Distribution and mobility of metal(loid)s at the sediment water interface

Verteilung und Mobilität von Metall(oid)en an der Sediment- Wasser-Grenzschicht

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Summary

The sediments of surface waters are temporary or final depository of many chemical compounds, including trace metals and metalloids (metal(loid)s) from natural and anthropogenic sources. Whether they act as a source or sink of metal(loid)s depends strongly on the dynamics of the biogeochemical processes that take place at the sediment-water interface (SWI). Important information on biogeochemical processes as well as on the exposure, the fate and the transport of pollutants at the SWI can be obtained by determining chemical concentration profiles in the sediment pore water. A major challenge is to conduct experiments with a spatial resolution, which allows to adequately record existing gradients and to log all the parameters needed, to describe and better understand the complex processes at the SWIs. At the same time, it is from major importance to prevent the formation of any artifacts during sampling, which may occur due to the labile nature of the SWIs and the very steep biogeochemical gradients.

In this context, in the first part of this work, a system was developed and tested that enables the automated, minimal invasive sampling of sediment pore water of undisturbed or manipulated sediments while simultaneously recording parameters such as redox potential, oxygen content and pH value. In an incubation experiment the impact of acidification and mechanical disturbance (re-suspension) on the mobility of 13 metal(loid)s was investigated using a triple quadrupole inductively coupled plasma-mass spectrometry (ICP-QQQ-MS) multi-element approach. Most metals were released as consequence of sulfide weathering whereas mechanical disturbance had a major impact on the mobility of the oxide forming elements As, Mo, Sb, U and V. Additionally, options were demonstrated to address with the system the size fractionation of metal(loid)s in pore water samples and the speciation of As(III/V) and Sb(III/V).

In the second part, the focus, with a similar experimental design, was placed on the processes leading to the release of metal(loid)s. For this purpose, two incubation experiments with different oxygen supply were conducted in parallel. For the first time the nonmetals carbon, phosphorus and sulfur were analyzed simultaneous to 13 metal(loid)s in sediment pore water by ICP-QQQ-MS. Throughout the experiment metal(loid) size fractionation was monitored. It was confirmed that resuspension promotes the mobility of metalloids such as As, Sb and V, while the release of most metals was largely attributed to pyrite weathering. The colloidal (0.45-16 µm) contribution in terms of mobilization was only relevant for a few elements.

Finally, the sampling system was used as part of a new approach to sediment risk assessment. Undisturbed sediment cores from differently contaminated positions in the Trave estuary were examined, considering 16 metal(loid)s, the non-metals C, P and S and the ions NH_4^+, PO_4^{3-} and SO_4^{2-}. By the first in-depth comparison with in-situ dialysis-based pore water sampling the ability of the suction-based approach to represent field conditions was proven. The pore water studies together with supplementing resuspension experiments in bio-geochemical microcosms and sequential extraction identified the most “pristine” sediment of the study area as posing the greatest risk of metal(loid) release. However, the potentially released amounts per kg of sediment are only a few parts per thousand of the average daily loads of the Trave river.

Zusammenfassung

Viele chemische Verbindungen, einschließlich Spurenelemente aus natürlichen und anthropogenen Quellen, verbleiben temporär oder endgültig in den Sedimenten der Oberflächengewässer. Ob diese als Quelle oder Senke von Metallen und Metalloiden (Metall(oid)e) fungieren, hängt von der Dynamik der biogeochemischen Prozesse ab, die an der Wasser-Sediment-Grenzschicht (sediment water interface - SWI) ablaufen. Wichtige Informationen zu biogeochemischen Prozessen sowie zur Exposition, zum Verbleib und zum Transport von Schadstoffen an der SWI lassen sich durch die Ermittlung von Konzentrationsprofilen im Sedimentporenwasser gewinnen. Dabei besteht die Herausforderung zum einen darin eine räumliche Auflösung zu realisieren, die es erlaubt, bestehende Gradienten adäquat zu erfassen und zu gleich hinreichend viele Parameter aufzunehmen, um die komplexen Prozesse zu verstehen. Zum anderen gilt es die Bildung von Probenahme-Artefakten zu verhindern, die durch die labile Natur der SWI sowie die steilen biogeochemischen Gradienten verursacht werden.

Vor diesem Hintergrund wurde im ersten Teil dieser Arbeit ein System zur automatisierten, minimal-invasiven Untersuchung der SWI entwickelt und erprobt. Das System ermöglicht die Beprobung des Sedimentporenwassers ungestörter oder manipulierter Sedimente bei gleichzeitiger Erfassung von Parametern wie Redoxpotential, Sauerstoffgehalt und pH-Wert. Im Rahmen eines Inkubationsexperimentes wurde der Einfluss von Versauerung und mechanischer Störung (Resuspension) auf die Mobilität von 13 Metall(oid)en untersucht, die mittels Tripel-Quadrupol induktiv gekoppelter Plasma-Massenspektrometrie (ICP-QQQ-MS) quantifiziert wurden. Während die meisten Metalle in Folge von Sulfid-Verwitterung freigesetzt wurden hatte die mechanische Störung einen großen Einfluss auf die Mobilität der oxidbildenden Elemente As, Mo, Sb, U und V. Zusätzlich wurde gezeigt, dass das Probenahme-System zudem Optionen zur Untersuchung der Größenfraktionierung von Metall(oid)en sowie der Speziierung von As(III/V) und Sb(III/V) bietet.

Im zweiten Teil dieser Arbeit wurde der Fokus - mit einem ähnlichen experimentellen Design - auf die Prozesse gelegt, die zur Freisetzung von Metall(oid)en führen. Zu diesem Zweck wurden zwei Inkubationsexperimente mit unterschiedlicher Sauerstoffversorgung parallel durchgeführt. Erstmals wurden mittels ICP-QQQ-MS die Nichtmetalle Kohlenstoff, Phosphor und Schwefel in einem Analyselauf gemeinsam mit 13 Metall(oid)en in Sedimentporenwasser quantifiziert. Die Größenfraktionierung der Metall(oid)e wurde über den gesamten Verlauf der Experimente überwacht. Es bestätigte sich, dass Sediment-Resuspension die Mobilität von Metalloiden wie As, Sb und V fördert, während die Freisetzung der meisten Metalle weitgehend auf die Verwitterung von Pyrit zurückzuführen war. Der kolloidale Beitrag (0,45 - 16 µm) zur Mobilisierung war nur für wenige Elemente relevant.

Schließlich wurde das Probenahmesystem im Rahmen eines neuen Ansatzes zur Sedimentbewertung eingesetzt. Dabei wurden ungestörte Sedimentkerne unterschiedlich kontaminierter Positionen im Trave-Ästuar untersucht und neben 16 Metall(oid)en, die Nichtmetalle C, P und S sowie die Ionen NH_4^+, PO_4^{3-} und SO_4^{2-} berücksichtigt. Durch den ersten umfangreichen Vergleich mit *in-situ* Dialyse-basierter Porenwasserbeprobung wurde die Eignung des entwickelten Ansatzes zur Erfassung der Feldbedingungen nachgewiesen. Die Porenwasseruntersuchungen zusammen mit ergänzenden Resuspensionsexperimenten in biogeochemischen Mikrokosmen und sequentieller Extraktion ergaben, dass das am geringsten „belastetste“ Sediment des Untersuchungsgebiets das größte Risiko für die Freisetzung von Metall(oid)en darstellt. Jedoch betrugen die potenziell freigesetzten Mengen je kg Sediment nur wenige Promille der durchschnittlichen täglichen Fracht der Trave.

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1
General Introduction

Sediment is an essential part of surface water bodies with regard to both morphological and qualitative aspects, and also offers numerous aquatic species a variety of habitats. Due to the affinity of many chemical species to attach to particle surfaces, sediments also reflect the history of impact and pollution in a given catchment area. Thus, monitoring and assessment of sediment contamination is an integral part of environmental monitoring[1,2] and is in particular recurrently of concern in the context of waterway maintenance and development.[3] Sediment contaminations do not always result in toxic effects due to decreased bioavailability of sediment-associated contaminants.[2] Therefore, measuring contaminant concentrations in the interstitial water has been identified as a useful tool for also estimating aquatic toxicity,[4] since pore water is a key route of exposure to aquatic organisms.[5,6]

Metals and metalloids (metal(loid)s) as natural components of the earth crust, on the one hand, are ubiquitous in the environment in trace concentrations. On the other hand, they are increasingly released in the course of anthropogenic activities and accumulate in certain environmental compartments, creating a threat to the environment and human health.[7,8] When studying metal(loid)s at the sediment-water interface (SWI), one challenge is to achieve a sufficiently high spatial resolution, while in parallel capturing a variety of parameters. The geochemical behavior of metal(loid)s is determined by a complex interplay of various processes. Their geochemical cycles are strongly related to (micro-)biological processes and the cycles of major elements such as C, S, N and P. Elucidating the fate of a certain element in a particular ecosystem therefore requires to collect a multitude of information in parallel including sediment parameters such as the pH value, redox potential, O_2 concentration as well as the concentrations of trace and major elements and nutrients. The simultaneous detection of these parameters on the other hand is complicated by the spatial heterogeneity of natural sediments and the steep geochemical gradients at the sediment surface. Inevitably, a compromise has to be made between the sample volume required for different measurement techniques and the spatial resolution studied. However, thanks to modern instrumental analytical techniques, only comparatively small sample volumes are required to quantify a large number of analytes. In the field of environmental analytical chemistry of metal(loid)s, in particular inductively coupled plasma-mass spectrometry (ICP-MS) with its multi-element capabilities and low detection limits is one of the most common and powerful techniques. Recent developments such as the introduction of collision and reaction cell technology, combined with two scanning quadrupoles, not only make it possible to quantify a large number of metal(loid)s but also to integrate non-metals into the same analytical run.[9]

In this context the aim of the present work was to study metal(loid)s at the sediment water interface with regard to fractionation, distribution and small-scale and short-term variabilities. Techniques should be developed and combined to sample sediment pore water in an automated and minimal-invasive manner with parallel detection of sediment parameters such as pH-value, redox potential and O_2 concentration. Analytical techniques taking advantage of state-of-the-art quadrupole ICP-MS devices including major and trace metal(loid)s as well as polyatomic nonmetals were envisaged to be developed and applied.

The following paragraphs give an overview of sediment water interfaces and the behavior of metal(loid)s in the environment as the subjects of investigation, as well as of pore water sampling techniques and triple quadrupole ICP-MS (ICP-QQQ-MS) as the essentially applied methods.

1.1 Sediment water interfaces

Sediments represent a significant portion of the surface of the solid earth wherever it is covered by waters. Their interface to supernatant water manifests not only the boundary of the two phases water and sediment, it also often sets the transition from a highly oxidizing surface environment to conditions rich in highly reduced biogenic products such as organic matter, sulfide minerals, or methane. Thereby, the sediment water interface is both, the habitat for the highest density of organisms and the area in which exchange processes take place between the sediment and the water column. Typically, this transition zone is characterized by steep geochemical gradients concerning not only the parameters O_2-concentration and redox potential but also the pH value and the dissolved concentrations of different compounds and elements. However, the actual conditions at a particular location are influenced by a variety of factors including chemical properties of sediment and overlying water, content and composition of the organic material, or the microbial and other biological activity. The most impacting key parameter is the availability of O_2 and its penetration depth at the sediment surface. The latter is - in absence of mechanical disturbance - mainly dependent on diffusive fluxes and consumption. In turn, the consumption of O_2 occurs mainly through biologically catalyzed processes such as organic matter degradation and the biologically mediated oxidation of inorganic components such as NH_3, Mn^{2+}, Fe^{2+}, H_2S or CH_4 and often leads to its depletion within the uppermost millimeters of the sediment. The transition from oxic to anoxic conditions at the SWI is usually reflected in a characteristic sequence of redox processes (Figure 1). According to their energetic favorability microorganisms substitute O_2 by compounds such as NO_3^-, NO_2^-, Mn(IV), Fe(III) or SO_4^{2-} as electron acceptors during organic matter degradation. Typically, a decrease of dissolved NO_3^- and NO_2^- close to the SWI, followed by increasing concentrations of dissolved Mn and Fe and, with increasing depth, SO_4^{2-} depletion is the consequence.[10-14]

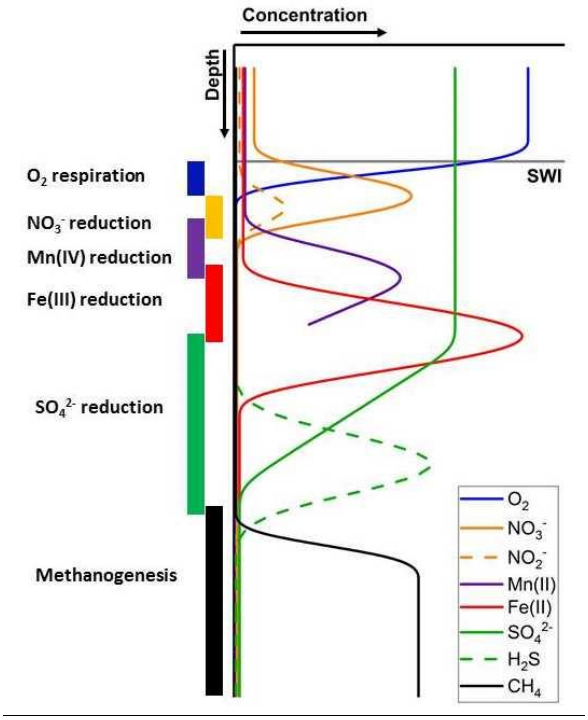

Figure 1: *Redox processes and generalized resulting concentration profiles of dissolved species at the sediment water interface (modified from* Jørgensen and Kasten 2006[14]*).*

In practice, the reaction sequence is altered by the availability of oxidants and kinetic constraints, including the dominance of certain microbial populations.[15] Additionally, the surface of natural sediments is often characterized by small scale spatial heterogeneities caused by a variety of physical, biological and geochemical processes. Examples are the activity of filtrating or dwelling benthic organisms, that can introduce O_2 into upper sediment layers or the formation of micro niches due to heterogeneously distributed organic matter and associated localized O_2 depletion.[16,17] An integrative measure for the oxidation-reduction status of surface environments is the redox potential. It describes the overall reducing or oxidizing capacity of a system. It is defined relative to a standard hydrogen electrode. Whether a system has a negative or a positive potential depends on whether it donates electrons to the hydrogen electrode or takes up electrons from the electrode.[18] While in oxygenated waters the redox potential remains between 300 and 500 mV it can be decreased by microbial mediated processes to below -300 mV. Due to the various redox couples present in natural systems that are often not in thermodynamic equilibrium the redox potential is rather a measure of a systems overall reaction potential than the description of a specific redox couple.[18-20] Changing redox conditions can go along with alterations in pH value as during reduction protons are consumed whereas oxidation tends to cause acidification.[21]

1.2 Metals and metalloids in the environment

Metals and metalloids (metal(loid)s) are naturally occurring elements that are ubiquitous in the environment (usually) in trace concentrations. They are released to surface waters by natural means such as soil erosion and natural weathering and human activities including mining, industrial effluents urban runoff, or sewage discharge.[22] Some metal(loid)s are important micro nutrients, essential for plant growth, animal life or both. They act as important constituents of several key enzymes and play important roles in various oxidation-reduction reactions.[23] Others, such as Cd, Pb, Sb, own no known biological function and are considered as not essential to living organisms.[24] However, both essential and non-essential metal(loid)s have toxic effects to many organisms above the respective concentration threshold. To mammals, different metal(loid)s may cause adverse health effects such as organ or nervous system damage or cause cancer.

In aquatic ecosystems metal(loid)s may occur in a variety of species and fractions that are significantly different in toxicity, mobility and (bio-)availability. Many metal(loid) associations (e.g., with organic substances) are dynamic and reversible and reflect changing physical-chemical conditions.[25] The processes generally determining metal(loid) partitioning between dissolved and particulate phases include sorption/desorption on/from particles, precipitation/dissolution reactions, oxidation-reduction and complexation. However, speciation and fractionation are decisively influenced by environmental factors such as pH-value, redox conditions and sediment composition.[26]

Sorption-desorption reactions are among the most important processes determining the partitioning of metal(loid)s between dissolved and solid phase. They occur on the surfaces of a variety of particulate components including Fe- and Mn-(hydr)oxides, clay minerals, carbonates, organic colloids / particles and organisms. The different components vary significantly with regard to both their sorption capacity and the strength with which metal(loid)s are bound.[26] Depending on the sorption mechanism, the process of sorption can be further subdivided into absorption, surface precipitation and adsorption.[26] Absorption refers to the diffusion of a dissolved chemical species into a solid phase, wherein the penetration depth into the solid phase must be greater than several nanometers. Surface precipitation is referred to as the growth of a solid phase on an already pre-existing solid phase that forms a primitive, repeating three-dimensional molecular unit. Adsorption is defined as the two-dimensional accumulation of an adsorbate at a solid surface and includes several mechanisms such as cation exchange (or unspecific adsorption), specific adsorption and surface complexation.[26] Ions directly bond to the sorbent through covalent and ionic bonds are referred to as inner-sphere complexes, while ions held adjacent to a sorbent through strictly electrostatic forces are called outer-sphere complexes.[27] The sorption capacity of a sorbent depends on the number of existing binding-sites and its specific surface area and the binding intensity is related to the strength of interaction between the sorbate and

the sorbent. Functional groups such as hydroxyl-, carboxyl-, amine and sulfhydryl-groups on the surfaces function as binding sites due to the surface charge that may develop as a result of their dissociation.[10] In sediments and soils competition between different elements for binding sites and their affinity to specific binding sites impact the sorption behavior.[28] Additionally, the pH value decisively affects sorption processes. Generally neutral or alkaline conditions result in net negatively charged surfaces while under acidic conditions retained protons yield a net positive charge. Accordingly, cations and anions sorb with opposite pH dependence.[26]

Depending on the concentration of the ions involved and the prevailing environmental conditions, mineral phases such as hydroxides, phosphates, carbonates or sulfides can precipitate or be dissolved. For example, the reduction of SO_4^{2-} to H_2S under anoxic conditions can lead to the formation of secondary sulfide minerals. At the same time in a few millimeters distance, the oxidative dissolution of the secondary minerals can occur under aerobic conditions. This can significantly limit the mobility of chalcophilic elements in anoxic sediments, while in contrast their release might occur under aerobic conditions. Next to the precipitation of discrete mineral phases many metal(loid)s can be scavenged by co-precipitation with mineral phases such as Fe- and Mn- (hydr)oxides or sulfides. As the solubility of many mineral phases is generally increased under acidic conditions, the pH value also has a decisive influence on these precipitation / dissolution reactions.[26]

Redox processes, both biotic and abiotic, have a critical impact on the speciation, bioavailability, toxicity and mobility of many metal(loid)s as well as major elements such as C, S and N. Thus, redox processes can cause the mobilization or immobilization of metal(loid)s in different ways depending on the particular element and prevailing environmental conditions.[15,27] Trace elements which themselves undergo redox transformations such as As, Cr or Se undergo different processes, in terms of reactivity, mobility and toxicity depending on their redox state.[15,29] As a rule by thumb, metals are generally less soluble in their higher oxidation state, whereas the solubility and mobility of metalloids depend on both the oxidation state and the ionic form.[29] Not redox-active elements may be indirectly coupled to redox processes, for example via changes in sorption and precipitation equilibria of metal(loid)-binding sorbents such as Fe- and Mn-(hydr)oxides and –sulfides, or by complexation with organic material.[10,21] One can sort abiotic driven redox processes, such as the reduction of Cu(II) to Cu(I) by Fe^{2+} or H_2S, [30,31] from biotic, mostly microbial, driven transformations which are environmentally from significant importance.[10] Not only do microbes, as all life on earth, derive energy from redox processes and transfer electrons to bring macronutrients such as N and S and micronutrients (e.g. Fe, Mn) into the proper oxidation states to incorporate them into biomolecules.[10] They are also able to directly reduce a wide range of metal(loid)s including highly toxic elements such as Cr or Hg.[32]

The complexation by dissolved organic ligands such as humic and fulvic acids[33] or inorganic complexing agents such as chloride, sulfate, ammonia and others has a significant influence on the solubility and thus mobility of metal(loid)s.[28] The formation of complexes with non-adsorbing ligands prevents precipitation by changing the state of the dynamic equibrilium.[27] On the other hand trace metal(loid) adsorption can be enhanced by ligand-adsorption and the formation of ternary complexes (e.g., adsorbent-ligand-cation).[28] Thus, depending on the ligands and their affinity for sorption to particle surfaces complexation reactions either enhance or reduce the solubility of metal(loid)s.[34]

1.3 Pore water sampling

In addition to mineral and organic material, the water that fills the pores between the solid grains often accounts for the largest share of the total sediment. In the surface sediment, the proportion of pore water often exceeds 50%.[35] Its exceptional relevance as habitat, means of transport and as reaction medium, makes it an important subject in various environmental scientific disciplines. The pore water composition allows to draw conclusions about metabolic processes (activities) of the active microbial communities of the sediment and pore water is the medium in which diagenetic processes occur and mineral precipitation / dissolution takes place and it mediates substance fluxes between sediments and the overlying water.[3] Additionally, the sediment pore water represents an important source of bioavailable contaminants for benthic organisms and is therefore increasingly considered as an important measure for sediment quality evaluations.[5]

Due to the relevance of pore water for various scientific disciplines and the difficulties associated to its access and the conservation of the prevailing conditions various techniques have been developed for pore water sampling. These can generally be distinguished in *ex-situ* and *in-situ* methods.[6,36,37] The *ex-situ* methods require the sediment to be removed from the natural system by coring devices or grab samplers before the aqueous fraction is separated from the solid fraction by techniques including centrifugation, squeezing, sedimentation and filtration. These methods enable the sampling of both sediments at great depth below water surface and the sampling of pore water in great depth below the SWI as well as the processing of large sampling volumes. Also, since the sediment is sampled together with the pore water, parallel analyzes and relation of the results is possible.[36] However, *ex-situ* sampling of sediment pore waters generally suffers from difficulties concerning the conservation of prevailing conditions. A risk of artifact formation exists, for example, by contaminated sampling equipment, changes in temperature and pressure conditions and most important by the contact with oxygen.[37] In particular, the oxidation of anoxic sediments in contact with air can only be prevented by performing the sampling and sample preparation under an inert atmosphere.[36,37]

The methods applied to sample sediment pore water *in-situ*, without removing the sediment from the natural system, include dialyses based approaches such as pore water peepers,[38-40] diffusive

equilibrium in thin film (DET)[41] and diffusive gradient in thin film (DGT)[42] as well as suction-based filtration techniques. Basic principle of the dialyses based approaches is the establishment of a diffusion driven equilibration of a sampling medium with the surrounding water and its solutes. Sediment peepers are one of the most widely used sampling devices and basically consist of (acryl) plates with a vertical series of cavities that are covered with a membrane and filled with ultra-pure water as sampling medium.[36,37] Employed at the sediment surface for several days or weeks samples of the pore water are obtained by diffusive equilibration with the surrounding water and its solutes through the membrane. After their recovery, the aqueous samples can be extracted from the cavities by pipetting.[38-40] DET samplers use a thin layer of hydrogel as sampling medium which reduces equilibration time to <1 hour and enables a higher spatial resolution at the millimeter (or even sub-millimeter) scale.[41,43] However, fixation or elution of the analytes from the sampling medium is necessary after the sampling devices are recovered.[44-46] As advancement ion exchange resins are placed behind the diffusive gel in DGT samplers to accumulate the dissolved species. Due to a linear relationship between the accumulation of analytes and deployment time that exists as long as the capacity of the binding layer is not exceeded, sampling can be performed based on a constant diffusive gradient.[36,42] Following sampling, the extraction of the analytes from the binding phase is necessary.[44] A common characteristic of all passive sampling techniques is the averaging the analytes concentrations over exposure time, which reflects the concentrations relevant in the case of long-term exposure of aquatic organisms. Additionally, due to long exposure times short-term episodic events can be detected that may be missed by spot-sampling, even though the associated concentrations are underestimated.[47,48] Further advantages are a reduced risk for the formation of sampling artefacts, improved detection limits and the capability of two-dimensional (depth and width) measurements.[44] Recognized limitations of passive sampling techniques include often small sample volumes, the need of divers for their installation in deep waters and the impossibility for studying short-term episodic events.[44]

Suction-based pore water sampling describes the process of pore water extraction by applying a weak negative pressure to a sampling probe by peristaltic, syringe-[51,52] or vacuum pumps.[48-51] Using a variety of sampling probes, from perforated volumetric pipettes to porous suction cups and rhizons,[53] single- or multi-level samplings were carried out with a spatial resolution in the mm range and a maximum sampling depth of up to 5 m below the SWI.[54] The immediate character of the obtained samples and the comparable rapid sampling process allow for combination with different sample preservation procedures, analyses of a variety of analytes and the examination of short-term events. However, similar to passive sampling divers or complex technical solutions (e.g., lander systems) are required to perform the sampling in deep waters. Fabricius et. al (2014)[55] developed a system that combines automatic spatially high-resolution suction-based sampling with the measurement of environmental

parameters such as O_2-saturation, redox potential and pH value. However, this system is limited to a maximum sampling depth of 4 cm and the high spatial resolution (in the mm range) is associated to small sample volumes (~2ml).[55]

1.4 Multi-element analyses

The development of instrumental analytical techniques nowadays enables the fast, comparable inexpensive, accurate and selective identification and quantification of numerous analytes with sample volumes of few mL. One of the most powerful tools for the quantification of element concentrations in environmental samples is inductively coupled plasma quadrupole mass spectrometry (ICP-QMS). It offers excellent detection limits, a wide dynamic range and the capability of accurate multi-element analysis.[56] However, the resolution is limited compared to other MS principles. Basic ICP principle is the ionization of the (usually liquid) sample in an argon plasma that is generated by a high frequency current in the plasma torch. In the plasma molecules are dissociated and the free atoms are ionized. The singly-charged ions are directed into a mass-filtering unit through an interface consisting of two or three metallic cones, referred to as skimmer cones, and electrostatic lenses, called ion optics, which focus the ion beam. In the heart of the mass spectrometer, the separation device, the ion beam is separated by mass-to-charge ratio. Of the different types of mass separation devices quadrupole, magnetic sector and multi collector time-of-flight technology are the most common. Here only the quadrupole technique is discussed, since it was used for analysis in this work. It uses a quadrupole, consisting of four parallel metal rods, as mass filtering device. The ions travelling parallel to the rods are separated by application of an electrical field that allows only the mass-to-charge-ratio of interest to pass. The passing ions are detected upon exiting the mass spectrometer as they strike the first dynode of an electron multiplier that amplifies their impact. An electronic signal results that can be processed by a data handling system and be converted into the analytes concentration by comparison to calibration standards.[56,57] Repeated scans over the entire analyte masses enables to quantify several isotopes in a multi-element run.

In classical quadrupole ICP-MS designs, the detection of certain elements is severely biased by polyatomic or molecular spectral interferences that are generated by a combination of plasma / nebulizer gas, solvent and matrix derived ions having the same mass-to-charge ratio as the analyte ion. For example, the measurement of Fe on its most abundant isotope ^{56}Fe is impacted by the occurrence of polyatomic ArO^+ ions with mass 56 that form from argon from the plasma and oxygen from the sample matrix. However, these interference problems were largely overcome by the introduction of collision/reaction cells in combination with two scanning quadrupoles.[9] A quadrupole that is enclosed and can be pressurized with collision or reaction gases such as oxygen, hydrogen, ammonia or methane

is located before the mass analyzer. Gas phase ion/molecule interactions are responsible for the removal of polyatomic interfering ions.

1.5 Objectives

The general objective was to develop and apply an approach to evaluate metal(loid) contaminated sediments in the context of different aspects of sediment handling operations based on the expected release into the environment. The possibilities of modern instrumental analysis should be exploited to extend the number of analytes beyond the elements considered in former risk assessment and to gain insights into underlying geochemical processes.

For this purpose, an approach was needed to sample the pore water from manipulated or undisturbed sediments to an appropriate depth and with an adequate spatial resolution that enables to obtain sufficient sample volume to carry out the required multi-element analyses. The aim of **chapter 2** was the development of a corresponding sampling system and its application to address the impact of mechanical disturbance and acidification on the mobility of metal(loid)s, as well as metal(loid) size fractionation and As(III/V) and Sb(III/V) speciation.

The purpose of **chapter 3** was to examine in detail individual questions raised during the development of the sampling system. In particular, it should be better differentiated between the impact of mechanical disturbance and acidification on metal(loid) mobility and size fractionation by running two incubation experiments in parallel. In addition, the task was to develop an ICP-QQQ-MS approach that involves polyatomic non-metals to better understand geochemical processes.

The aim of **chapter 4** was to investigate sites with differently contaminated sediments in terms of metal(loid) mobility and to contrast the results obtained with the developed sampling system with *in-situ* sampling. Additionally, pore water sampling should be accompanied with additional techniques to perform a comprehensive risk assessment.

1.6 Thesis outline

Chapter 2 describes the setup of the meso profiling and sampling system (*messy*). It is an adaptation of the micro profiling and sampling system (*missy*);[54] enabling the sampling of pore water profiles down to a depth of about 20 cm. Its suitability to address the distribution of metal(loid)s across the SWI as well as their size fractionation and speciation is demonstrated in the context of an incubation / acidification experiment that was conducted to investigate the impact of mechanical disturbance and acidification on the metal(loid)s mobility.

Chapter 3 closes knowledge gaps identified during the development of the *messy*. The sampling-system is applied in two incubation experiments to better differentiate between impacts of mechanical

disturbance and oxygen induced acidification on the mobility of metal(loid)s at sediment water interfaces in the two size fractions dissolved and colloidal. Additionally, the set of analytes simultaneously quantified in the complex matrix from sediment pore water by ICP-QQQ-MS was extended to polyatomic nonmetals for a better understanding of geochemical processes.

Chapter 4 pictures the application of *messy* for studying metal(loid) mobility in undisturbed sediments in the context of sediment risk assessment. A comparison with *in-situ* sampling takes place to prove its suitability for determination of in-field conditions in the laboratory. Additionally, the information obtained from pore water sampling is complemented by examination of the metal(loid)s binding forms in the studied sediments by sequential extraction and by results from bio-geochemical microcosms.

Chapter 5 critically summarizes the results and conclusions of the previous chapters and gives an outlook on potential future applications, possible improvements and further developments.

1.7 References

1. Förstner, U., Sediments and the EU-Water Framework Directive: revisiting the Elbe 2015 River Basin Management Plan. *Journal of Soils and Sediments* **2015,** *15*, (9), 1863-1864.
2. Brils, J., Sediment monitoring and the European Water Framework Directive. *Annali dell'Istituto superiore di sanita* **2008,** *44*, (3), 218-23.
3. Calmano, W., *Untersuchung und Bewertung von Sedimenten*. Springer: Berlin, Heidelberg, 2001.
4. Ankley, G. T.; Di Toro, D. M.; Hansen, D. J.; Berry, W. J., Technical basis and proposal for deriving sediment quality criteria for metals. *Environ Toxicol Chem* **1996,** *15*, (12), 2056-2066.
5. Chapman, P. M.; Wang, F.; Germano, J. D.; Batley, G., Pore water testing and analysis: the good, the bad, and the ugly. *Marine Pollution Bulletin* **2002,** *44*, (5), 359-366.
6. Gruzalski, J. G.; Markwiese, J. T.; Carriker, N. E.; Rogers, W. J.; Vitale, R. J.; Thal, D. I., Pore Water Collection, Analysis and Evolution: The Need for Standardization. *Rev Environ Contam Toxicol* **2016,** *237*, 37-51.
7. Schulz-Zunkel, C.; Krueger, F., Trace metal dynamics in floodplain soils of the river Elbe: a review. *J Environ Qual* **2009,** *38*, (4), 1349-62.
8. Jaishankar, M.; Tseten, T.; Anbalagan, N.; Mathew, B. B.; Beeregowda, K. N., Toxicity, mechanism and health effects of some heavy metals. *Interdiscip Toxicol* **2014,** *7*, (2), 60-72.
9. Profrock, D.; Prange, A., Inductively coupled plasma-mass spectrometry (ICP-MS) for quantitative analysis in environmental and life sciences: a review of challenges, solutions, and trends. *Appl Spectrosc* **2012,** *66*, (8), 843-68.
10. Borch, T.; Kretzschmar, R.; Kappler, A.; Cappellen, P. V.; Ginder-Vogel, M.; Voegelin, A.; Campbell, K., Biogeochemical redox processes and their impact on contaminant dynamics. *Environ Sci Technol* **2010,** *44*, (1), 15-23.

11. Santschi, P.; Höhener, P.; Benoit, G.; Buchholtz-ten Brink, M., Chemical processes at the sediment-water interface. *Marine Chemistry* **1990,** *30*, 269-315.
12. Ritzrau, W.; Graf, G.; Schlüter, M., Exchange Processes Across the Sediment Water Interface. In *The Northern North Atlantic: A Changing Environment*, Schäfer, P.; Ritzrau, W.; Schlüter, M.; Thiede, J., Eds. Springer Berlin Heidelberg: Berlin, Heidelberg, 2001; pp 199-206.
13. Libes, S., *Introduction to Marine Biogeochemistry*. Elsevier Science: 2011.
14. Jørgensen, B. B.; Kasten, S., Sulfur Cycling and Methane Oxidation. In *Marine Geochemistry,* Schulz H. D., Zabel M., Eds. Springer, Berlin, Heidelberg. 2006; pp 271-309.
15. Hamilton-Taylor, J.; Davison, W., Redox-Driven Cycling of Trace Elements in Lakes. In *Physics and Chemistry of Lakes*, Lerman, A.; Imboden, D. M.; Gat, J. R., Eds. Springer Berlin Heidelberg: Berlin, Heidelberg, 1995; pp 217-263.
16. Stockdale, A.; Davison, W.; Zhang, H., Micro-scale biogeochemical heterogeneity in sediments: A review of available technology and observed evidence. *Earth-Science Reviews* **2009,** *92*, (1-2), 81-97.
17. Lehto, N.; Glud, R. N.; á Norði, G.; Zhang, H.; Davison, W., Anoxic microniches in marine sediments induced by aggregate settlement: biogeochemical dynamics and implications. *Biogeochemistry* **2014**.
18. Søndergaard, M., Redox Potential. In *Encyclopedia of Inland Waters*, Likens, G. E., Ed. 2009; pp 852-859.
19. DeLaune, R. D.; Reddy, K. R., Redox Potential. In *Encyclopedia of Soils in the Environment*, Hillel, D., Ed. Academic Press: 2005; pp 366-371.
20. Schüring, J.; Schulz, H. D.; Fischer, W. R.; Böttcher, J.; Duijnisveld, W. H. M., *Redox: Fundamentals, Processes and Applications*. Springer: Heidelberg, 2000.
21. Du Laing, G.; Rinklebe, J.; Vandecasteele, B.; Meers, E.; Tack, F. M., Trace metal behaviour in estuarine and riverine floodplain soils and sediments: a review. *Sci Total Environ* **2009,** *407*, (13), 3972-85.
22. Morais, S.; e Costa, F. G.; Lourdes Pereir, M. d., Heavy Metals and Human Health. In *Environmental Health - Emerging Issues and Practice*, 2012.
23. WHO *Trace elements in human nutrition and health*; 92 4 156173 4; 1996.
24. Chang, L. W.; Magos, L.; Suzuki, T.; eds *Toxicology of metals*; CIS/96/02236; Health and Safety Executive, Health and Safety Laboratory: 1996.
25. Warren, L. A.; Haack, E. A., Biogeochemical controls on metal behaviour in freshwater environments. *Earth-Science Reviews* **2001,** *54*, (4), 261-320.
26. Smith, K. S., Metal sorption on mineral surfaces: An overview with examples relating to mineral deposits. In *The Environmental Geochemistry of Mineral Deposits: Part A: Processes, Techniques,*

and Health Issues Part B: Case Studies and Research Topics, Plumlee, G. S.; Logsdon, M. J.; Filipek, L. F., Eds. Society of Economic Geologists: 1999; Vol. 6.

27. Violante, A.; Cozzolino, V.; Perelomov, L.; Caporale, A. G.; Pigna, M., Mobility and Bioavailability of Heavy Metals and Metalloids in Soil Environments. *Journal of soil science and plant nutrition* **2010,** *10*, (3).
28. Caporale, A. G.; Violante, A., Chemical Processes Affecting the Mobility of Heavy Metals and Metalloids in Soil Environments. *Current Pollution Reports* **2015,** *2*, (1), 15-27.
29. Rinklebe, J.; Knox, A. S.; Paller, M., Redox Reactions of Heavy Metal(loid)s in Soils and Sediments in Relation to Bioavailability and Remediation. In *Trace Elements in Waterlogged Soils and Sediments*, CRC Press: 2016.
30. Matocha, C. J.; Karathanasis, A. D.; Rakshit, S.; Wagner, K. M., Reduction of copper(II) by iron(II). *J Environ Qual* **2005,** *34*, (5), 1539-46.
31. Pattrick, R. A. D.; Mosselmans, J. F. W.; Charnock, J. M.; England, K. E. R.; Helz, G. R.; Garner, C. D.; Vaughan, D. J., The structure of amorphous copper sulfide precipitates: An X-ray absorption study. *Geochimica et Cosmochimica Acta* **1997,** *61*, (10), 2023-2036.
32. Lovley, D. R., Dissimilatory metal reduction. *Annu Rev Microbiol* **1993,** *47*, 263-90.
33. Weng, L.; Temminghoff, E. J.; Lofts, S.; Tipping, E.; Van Riemsdijk, W. H., Complexation with dissolved organic matter and solubility control of heavy metals in a sandy soil. *Environ Sci Technol* **2002,** *36*, (22), 4804-10.
34. Zhang, C.; Yu, Z. G.; Zeng, G. M.; Jiang, M.; Yang, Z. Z.; Cui, F.; Zhu, M. Y.; Shen, L. Q.; Hu, L., Effects of sediment geochemical properties on heavy metal bioavailability. *Environ Int* **2014,** *73*, 270-81.
35. Zimmer, M., *Erarbeitung von Kriterien zur Ableitung von Qualitätszielen für Sedimente und Schwebstoffe: Literaturstudie : Forschungsbericht 10204384/01 / von Manfred Zimmer ; Wolfgang Ahlf*. Umweltbundesamt: 1994.
36. Murdoch, A.; Azcue, J. M., *Manual of aquatic sediment sampling*. Lewis Publishers: Boca Raton, 1995; p 219.
37. Bufflap, S. E.; Allen, H. E., Sediment pore water collection methods for trace metal analysis: A review. *Water Research* **1995,** *29*, (1), 165-177.
38. Hesslein, R. H., An in situ sampler for close interval pore water studies1. *Limnology and Oceanography* **1976,** *21*, (6), 912-914.
39. Lewandowski, J.; Rüter, K.; Hupfer, M., Two-Dimensional Small-Scale Variability of Pore Water Phosphate in Freshwater Lakes: Results from a Novel Dialysis Sampler. *Environmental Science & Technology* **2002,** *36*, (9), 2039-2047.

40. Teasdale, P., Pore water sampling with sediment peepers. *TrAC Trends in Analytical Chemistry* **1995,** *14*, (6), 250-256.
41. Davison, W.; Grime, G. W.; Morgan, J. A. W.; Clarke, K., Distribution of dissolved iron in sediment pore waters at submillimetre resolution. *Nature* **1991,** *352*, (6333), 323-325.
42. Davison, W.; Zhang, H., In situ speciation measurements of trace components in natural waters using thin-film gels. *Nature* **1994,** *367*, (6463), 546-548.
43. Davison, W.; Fones, G. R.; Grime, G. W., Dissolved metals in surface sediment and a microbial mat at 100-µm resolution. *Nature* **1997,** *387*, (6636), 885-888.
44. Peijnenburg, W. J.; Teasdale, P. R.; Reible, D.; Mondon, J.; Bennett, W. W.; Campbell, P. G., Passive sampling methods for contaminated sediments: state of the science for metals. *Integr Environ Assess Manag* **2014,** *10*, (2), 179-96.
45. Mortimer, R. J. G.; Krom, M. D.; Hall, P. O. J.; Hulth, S.; Ståhl, H., Use of gel probes for the determination of high resolution solute distributions in marine and estuarine pore waters. *Marine Chemistry* **1998,** *63*, (1-2), 119-129.
46. Pagès, A.; Welsh, D. T.; Robertson, D.; Panther, J. G.; Schäfer, J.; Tomlinson, R. B.; Teasdale, P. R., Diurnal shifts in co-distributions of sulfide and iron(II) and profiles of phosphate and ammonium in the rhizosphere of Zostera capricorni. *Estuarine, Coastal and Shelf Science* **2012,** *115*, 282-290.
47. Dunn, R. J. K.; Teasdale, P. R.; Warnken, J.; Schleich, R. R., Evaluation of the Diffusive Gradient in a Thin Film Technique for Monitoring Trace Metal Concentrations in Estuarine Waters. *Environmental Science & Technology* **2003,** *37*, (12), 2794-2800.
48. Jordan, M. A.; Teasdale, P. R.; Dunn, R. J. K.; Lee, S. Y., Modelling copper uptake by Saccostrea glomerata with diffusive gradients in a thin film measurements. *Environmental Chemistry* **2008,** *5*, (4).
49. Barnes, R. O., An in situ interstitial water sampler for use in unconsolidated sediments. *Deep Sea Research and Oceanographic Abstracts* **1973,** *20*, (12), 1125-1128.
50. Sayles, F. L.; Mangelsdorf, P. C.; Wilson, T. R. S.; Hume, D. N., A sampler for the in situ collection of marine sedimentary pore waters. *Deep Sea Research and Oceanographic Abstracts* **1976,** *23*, (3), 259-264.
51. Howes, B. L.; Dacey, J. W. H.; Wakeham, S. G., Effects of sampling technique on measurements of porewater constituents in salt marsh sediments1. *Limnology and Oceanography* **1985,** *30*, (1), 221-227.
52. Goodman, K. S. J. H. B., An apparatus for sampling interstitial water throughout tidal cycles. **1979,** *13*, (1), 30-33.

53. Seeberg-Elverfeldt, J.; Schlüter, M.; Feseker, T.; Kölling, M., Rhizon sampling of porewaters near the sediment-water interface of aquatic systems. *Limnology and Oceanography: Methods* **2005,** *3*, (8), 361-371.
54. Beck, M.; Dellwig, O.; Kolditz, K.; Freund, H.; Liebezeit, G.; Schnetger, B.; Brumsack, H.-J., In situ pore water sampling in deep intertidal flat sediments. *Limnology and Oceanography: Methods* **2007,** *5*, (5), 136-144.
55. Fabricius, A.-L.; Duester, L.; Ecker, D.; Ternes, T. A., New Microprofiling and Micro Sampling System for Water Saturated Environmental Boundary Layers. *Environmental Science & Technology* **2014,** *48*, (14), 8053-8061.
56. Nelms, S. M., *Inductively Coupled Plasma Mass Spectrometry Handbook*. CRC Press: Boca Raton, 2005.
57. Thomas, R., *Practical Guide to ICP-MS*. CRC Press: Boca Raton 2013.

2

Metal(loid) speciation and size fractionation in sediment pore water depth profiles examined with a new meso profiling system

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2.1 Abstract

In an exemplary incubation study with an anaerobic sediment sampled at an oxbow of the river Lahn in Germany (50°18'56.87"N; 7°37'41.25"E) and contaminated by former mining activity, a novel meso profiling and sampling system (*messy*) is presented. *Messy* enables a low invasive, automated sampling of pore water profiles across the sediment water interface (SWI), down to ~20 cm depth with a special resolution of 1 cm. In parallel to the pore water sampling it collects physicochemical sediment parameters such as redox potential and pH value. In an incubation experiment of 151 days the ability of the setup was proven to address several different aspects relevant for fresh water and marine sediment studies. (i) The influence of mechanical disturbance and oxygen induced acidification was quantified on the mobility of 13 metals and metalloids (Cd, Co, Cu, Fe, Mn, Mo, Ni, Sb, U, V, Zn) based on 11 profiles. The analytes were quantified by inductively coupled plasma mass spectrometry. Three groups of elements were identified with respect to the release into the pore water and the overlying water under different experimental conditions. (ii) The capability to investigate the impacts of changing physicochemical sediment properties on arsenic and antimony (III/V) speciation is shown. (iii) An approach to obtain information on size fractionation effects and to address the colloidal pore water fractions (0.45 µm to 16 µm) was successfully conducted for the elements Ag, As, Cu, Fe and Mn.

2.2 Introduction

Biogeochemical processes at the boundary layers of sediment water interfaces determining the distribution and cycling of analytes such as trace metals, nutrients or organic compounds are closely linked to sediment parameters like O_2 saturation, redox potential or pH value. The development of different measurement techniques using microsensors or –electrodes enables the determination of analytes like O_2, the redox potential, the pH value, H_2S or N_2O with a spatial high resolution[1]. The examination of further analytes like metals or metalloids (metal(loid)s) is mostly performed on the basis of pore water samples[2] obtained either by ex-situ methods such as centrifugation and squeezing[3, 4] or in-situ methods such as dialyses[5, 6] or suction based techniques.[7-9]

In order to understand the biogeochemical processes determining the mobility and transformation of chemical species and to assess potential risks arising from contaminated sediments the distribution of metal(loid)s needs to be determined parallel to different physicochemical parameters. In 2014 the authors presented a novel microprofiling and sampling system (*missy*) that combines the measurement of O_2 saturation, redox potential and pH value across the SWI with suction based pore water sampling using hollow fibers with a size cut-off of 0.45 µm.[10] *Missy* is limited to provide pore water samples down to a maximum depth of 4 cm mainly due to the robustness of the microsensors. To answer questions on the fate of metals and metalloids (metal(loid)s) under changing environmental conditions and to include deeper sediment layers, *missy* was extended to a meso profiling and sampling system

(*messy*). Both systems enable to analyze the pore water samples by application of inductive coupled plasma-mass spectroscopy (ICP-MS), one of the most powerful analytical techniques for determining metal(loid) concentrations.

In the sediment incubation experiment presented here: (i) the *messy* setup was tested and optimized. Across the sediment water interface (SWI) of a natural contaminated organic rich sediment down to a depth of 16 cm the release of 13 metalloids (Ag, As, Cd, Co, Cu, Fe, Mn, Mo, Ni, Sb, U, V, Zn) impacted by (ii) physical as well as (iii) chemical disturbance was monitored over a period of 151 days. In addition, the capability to use *messy* in (iv) speciation studies (here inorganic arsenic and antimony (III/V)) was tested. (v) Finally, by using a size cut-off <16 µm, the basis to address colloidal pore water fractions (here, lower cut-off 0.45 µm and upper 16 µm) in future studies was acquired.

2.3 Materials and methods

2.3.1 Meso profiling and sampling system (messy)

The basic principle of *messy* is to collect vertical profiles of suction-based pore water samples through the SWI. The constantly taken aqueous samples represent depth intervals in the cm range. Parallel movement of a sampling probe and a redox electrode enables to survey the redox state during the sampling of the sediment pore water. Figure 2.1 delivers an overview of the setup used.

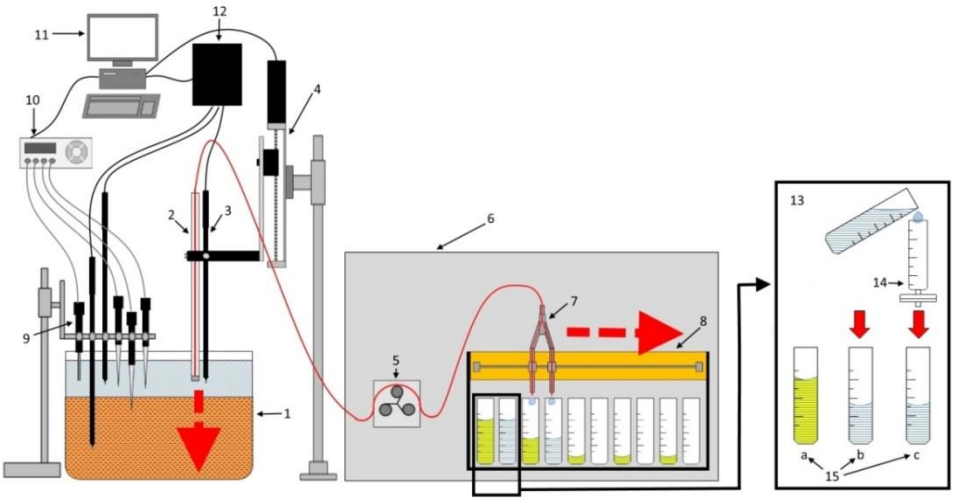

Figure 2.1: *Messy set up:1) sediment sample (disturbed or undisturbed); 2) sampling probe; 3) redox probe; 4) step motor; 5) peristaltic pump; 6) glove box with argon-atmosphere; 7) split valve; 8) fraction collector; 9) fixed probes: temperature, redox and O_2; 10) multimeter; 11) PC; 12) redox logger; 13) size fractionation step; 14) filtration cut-off 0.45 µm; 15) a = EDTA preserved subsample, b = <16 µm cut-off, c = <0.45 µm cut-off*

In the experiment, conducted to perform the method development and to examine the metal(loid) release into the pore water under varying conditions, aqueous samples were taken through a self-manufactured sampling probe from the sediment. The borosilicate probe head provides a cut-off of <16 µm (EcoTech, Germany) and the suction based sampling is basically comparable to.[11] The probe head was placed in a polycarbonate tube which was lined with two component polyurethane and connected via polytetrafluoroethylene (PTFE) tube with a peristaltic pump (Preciflow, LAMBDA Laboratory Systems, Switzerland). Vertical movement of the sampling probe and a redox electrode was conducted constantly by a motor operated with the profiling software SensorTrace Suite (both Unisense, Denmark) in steps of 200 µm every 154.6 seconds. A fraction collector (Omnicoll, LAMBDA Laboratory Systems, Switzerland) synchronized to the profiling software was programmed to change vessels every 261.8 minutes. In order to meet all minimum thresholds for analytical detection an intended volume of 7.9 mL was sampled at a flow rate of 30 µL/min for ~4.3 h. Sampling probe, peristaltic pump and fraction collector were connected via tubing with an inner diameter of 500 µm. All tubing and connectors used consisted of perfluoroalkoxy alkane (PFA), fluorinated ethylene propylene (FEP), polyether ether ketone (PEEK) or (only used under argon atmosphere) poly(organo)siloxane. To prevent re-oxidation of the samples, the peristaltic pump and the fraction collector were positioned in a glovebox under an argon-atmosphere (Weidner Laboreinrichtungs GmbH, Germany). A comparison of the features of the previously published *missy* and the new *messy* is provided in Table 2.1.

Table 2.1: *Comparison of the missy-setup published by Fabricius et al. (2014)[10] and the presented messy-setup.*

Characteristic	***missy*** (microprofiling and sampling system)	***messy*** (mesoprofiling and sampling system)
Probe head	~3 mm	~5-10 mm
Cut-off	0.45 µm	16 µm
Pump speed	~5 µL/min	~20-80 µL/min
Depth	~2-4 cm	~20 cm
Sampling resolution	<<1 cm	>1 cm

2.3.2 Measurements of the redox potential, the pH value and O_2 concentration

Profiles of the redox potential were obtained by a Mansfeldt-type electrode (ecoTech Umweltmeßsysteme GmbH, Germany) parallel mounted to the sampling probe (Figure 2.1) and connected to an Ag/AgCl-reference electrode (REF321, Radiometer Analytical, Germany). The “redox potential” measured by the platinum electrode represents the operationally determined and not the

thermodynamic value. The term "redox potential" is, nevertheless, used to facilitate reading. Measured values were stored with an enviLog data logger (ecoTech, Germany).

Throughout the experiment O_2 concentrations, pH and temperatures were measured in the water column using a Clark-type O_2 microsensor (Ox 500, Unisense, Denmark), a microelectrode (pH-100 glass electrode, Unisense Denmark) connected to a Ag/AgCl-reference electrode (REF321, Radiometer Analytical, Germany) and a mineral insulated thermo coupler (TP2000, Unisense, Denmark).

2.3.3 Sampling and sample preparation

During the experiment presented, 22 samples were taken per profile each over an interval of 1 cm from 6 cm above to 16 cm below the SWI. Samples were collected in 15 mL centrifuge tubes (VWR catalyst Laboratory Services, USA), previously cleaned in 1.3% nitric acid for >24 h (HNO_3, 65%, w/w, p.a. purchased by Merck GmbH, Germany and sub-boiled using a dst-1000 Savillex, USA) and rinsed with ultrapure water (USF ELGA Purelab Plus system, ELGA LabWater, Germany). To avoid contaminations, pipes and tubes were rinsed >12 h with HNO_3 (1.3%) and ultrapure water (>2 h) and filled with overlying water from the experiment. During the first 8 profiles the entire volume of the samples was stabilized by EDTA (Sigma Aldrich, 99,995%, trace metal basis, final concentration 20 mM) and used for speciation (As(III/V) and Sb(III/V)) as well as for determination of the total concentration including colloids and suspended matter. To be able to add size fractionation analyses, the samples of profiles 9-11 (*cf.* Table A1. 1, Appendix A1) were split online using a programmable split valve (Cetoni, NEMESYS low pressure syringe pump valve). Half of the volume sampled for size fractionation was filtered with syringe filters (pore size 0.45 µm, Minisart NML Syringe Filters, surfactant-free cellulose acetate, Sartorius, Germany). In agreement with the general convention, the element concentrations of the filtered fraction are regarded as "dissolved" fraction (<0.45 µm) even though also colloids might pass the filter. Element concentrations of the unfiltered pore water (<16 µm) are referred to as total content fraction. Samples for size fractionation analyses were acidified to a concentration of 1.3% HNO_3 and stored frozen until measurement.

2.3.4 Incubation Experiment

The sediment used within the experiment was sampled at a former millstream at the river Lahn in Germany. Since several years the water body is not connected directly to the river and receives fresh water from the main stream approximately two to three times per year at flood events (Figure A1. 1, Appendix A1). Details on the sampling site and the sampling procedure are provided in Appendix A1, section A1. 2.

Table A1. 1 (Appendix A1) delivers an overview of the experimental setup. As mentioned, the aim of the study was to design, manufacture and test the *messy* with respect to different scientific questions.

Therefore, after an incubation time of two month the sediment was profiled two times at the beginning to characterize the actual conditions (profile 1, day -10 and profile 2, day -5). On day 0 the sediment was disturbed by fully mixing the sediment and water with a stainless steel stirrer (IKA, Germany) driven by a screw driller (Makita, Germany) for 5 minutes. Preliminary experiments (data not shown) showed a very low Sb release. In order to deal with Sb concentrations in the pore water above the detection limits the authors considering the suspension of Sb_2O_3 would contain approximately 1% Sb as dissolved species[12]. Therefore, Sb was spiked as diantimony trioxide *puriss.* (Sb_2O_3, Merck, Germany) to a concentration of 8 mg/L Sb (as particles) related to the total volume of sediment and the overlying water body. The mean diameter of the powder was 5 µm and the d90 value was 9 µm. It was decided to use Sb_2O_3, because it is one of the most common Sb species used in a multitude of products (e.g., as flame retardant). Moreover, a direct release into the aquatic environments from brake pads containing antimony sulfide (species transformation within the braking process) is possible via street run-off[13]. Directly before spiking Sb_2O_3 was suspended in 50 mL demineralized water (electric conductivity ~0.5 µS/cm; demineralization system by Grünbeck Wasseraufbereitung GmbH, Germany). The suspension was added dropwise during the physical disturbance. Subsequently, profile 3 was started. After the main sediment fraction was settled, air was bubbled into the water column via a glass air stone (JBL, Germany) and a membrane pump (Sera air 110 plus, Germany) to support oxygen induced slow "natural" pyrite weathering, resulting in a slow acidification over time. After the disturbance *messy* profiles were taken on day 5, 10, 15, 20, 57, 65, 77 and 141. As described in detail in chapter 2.3 the sampling procedure and stabilization of the samples was changed after profile 8, mainly to be able to perform size fractionation analyses. After profile 11 a sediment core was taken with a polyethylene terephthalate glycol tube (CT 46.2 ClearTec, Germany). The core was frozen and cut into 1 cm slices with a ceramic knife. The depth related pseudo total content of the sediment was determined after microwave assisted digestion with reverse *aqua regia* as described in Appendix A1, section A1. 3.

2.3.5 ICP-MS Analyses

Concentrations of the metalloids in the pore water as well as in different fractions were performed by means of inductively coupled plasma-quadrupole mass spectrometry (ICP-QMS, Agilent 7700 series; Agilent Technologies, Germany) equipped with a ST Micro Flow nebulizer (ES-2040) and an inert sample introduction kit (both PFA) with a sapphire injector (inner diameter of 2.5 mm, all Agilent Technologies, Germany). To determine the total concentrations, samples were introduced using an autosampler (ASX-500, CETAC Technologies, USA) and the integrated sample introduction system (ISIS) of the ICP device. The arsenic and antimony (III/V) speciation preservation was applied based on the procedure from.[14] Analyses were performed by coupling a HPLC (Agilent, 1290, Germany) to the ICP-QMS (*cf.* Appendix A1, section A.1 5). The separation of the species was undertaken using a Hamilton

PRP-X100 250x4.6 mm (pore size 10 µm) column and two mobile phases with 3% MeOH (Sigma Aldrich, CHROMASOL, 99.9%) and different EDTA concentrations (A: 5 mM EDTA and B: 30 mM EDTA). Instead of the Micro Flow nebulizer a PEEK Mira Mist nebulizer was used (Burgener research, Canada) for the EDTA-containing samples.

2.3.6 Calculations and graphs

All analyses were performed with SPSS 17.0. Bivariate correlation analyses were performed with Spearman's rank correlation test, since some of the profile data was not normal distributed. All graphs were prepared with Origin 2016 or Excel. Redox potentials measured under acidic conditions were corrected in accordance to.[15]

2.4 Results and discussion

The results will be presented and discussed in 4 sections: First the development of the sediment parameters (redox and pH) during the incubation experiment is presented. Subsequently their impact is shown on the total metal(loid) fraction (<16 µm). The results of As and Sb speciation and of the size fractionation analyses are discussed in two separate paragraphs.

2.4.1 Sediment parameters

During the first two profiles (conducted prior to the disturbance and addition of oxygen) of the experiment a redox potential averaging about 200 mV was measured in the water column at near neutral pH values of ~7.3. Below the SWI it decreased to values <-200 mV (*cf.* Figure A1. 2, Appendix A1).

On day 0 of the incubation experiment two processes were initiated to simulate events known to influence the physicochemical parameters of sediments: first, a resuspension event was simulated by the mechanical disturbance of the sediment and, second, sulfide weathering was initiated by the aeration of the water column resulting in an acidification process.

The effects detected directly after the disturbance were low compared to the mid and long term changes over the experimental period of 140 days. The pH value in the water above the SWI dropped slightly from 7.3 to 7.0 within the first three profiles measured after the disturbance (at days 0, 5 and 10) (*cf.* Figure A1. 3, Appendix A1). Also mixing and related oxygenation led to a less pronounced redox gradient compared to the former profiles.

The main shift of the pH in the water body took place between day 30 and 50 leading to a pH of <4.5. This acidification was followed by the development of a steep redox gradient (from day 60 on) showing values of ~500 mV in the overlaying water body and the upper 5 cm of the sediment and of ~-450 mV in the deeper sediment layers (*cf.* Figure A1. 2, Appendix A1).

The acidification detected can be related to sulfide weathering caused by the aeration of the anoxic sediment containing high sulfur quantities (*cf.* Table A1. 2, Appendix A1). This is comparable to studies from other sites with sediments[16,17] or bedrocks[18] containing high sulfur concentrations. Especially in association with (former) mining activities where pyrite weathering is known to cause significant environmental problems[19,20] by acid mine drainage[21,22] (see also paragraph 3.2). A detailed description of the sulfide weathering can be found elsewhere.[23,24] However, the question, if the pyrite weathering was driven by bedrock weathering or secondary sulfide containing minerals, was not within the scope of this study and should be addressed in future experiments.

2.4.2 The release of metal(loid)s into the pore water

During the first two profiles (day -10 and -5) with exception of Cd all remaining analytes discussed (Ag, As, Cd, Co, Cu, Fe, Mn, Mo, Ni, Sb, U, V, Zn) were present in the water column in concentrations above the respective detection limit (>LOD).

With increasing depth the concentrations of Fe and Mn increased from values in the water column between 7 and 150 µg/L for Fe and 86 and 188 µg/L for Mn, to about 9000 µg/L (Fe) and >650 µg/L (Mn) in the sediment pore water at 15 cm depth (*cf.* Figure 2.2 and Figure A1. 5 and Tables A1. 9 and A1. 10, Appendix A1). This displays the solubility of Mn^{2+} and Fe^{2+} species released due to the reduction of Mn- and Fe oxy(hydr)oxides under low redox conditions.[6,25,26] The concentrations of all other elements analyzed decreased in the sediment pore water with increasing depth. This is likely to be the result of an increasing availability of H_2S in deeper sediment layers and the formation of insoluble metal-sulfides.[27-29] For As, Co, Cu and Zn a subsurface peak was detected in the first profiles at a depth of 1-4 cm. This can be explained by the degradation of organic matter in the cause of the reduction during the incubation period and the release of associated metal(loid)s.[30]

Based on the element distributions, three different patterns can be distinguished initiated by the mechanical disturbance and the acidification process. These are exemplary illustrated by the concentrations of Mo, Cd and Mn (Figure 2.2).

The first group of elements (As, Mo, U and V; Figure 2.2 and 2.3; Figures A1. 6-A1. 7, Appendix A1) showed a direct but temporary increase of the concentration in the water column after the mechanical disturbance followed by a decrease over the course of the experiment. All these metal(loid)s are oxides-forming elements. In the case of V, U and As, the concentration peak was detected in the first profile after the disturbance, probably caused by a resuspension of particulate matter containing metal(loid)s.[31] In contrast to that, the results of Mo indicate that the mixing led to a more homogenous distribution over the entire profile (*cf.* Table A1. 15, Appendix A1). All elements of this group showed an ongoing decrease of the concentration in the water column (*cf*. tables A1. 11 and A1. 15-A1. 17,

Appendix A1) that can be explained by sorption to iron(hydr)oxides of the oxy-anionic species.[32] However, since the concentrations, especially of U and V, are in the low µg/L range and close to the LODs, small changes in concentrations should not be over-interpreted. The heatplots chosen enable a fast and simple access to data sets with three dimensions (here: time, depth and concentration), but include the risk of an over-interpretation if the analytical circumstances are not taken into account. For example the apparent concentration peak of Mo in the SWI near sediment pore water at day 65 (Figure 2.2) is related to high limits of detection on the previous profile at day 57 and comparatively lower LODs on the following days (*cf* Table A1. 15, Appendix A1; all measurements were close to the LODs).

The second group contains the metals Co, Fe, Mn, Ni and Zn (*cf*. Tables A1. 12, A1. 9, A1. 10, A1. 18, A1. 14 and Figures A1. 5, A1. 8-A1. 10, Appendix A1) characterized by a long-term progressive accumulation in the water column and in the SWI near sediment pore water impacted by the acidification process. Subsequent to the mechanical disturbance only Mn, which concentrations sextupled, and Co were released to the water column, while Zn, Ni and (less pronounced) Fe were removed. In all cases the mixing process led to less pronounced differences between the concentrations in the water column and the pore water of the sediment. As an effect of the acidification process the elements Ni, Co, Zn and Mn were progressively released from the sediment and accumulated in the water column multiplying their initial concentrations by the factors 3, 10, 10 and 200, respectively. Concentrations of Mn and Zn also tripled in the surface-near pore water. In a comparable manner, a tenfold increase of the Fe concentration is restricted to the first cm below the SWI. An increase of the Fe concentration in the water column was hampered by a visible iron-ochre precipitation on the sediment surface.

In contrast to Fe, which was almost completely removed from the water during the mechanical disturbance, Mn remained available in the system and disappeared after settling of the sediment from the overlying water body. Since the oxidation of Mn^{2+} proceeds orders of magnitudes slower than this of Fe^{2+} [26], the element remained longer in the water phase during the disturbance.

The decrease of Ni and Zn during the disturbance in the water column is most likely related to an association with the organic carbon of the sediment[33] (*cf*. Tables A1. 18 and A1. 14, Appendix A1). Scavenging of these organic complexes by the suspended particulate matter during mixing is hypothesized to explain the difference in the behavior of these elements in comparison to Co and Mn. This is in accordance with the findings of Vink et al. (2010)[30] that the production of dissolved organic matter is enhanced in case of available Mn.

The comparable high sulfur content of the sediment (cf. Table A1. 2, Appendix A1) and the location of the sampling site in a former mining area of the chalcophile elements Ag and Pb cause an oxygen

induced acidification. In most anoxic sediments sulfides are considered to be the predominant solid phase of metal(loid)s.[34] While FeS_2 is the most widespread sulfide mineral in nature,[24] trace elements are associated to it.[27,29,35] The self-energizing process of pyrite-weathering and the co-release of metal(loid)s from primary and secondary sulfides can thus be regarded as a main process causing the observed metal release.

Under oxic conditions Fe and Mn (hydr)oxides are important carriers for metal(loid)s. The precipitation of Fe (hydr)oxides could thus be expected to cause scavenging of the released metal(loid)s and limit their accumulation in the water column. However, as shown by Frohne et al. (2014)[36] and Shaheen et al. (2016)[37] acidic conditions might prevent metal(loid)s like Co, Ni and Zn from co-precipitation with Fe (hydr)oxides. The accumulation of Mn in the water column suggests that precipitation of Mn (hydr)oxides was prohibited by the prevalent acidic conditions which is in according with findings of Frohne et al. (2011).[36]

Next to sulfides and Fe and Mn (hydr)oxides the mobility of metal(loid)s is decisively determined by reactions with organic matter (OM). Processes as desorption of metal(loid)s from OM (as well as clay minerals and other sorbents) due to the acidic conditions and the release of metal(loid)s caused by degradation of OM might contribute to the observed releases. On the other hand dissolved organic carbon (DOC) promotes the solubility of metal(loid)s and prevents them from co-precipitation with minerals such as Fe (hydr)oxides. The importance of these processes is discussed by e.g., Frohne et al. (2014)[37] and Shaheen et al. (2016)[38]. Their contribution in comparison to the pyrite weathering can be examined in future experiments with *messy* by parallel analyses of the SO_4^{2-} or totals S and DOC or total C concentration of the pore water.

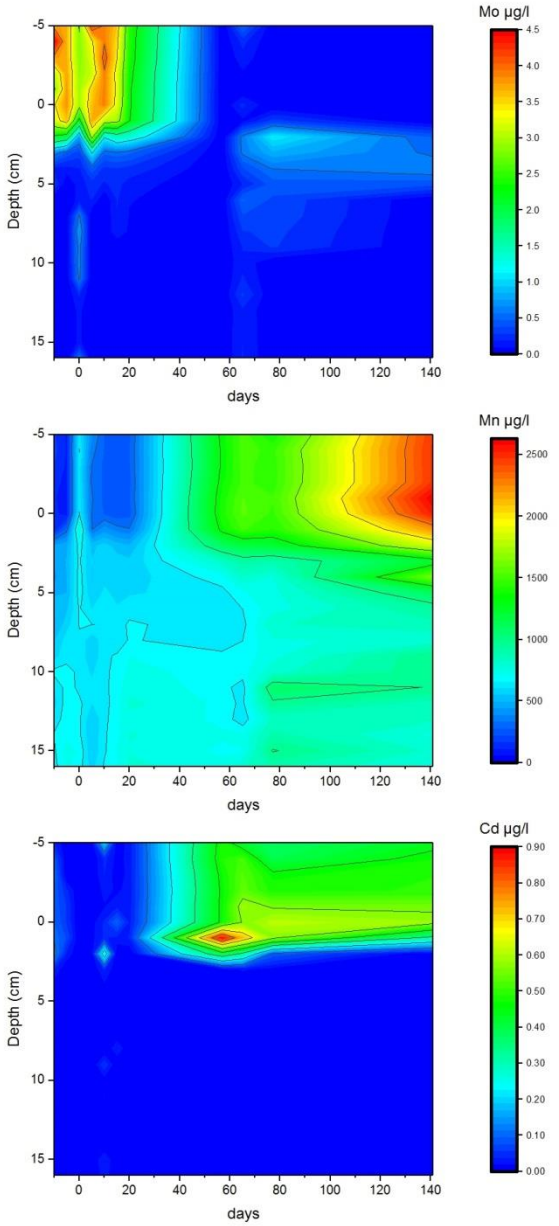

Figure 2.2: *Concentration of cadmium, manganese and molybdenum in the <16 µm filtered pore water across the sediment water interface.*

The elements of the third group, including Ag, Cd and Cu (Tables A1. 19, A1. 20, A1. 13 and Figure A1. 11-A1. 12, Appendix A1) were removed from the water column during the simulated resuspension event. A sudden but temporary release of Cd and Cu following the main pH shift is reflected by distinct concentration maxima of 0.89 (Cd) and 289 (Cu) µg/L in the near-surface pore water during profiles 8 (day 57) and 9 (day 65). A peak in Ag concentrations (1.5 µg/L) followed delayed in profile 10 (day 77). These high concentrations were only detected in pore water samples directly below the SWI. Ag, Cd and Cu were found to be essentially associated with the organic phase in several studies and the oxidation of organic matter was observed to cause substantial release of all three elements [39-44]. This most likely explains their concentration maxima and indicates that even higher concentrations may

occur in the thin boundary layer at the sediment surface directly impacted by the aerated water which could not be captured by the *messy* due to the coarse resolution.

Even though Cu and Cd seem to behave differently compared to the elements of group 2 (Co, Mn, Ni, Zn), Spearmann based calculated correlations (*cf.* Table A1. 17, Appendix A1) suggest similar processes during the acidification process. All 6 elements were positively correlated (correlation coefficients >0.7) in the profiles affected by acidification (profiles 8-11). Also regarding the whole 140 day period of the experiment, highest correlation coefficients (>0.7) were calculated for the elements Cd, Cu, Zn and Ni. Comparably, within the group of the anion-forming elements, positive correlation coefficients (>0.7) were determined for Mo/Sb (profile 1-4) and As/U and As/V (profile 8-11). Differences between the anion forming elements As, Mo, U and V and the divalent cation forming elements are reflected by negative correlations during the acidification process. Values <-0.7 were found for V/Cd, V/Mn, V/Mo and V/Zn as well as for As/Cd and Mo/U considering profiles 8-11. Correlation coefficients >0.6 between Sb and Mo, Ni and Zn might result from the Sb_2O_3 spike and the visible short and low initial Sb release. Taken together, the correlation coefficients presented in Table A1. 21 (Appendix 1) support and extend the grouping of the elements undertaken by observation (heatplots) and basic theory previously published on the fate of cation- and oxyanion forming metal(loid)s in the SWI.

2.4.3 Speciation of As(III/V) and Sb(III/V)

Species related concentrations of As and Sb were determined throughout the incubation experiment by coupling an HPLC to the ICP-QMS as detailed in section 2.3.3.

Before mixing arsenic concentrations in the water column above the sediment were ~1 µg/L, exhibited a subsurface peak (>1.5 µg/L) and decreased in the pore water of deeper sediment layers. This distribution pattern was equally found for As(III) and As(V) (*cf.* Figure 2.3 and Tables A1. 22-A1. 23, Appendix A1), with As(III) being the dominant species across all depth profiles. The dominance of As(III) prevailed within all samples throughout the experiment, but was less prominent in pore water samples near the SWI after the mechanical disturbance. Together with the more pronounced redox gradient and also affected by the re-oxidation and acidification process, the subsurface peak of As shifted deeper into the sediment (Figure 2.3 and Figure A1. 2, Appendix A1). The observed dominance of As(III) species in the water column differs from the findings of others, where usually As appears in the oxidation state +5 under oxic conditions.[32,45] A potential explanation for this effect in this study is that As(V) was quickly removed from the water column, whereas As(III) concentrations remained stable. This presumably reflects the preferential scavenging of As by Fe (hydr)oxides[46] with As(V) being more effectively adsorbed than As(III).[46,47] Accordingly, the iron-ochre layer formed on the sediment probably acts as an effective As barrier.

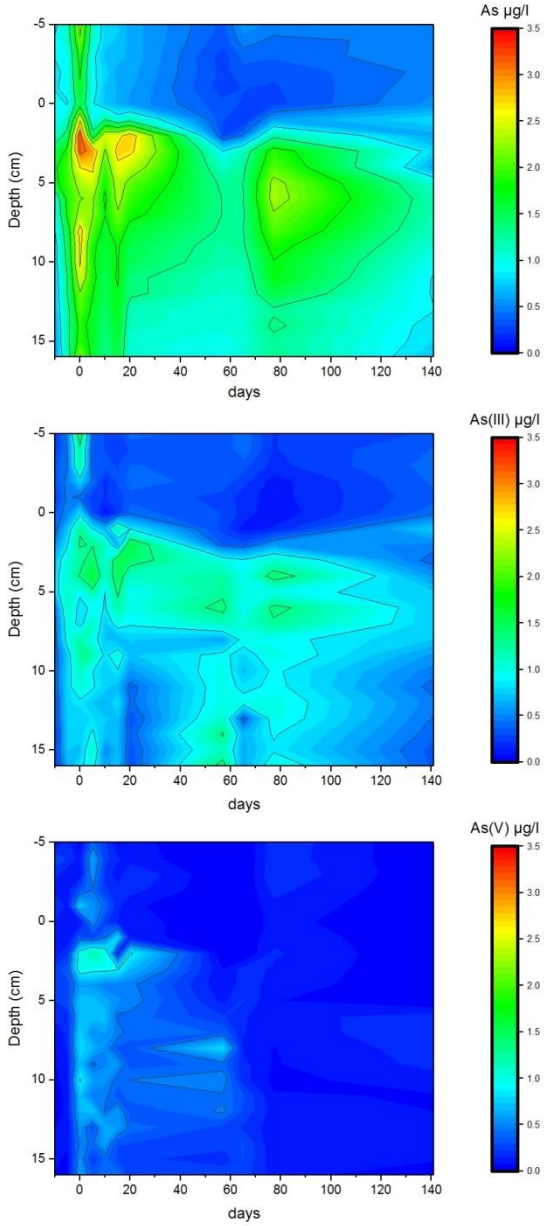

Figure 2.3: *Concentration of arsenic, arsenite and arsenate in the <16 µm filtered pore water across the sediment water interface.*

Throughout the experiment the sum of As(III) and As(V) only explains ~50% of the total As detected. Within this context, two aspects must be taken into account, whereas the first is most likely more relevant: (i) The total content is based on the size fraction <16 µm and not on the fraction <0.45 µm. Additionally, the method applied to separate As(III and V) capture compounds bound to EDTA and, hence, does not include size fractions/species which display a higher bonding strength than EDTA. These considerations are supported by the fractionation approach (*cf.* paragraph 3.4) where a significant portion of arsenic was proven to be associated to the size fraction between 0.45 and 16 µm especially in the SWI-near pore water. (ii) In contrast to Sb, As is an element with very divers biogeochemical species that are not entirely addressed by the method applied separating the

inorganic, but not the organic As species. Further details on As speciation can be found in e.g., Oremland & Stolz (2003)[48] or Mestrot (2013)[49]. However, the overall picture shows the dominance of inorganic As(III) species as well as the fact that the SWI is an efficient barrier for As under the prevalent experimental conditions.

The spike of Sb_2O_3 (final concentration 8 mg/L) performed during the mechanical disturbance (see section 2.3.4) has to be considered during the interpretation of the Sb concentrations. Sb was present in the water column in concentrations of about 0.6 µg/L and dropped below 0.1 µg/L in the pore water in the first two profiles (day -10 and -5). Sb(V) was the dominant species throughout the experiment, but the Sb(III) concentrations were always below the respective LOD (*cf.* Tables A1. 24-A1. 25 and Figures A1. 13-A1. 14, Appendix A1). Even after spiking Sb_2O_3 only the concentrations of total Sb and Sb(V) increased, whereas Sb(III) was still not detectable. Regardless of the concentrations of the different species, the contribution of the spike to the total Sb pore water concentration was remarkably low. Even considering the low solubility of Sb_2O_3, it can (based on theory and practice) be expected that a spike of 8 mg/L leads to increased Sb concentrations in the course of the experiment.[7,12] However, only during disturbance/spiking the total and the Sb(V) concentration raised in the overlying water body, but remained in the ng/L range and, hence, close to the LODs. Following the hypothesis that Sb_2O_3 releases dissolved species under the prevalent conditions, the low concentrations might be explained by a direct removal from the <16 µm fraction due to the attachment of the spiked particles to suspended material and due the affinity of Sb to Fe and Mn hydroxides.[50] The release in the SWI-near pore water can be related to the sulfide weathering process since the solubility of Sb is known to be controlled by sorption on Fe sulfides under anoxic conditions.[51] Moreover, the nearly equal concentrations of total Sb and Sb(V) are in accordance with the finding that, in contrast to As, methylated or organic compounds usually represent only a small percentage of the total Sb fraction[52] and that the oxidation of Sb(III) to Sb(V) occurs fast under oxic conditions.[53]

2.4.4 Size fractionation

The ability of the *messy*-system to obtain information on different size fractionations was tested during the last 3 profiles (profile 9, 10 and 11, day 65, 77 and 141) of the experiment. Therefore, half of the sample volume was filtered through 0.45 µm membrane filters (*cf.* section 2.3.3 and Figure 2.1). Colloidal element concentrations were calculated by subtracting the dissolved fraction (<0.45 µm) from the total concentration (<16 µm). It thus includes larger colloids and small particles, but does not cover the size range between 0.001 and 1000 µm often defined as colloids (e.g. Guo & Santschi (2006)[54]). However, the term "colloidal size fraction" is not covered by a strict experimental convention like the term "dissolved fraction" (<0.45 µm) and the aim of the approach presented here was to test the general applicability of the experimental concept. Regarding the ICP-MS measurements, suspected

instabilities caused by large colloids or small particles (<16 µm) were not detected, probably because sample conservation with HNO_3 led to their dissolution. For the elements Ag, As, Cu, Fe and Mn it was possible to identify different fractions (Figure 2.4 and Figure A1. 15-A1. 18, Appendix A1). Negative values may occur due to rising uncertainties closer to the LODs and an overall combined uncertainty of about 25% assumed for this methodologic approach.

Generally only small percentages of most analytes were present in the colloidal fraction in samples originating from the water column, which most likely can be explained by the prevalent acidic conditions leading to dilution of existing colloids. An exception is Ag, which was found to be with about 50% colloidal size fraction in the water column (*cf.* Figure A1. 15, Appendix A1). This corresponds well with its tendency to form sulfide particles.[55] Regarding Fe and Mn the colloidal fraction is of increasing importance with increasing depth and often accounts for 60-95% of Fe below 4 cm and 20-40% of Mn below 12 cm depth (*cf.* Figure A1. 16-A1. 17, Appendix A1). Whether this can be linked to organic matter degradation cannot be answered with the presented data set. Also 70-100% of Cu in many pore water samples is presented in the colloidal size fraction (*cf.* Figure A1. 18, Appendix A1). Even though total Cu concentration in this samples is mostly <1 µg/L the results are in good agreement with the high affinity of Cu to organic ligands.[56,57] Interesting is the fate of As. Its highest proportions in the colloidal fraction (25-50%) were found close to the SWI in the zone where a decrease of the total concentrations took place with decreasing depth (Figure 2.4). This zone corresponds with the depth interval where Fe accumulates. An orders of magnitude larger amount of Fe compared to As is given and appears to be an additional evidence of the adsorption of As to Fe (hydr)oxides mentioned in section 2.4.3. Even a small percentage of the Fe present as hydroxides would offer sufficient bonding sites for the adsorption of most of the As species.

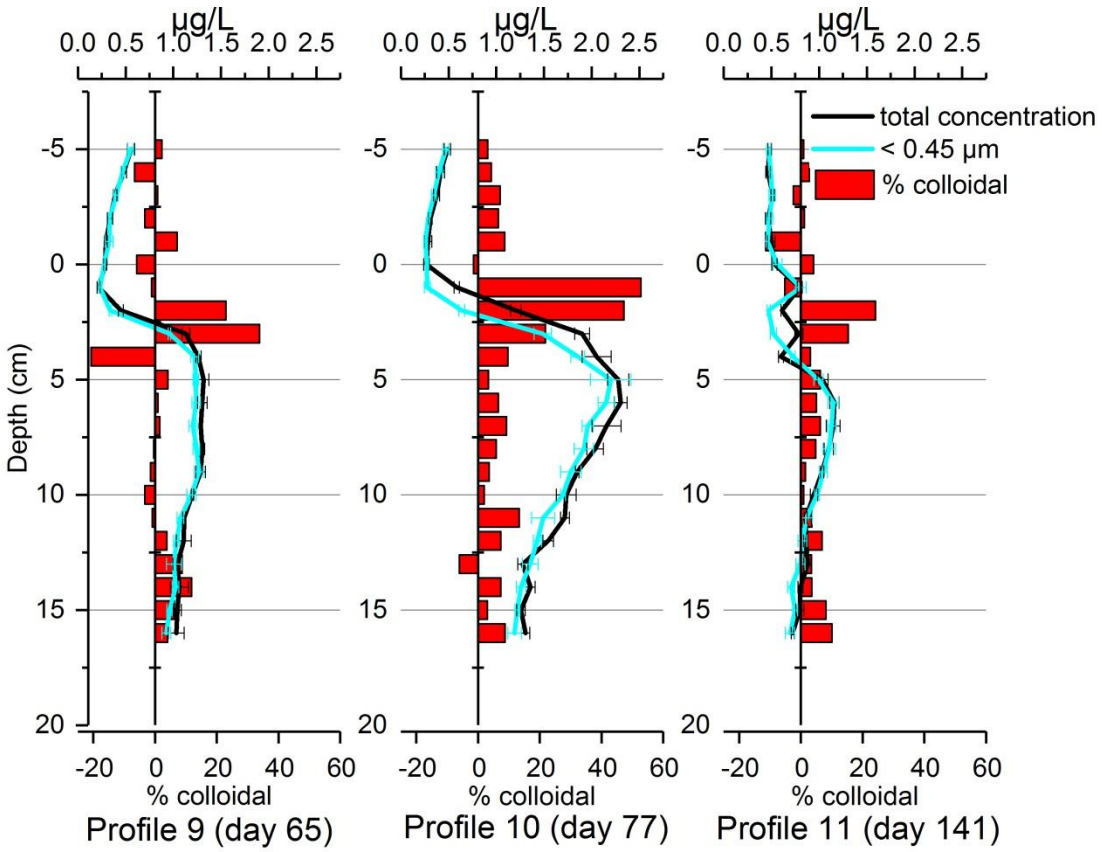

Figure 2.4: *Profiles of total (<16 µm) and dissolved (<0.45 µm) arsenic concentration and calculated colloidal fraction in % across the SWI. Exemplary diagrams for Ag, Cu, Fe and Mn are given in the SIs (Figure A1. 15– A1. 18, Appendix A1).*

Regarding potential future improvements several optimizations are possible: (i) The glove box environment can be adopted to trace analyze needs. (ii) By lowering the sampling resolution, more volume per depth can be sampled and fractionated. (iii). By using smaller syringe filters the dead volume can be lowered. In considering these steps in future studies, the promising first *messy* results on the contribution of colloidal pore water release may be extended in a systematic manner to better understand the mechanisms under varying environmental conditions.

2.5 Summary and conclusions

The *messy*-setup presented extends the experimental range with respect to depth and size fractionation. It provides a method for low invasive, automated sampling of pore water profiles across the SWI, delivering the possibility to monitor, locate and quantify metal(loid)s mobility during sediment manipulation and simulation of naturally occurring processes as resuspension and sulfide weathering induced acidification. It was proven that it is combinable with different techniques for sample preparation and analyses like size fractionation and speciation analyses. Therefore, *messy* delivers high

degree of freedom to design experiments with respect to time, depth and size resolution. By using a glass probe head also organic trace analytes could be addressed in future studies.

By increasing the amount of data available from *missy* or *messy* studies as well as dialyses based investigations (e.g., peeper based studies[5,58] or diffusive gradients in thin films,[59-61] it will be possible to setup or improve models that address the mobility of metal(loid)s at the SWI. Until now, suction based setups, like *messy*, are mainly applied in laboratory experiments, whereas diffusion based methods are more common in field studies. To better link the results from the different methods a direct comparison between diffusion based and suction based methods identifying their advantages and limitations, is desirable.

2.6 References

1. Stockdale, A.; Davison, W.; Zhang, H., Micro-scale biogeochemical heterogeneity in sediments: A review of available technology and observed evidence. *Earth-Science Reviews* **2009,** *92*, (1-2), 81-97.
2. Murdoch, A.; Azcue, J. M., *Manual of aquatic sediment sampling*. Lewis Publishers: Boca Raton, 1995; p 219.
3. Lourino-Cabana, B.; Lesven, L.; Billon, G.; Denis, L.; Ouddane, B.; Boughriet, A., Benthic exchange of sedimentary metals (Cd, Cu, Fe, Mn, Ni and Zn) in the Deûle River (Northern France). *Environmental Chemistry* **2012,** *9*, (5), 485.
4. Scholz, F.; Hensen, C.; Noffke, A.; Rohde, A.; Liebetrau, V.; Wallmann, K., Early diagenesis of redox-sensitive trace metals in the Peru upwelling area – response to ENSO-related oxygen fluctuations in the water column. *Geochimica et Cosmochimica Acta* **2011,** *75*, (22), 7257-7276.
5. Lewandowski, J.; Rüter, K.; Hupfer, M., Two-Dimensional Small-Scale Variability of Pore Water Phosphate in Freshwater Lakes: Results from a Novel Dialysis Sampler. *Environmental Science & Technology* **2002,** *36*, (9), 2039-2047.
6. Rigaud, S.; Radakovitch, O.; Couture, R.-M.; Deflandre, B.; Cossa, D.; Garnier, C.; Garnier, J.-M., Mobility and fluxes of trace elements and nutrients at the sediment–water interface of a lagoon under contrasting water column oxygenation conditions. *Applied Geochemistry* **2013,** *31*, 35-51.
7. Duester, L.; Prasse, C.; Vogel, J. V.; Vink, J. P. M.; Schaumann, G. E., Translocation of Sb and Ti in an undisturbed floodplain soil after application of Sb2O3 and TiO2 nanoparticles to the surface. *Journal of Environmental Monitoring* **2011,** *13*, (5), 1204.
8. Seeberg-Elverfeldt, J.; Schlüter, M.; Feseker, T.; Kölling, M., Rhizon sampling of porewaters near the sediment-water interface of aquatic systems: Rhizon porewater sampling. *Limnology and Oceanography: Methods* **2005,** *3*, (8), 361-371.

9. Vink, J. P. M., Measurement of Heavy Metal Speciation over Redox Gradients in Natural Water−Sediment Interfaces and Implications for Uptake by Benthic Organisms. *Environmental Science & Technology* **2002,** *36*, (23), 5130-5138.
10. Fabricius, A.-L.; Duester, L.; Ecker, D.; Ternes, T. A., New Microprofiling and Micro Sampling System for Water Saturated Environmental Boundary Layers. *Environmental Science & Technology* **2014,** *48*, (14), 8053-8061.
11. Hofacker, A. F.; Voegelin, A.; Kaegi, R.; Kretzschmar, R., Mercury Mobilization in a Flooded Soil by Incorporation into Metallic Copper and Metal Sulfide Nanoparticles. *Environmental Science & Technology* **2013,** *47*, (14), 7739-7746.
12. Dehnicke, K., Hollemann-Wiberg, Lehrbuch der Anorganischen Chemie. 101. Auflage. VonNils Wiberg. Walter de Gruyter, Berlin/New York, 1995. 2033 S., geb. 158.00 DM. ISBN 3–11–012641–9. *Angewandte Chemie* **1996,** *108*, (21), 2696-2696.
13. Iijima, A.; Sato, K.; Yano, K.; Kato, M.; Kozawa, K.; Furuta, N., Emission Factor for Antimony in Brake Abrasion Dusts as One of the Major Atmospheric Antimony Sources. *Environmental Science & Technology* **2008,** *42*, (8), 2937-2942.
14. Daus, B.; Wennrich, R., Investigation on stability and preservation of antimonite in iron rich water samples. *Analytica Chimica Acta* **2014,** *847*, 44-48.
15. DeLaune, R. D.; Reddy, K. R., Redox Potential. In *Encyclopedia of Soils in the Environment*, Hillel, D., Ed. Academic Press: 2005; pp 366-371.
16. Åström, M.; Åström, J., Geochemistry of stream water in a catchment in Finland affected by sulphidic fine sediments. *Applied Geochemistry* **1997,** *12*, (5), 593-605.
17. Cánovas, C. R.; Olías, M.; Macias, F.; Torres, E.; San Miguel, E. G.; Galván, L.; Ayora, C.; Nieto, J. M., Water acidification trends in a reservoir of the Iberian Pyrite Belt (SW Spain). *Science of The Total Environment* **2016,** *541*, 400-411.
18. Cameron, E. M.; Prévost, C. L.; McCurdy, M.; Hall, G. E. M.; Doidge, B., Recent (1930s) natural acidification and fish-kill in a lake that was an important food source for an Inuit community in northern Québec, Canada. *Journal of Geochemical Exploration* **1998,** *64*, (1-3), 197-213.
19. Mascaro, I.; Benvenuti, M.; Corsini, F.; Costagliola, P.; Lattanzi, P.; Parrini, P.; Tanelli, G., Mine wastes at the polymetallic deposit of Fenice Capanne (southern Tuscany, Italy). Mineralogy, geochemistry, and environmental impact. *Environmental Geology* **2001,** *41*, (3-4), 417-429.
20. Schuwirth, N.; Voegelin, A.; Kretzschmar, R.; Hofmann, T., Vertical Distribution and Speciation of Trace Metals in Weathering Flotation Residues of a Zinc/Lead Sulfide Mine. *Journal of Environment Quality* **2007,** *36*, (1), 61.
21. Akcil, A.; Koldas, S., Acid Mine Drainage (AMD): causes, treatment and case studies. *Journal of Cleaner Production* **2006,** *14*, (12-13), 1139-1145.

22. Blowes, D. W.; Ptacek, C. J.; Jambor, J. L.; Weisener, C. G., The Geochemistry of Acid Mine Drainage. In *Treatise on Geochemistry*, Elsevier: 2003; pp 149-204.
23. Schippers, A.; Sand, W., Bacterial Leaching of Metal Sulfides Proceeds by Two Indirect Mechanisms via Thiosulfate or via Polysulfides and Sulfur. *Applied and Environmental Microbiology* **1999,** *65*, (1), 319-321.
24. Schippers, A., Biogeochemistry of metal sulfide oxidation in mining environments, sediments, and soils. In *Special Paper 379: Sulfur Biogeochemistry - Past and Present*, Geological Society of America: 2004; Vol. 379, pp 49-62.
25. Balistrieri, L. S.; Murray, J. W.; Paul, B., The geochemical cycling of trace elements in a biogenic meromictic lake. *Geochimica et Cosmochimica Acta* **1994,** *58*, (19), 3993-4008.
26. Giblin, A. E., Iron and Manganese. In *Encyclopedia of Inland Waters*, Elsevier: 2009; pp 35-44.
27. Huerta-Diaz, M. A.; Morse, J. W., Pyritization of trace metals in anoxic marine sediments. *Geochimica et Cosmochimica Acta* **1992,** *56*, (7), 2681-2702.
28. Morse, J. W., Interactions of trace metals with authigenic sulfide minerals: implications for their bioavailability. *Marine Chemistry* **1994,** *46*, (1-2), 1-6.
29. Morse, J. W.; Luther, G. W., Chemical influences on trace metal-sulfide interactions in anoxic sediments. *Geochimica et Cosmochimica Acta* **1999,** *63*, (19-20), 3373-3378.
30. Vink, J. P. M.; Harmsen, J.; Rijnaarts, H., Delayed immobilization of heavy metals in soils and sediments under reducing and anaerobic conditions; consequences for flooding and storage. *Journal of Soils and Sediments* **2010,** *10*, (8), 1633-1645.
31. Namieśnik, J.; Rabajczyk, A., The speciation and physico-chemical forms of metals in surface waters and sediments. *Chemical Speciation & Bioavailability* **2010,** *22*, (1), 1-24.
32. Smedley, P. L.; Kinniburgh, D. G., A review of the source, behaviour and distribution of arsenic in natural waters. *Applied Geochemistry* **2002,** *17*, (5), 517-568.
33. Collins, R. N.; Kinsela, A. S., The aqueous phase speciation and chemistry of cobalt in terrestrial environments. *Chemosphere* **2010,** *79*, (8), 763-771.
34. Simpson, S. L.; Apte, S. C.; Batley, G. E., Effect of Short-Term Resuspension Events on Trace Metal Speciation in Polluted Anoxic Sediments. *Environmental Science & Technology* **1998,** *32*, (5), 620-625.
35. Huerta-Diaz, M. A.; Tessier, A.; Carignan, R., Geochemistry of trace metals associated with reduced sulfur in freshwater sediments. *Applied Geochemistry* **1998,** *13*, (2), 213-233.
36. Frohne, T.; Rinklebe, J.; Diaz-Bone, R. A.; Du Laing, G., Controlled variation of redox conditions in a floodplain soil: Impact on metal mobilization and biomethylation of arsenic and antimony. *Geoderma* **2011,** *160*, (3-4), 414-424.

37. Frohne, T.; Rinklebe, J.; Diaz-Bone, R. A., Contamination of Floodplain Soils along the Wupper River, Germany, with As, Co, Cu, Ni, Sb, and Zn and the Impact of Pre-definite Redox Variations on the Mobility of These Elements. *Soil and Sediment Contamination: An International Journal* **2014,** *23*, (7), 779-799.
38. Shaheen, S. M.; Rinklebe, J.; Frohne, T.; White, J. R.; DeLaune, R. D., Redox effects on release kinetics of arsenic, cadmium, cobalt, and vanadium in Wax Lake Deltaic freshwater marsh soils. *Chemosphere* **2016,** *150*, 740-748.
39. Gobeil, C.; Silverberg, N.; Sundby, B.; Cossa, D., Cadmium diagenesis in Laurentian Trough sediments. *Geochimica et Cosmochimica Acta* **1987,** *51*, (3), 589-596.
40. Huerta-Diaz, M. A.; Rivera-Duarte, I.; Sañudo-Wilhelmy, S. A.; Flegal, A. R., Comparative distributions of size fractionated metals in pore waters sampled by in situ dialysis and whole-core sediment squeezing: Implications for diffusive flux calculations. *Applied Geochemistry* **2007,** *22*, (11), 2509-2525.
41. Martin, J. H.; Knauer, G. A.; Gordon, R. M., Silver distributions and fluxes in north-east Pacific waters. *Nature* **1983,** *305*, (5932), 306-309.
42. Rivera-Duarte, I.; Flegal, A. R., Pore-water silver concentration gradients and benthic fluxes from contaminated sediments of San Francisco Bay, California, U.S.A. *Marine Chemistry* **1997,** *56*, (1-2), 15-26.
43. Sanudo-Wilhelmy, S. A.; Flegal, A. R., Anthropogenic silver in the Southern California Bight: a new tracer of sewage in coastal waters. *Environmental Science & Technology* **1992,** *26*, (11), 2147-2151.
44. Skrabal, S. A.; Donat, J. R.; Burdige, D. J., Pore water distributions of dissolved copper and copper-complexing ligands in estuarine and coastal marine sediments. *Geochimica et Cosmochimica Acta* **2000,** *64*, (11), 1843-1857.
45. Bissen, M.; Frimmel, F. H., Arsenic — a Review. Part I: Occurrence, Toxicity, Speciation, Mobility. *Acta hydrochimica et hydrobiologica* **2003,** *31*, (1), 9-18.
46. Gorny, J.; Billon, G.; Lesven, L.; Dumoulin, D.; Madé, B.; Noiriel, C., Arsenic behavior in river sediments under redox gradient: A review. *Science of The Total Environment* **2015,** *505*, 423-434.
47. Gupta, S. K.; Chen, K. Y., Arsenic Removal by Adsorption. *Journal (Water Pollution Control Federation)* **1978,** *50*, (3), 493-506.
48. Oremland, R. S.; Stolz, J. F., The Ecology of Arsenic. *Science* **2003,** *300*, (5621), 939-944.
49. Mestrot, A.; Planer-Friedrich, B.; Feldmann, J., Biovolatilisation: a poorly studied pathway of the arsenic biogeochemical cycle. *Environmental Science: Processes & Impacts* **2013,** *15*, (9), 1639.
50. Filella, M.; Belzile, N.; Chen, Y.-W., Antimony in the environment: a review focused on natural waters. *Earth-Science Reviews* **2002,** *59*, (1-4), 265-285.

51. Chen, Y.-W.; Deng, T.-L.; Filella, M.; Belzile, N., Distribution and early diagenesis of antimony species in sediments and porewaters of freshwater lakes. *Environmental Science & Technology* **2003,** *37*, (6), 1163-1168.
52. Filella, M.; Belzile, N.; Chen, Y.-W., Antimony in the environment: a review focused on natural waters. *Earth-Science Reviews* **2002,** *57*, (1-2), 125-176.
53. Oorts, K.; Smolders, E.; Degryse, F.; Buekers, J.; Gascó, G.; Cornelis, G.; Mertens, J., Solubility and toxicity of antimony trioxide (Sb2O3) in soil. *Environmental Science & Technology* **2008,** *42*, (12), 4378-4383.
54. Guo, L.; Santschi, P. H., Ultrafiltration and its Applications to Sampling and Characterisation of Aquatic Colloids. In *Environmental Colloids and Particles*, Associateessor, K. J. W. P. D.; Lecturer, J. R. L. P. D. p. r. S., Eds. John Wiley & Sons, Ltd: 2006; pp 159-221.
55. Levard, C.; Hotze, E. M.; Lowry, G. V.; Brown, G. E., Environmental Transformations of Silver Nanoparticles: Impact on Stability and Toxicity. *Environmental Science & Technology* **2012,** *46*, (13), 6900-6914.
56. Burton, E. D.; Hawker, D. W.; Tighe, M. R., Sludge-Derived Cu and Zn in a Humic-Gley Soil: Effect of Dissolved Metal-Organic Matter Complexes on Sorption and Partitioning. *Soil and Sediment Contamination* **2003,** *12*, (1), 23-46.
57. Schröder, T. J.; van Riemsdijk, W. H.; van der Zee, S. E. A. T. M.; Vink, J. P. M., Monitoring and modelling of the solid-solution partitioning of metals and As in a river floodplain redox sequence. *Applied Geochemistry* **2008,** *23*, (8), 2350-2363.
58. Peijnenburg, W. J. G. M.; Teasdale, P. R.; Reible, D.; Mondon, J.; Bennett, W. W.; Campbell, P. G. C., Passive sampling methods for contaminated sediments: State of the science for metals: PSMs for Metals in Assessment of Contaminated Sediments. *Integrated Environmental Assessment and Management* **2014,** *10*, (2), 179-196.
59. Dunn, R. J. K.; Teasdale, P. R.; Warnken, J.; Schleich, R. R., Evaluation of the Diffusive Gradient in a Thin Film Technique for Monitoring Trace Metal Concentrations in Estuarine Waters. *Environmental Science & Technology* **2003,** *37*, (12), 2794-2800.
60. Garmo, Ø. A.; Røyset, O.; Steinnes, E.; Flaten, T. P., Performance Study of Diffusive Gradients in Thin Films for 55 Elements. *Analytical Chemistry* **2003,** *75*, (14), 3573-3580.
61. Zhang, H.; Davison, W., Direct In Situ Measurements of Labile Inorganic and Organically Bound Metal Species in Synthetic Solutions and Natural Waters Using Diffusive Gradients in Thin Films. *Analytical Chemistry* **2000,** *72*, (18), 4447-4457.

3

Impact of mechanical disturbance and acidification on the metal(loid) and C, P, S mobility at the sediment water interface examined using a fractionation meso profiling ICP-QQQ-MS approach

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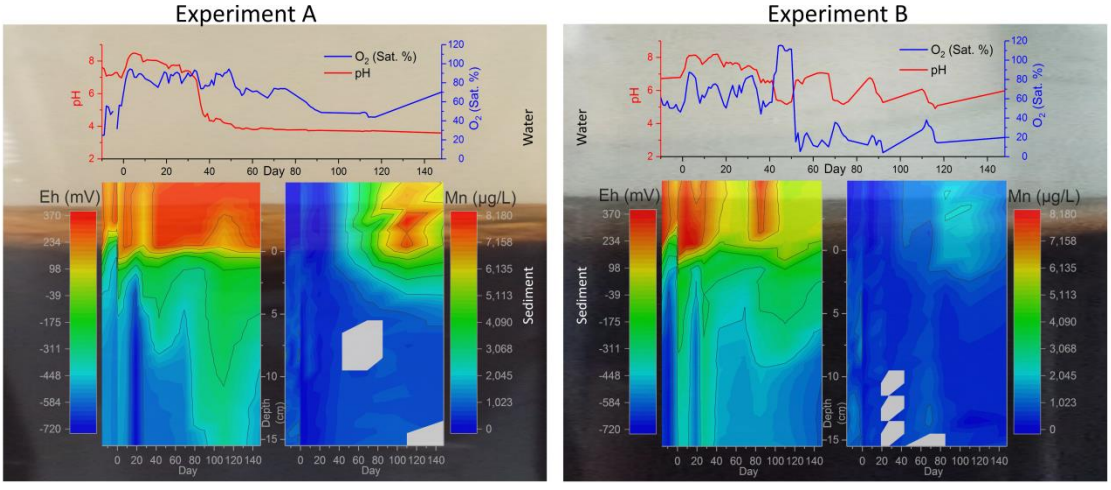


3.1 Abstract

The impact of mechanical disturbance and oxygen induced acidification on the concentration and size fractionation of the 12 metal(loid)s As, Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb, Sb, Tl, V and the polyatomic nonmetals C, P and S in the pore water was studied. Using the meso profiling and sampling system (messy) 12 pore water depth profiles were sampled from two incubation experiments undertaken in parallel, which were both mechanically disturbed in the lab and subsequently exposed to a different air supply. In parallel to the low invasive, automated sampling process the redox potential, the pH value and the O_2 concentration were detected. Simultaneous quantification of all analytes by inductively coupled plasma-triple quad-mass spectrometry in the two different size classes dissolved (<0.45 µm) and colloidal (0.45-16 µm) showed: i) the predominant influence of the pH on the mobility of metals; ii) the mobility of metalloids was strongly impacted by the mechanical disturbance; and iii) the colloidal release is less important except for Fe, P, and Ni.

3.2. Introduction

Sediments can serve as sinks, transformation matrix or sources of potentially environmentally harmful substances, depending on the environmental conditions. Processes that determine distribution, cycling, solubility and bio-availability of analytes such as trace metals, nutrients or organic compounds thus depend essentially on parameters such as O_2 saturation, redox potential and pH value. Steep gradients of these parameters characterize sediment water interfaces (SWI), leading to the fact that the analytes speciation and fractionation may vary significantly with depth.[1] Therefore, on the one hand side it is necessary to study different parameters and analytes in parallel with high spatial resolution, for a comprehensive understanding of the geochemical processes determining distribution and transport of substances at SWI. On the other hand, disturbances, mechanically or chemically, alter existing equilibria and can thus change the partitioning and hence, availability of certain analytes.[2] Such disturbances are often caused by human activities like construction and maintenance measures in waterways. Hence an understanding of processes occurring at the SWI is of interest, especially in the context of environmental risk assessments.

The determination of parameters such as O_2 saturation, redox potential or pH value (next to others) *in-situ* with a spatial high resolution is facilitated by the development of micro-sensors and –electrodes.[3] Contrary, the detection of many contaminants, nutrients and organic matter (OM) can be performed with great accuracy using different state of the art analytical techniques. The extraction of pore water samples, using *ex-situ* methods such as squeezing and centrifugation.[4,5] or *in-situ* methods such as dialyses[6,7] including diffusive gradients/equilibration in thin film[8] or suction based techniques[9-11] remains the most challenging part, due to its vulnerability to the formation of artefacts.

An option to combine suction based pore water sampling with *in-situ* measurements on O_2, the redox potential and the pH value for sediment depth profiles was presented by Fabricius et al. (2014).[12] This setup, restricted to high-resolution investigations of the first cm of the sediment, was modified by the authors to sample pore waters to a depth of >15 cm while measuring accompanying parameters in parallel. In a first study the system was tested for the simulation of processes related to sediment handling operations such as re-suspension and oxygenation.[13] The necessity was identified to better distinguish between the processes triggered by the different types of disturbance (mechanical or chemical) by extending the set of analytes and by systematical consideration of the colloidal fraction during metal(loid) releases into the pore and surface water.

In the present study the latter setup was used to (i) simulate a resuspension event and the acidification of an oxbow sediment as consequence of aeration. Therefore, two incubation experiments run in parallel were mechanically disturbed in the lab and subsequently either aerated or left untreated. (ii) The impact on the release of 12 metal(loid)s (As, Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb, Sb, Tl, V) was analyzed for 12 pore water profiles sampled across the SWI of both experiments. (iii) Additionally, the pore water concentrations of C, S and P as well as the redox-potential and the O_2 concentration were determined at the same spatial resolution to deliver mechanistic explanations of observed metal(loid) releases. (iv) To examine the potential contribution of the colloidal fraction between 0.45 and 16 µm during the metal(loid) release, a previously presented size fractionation approach[13] was applied in a systematic manner throughout the whole experiment.

3.3 Materials and methods

3.3.1 Incubation experiment

Sediment was sampled at an oxbow (former millstream) of river Lahn in Germany (50°18'56.87"N; 7°37'41.25"E), that only receives fresh water from the stream during flood events (approximately twice a year) and is known for increased metal(loid) concentrations due to former lead and silver mining activities. The sediment was sieved <2 mm to remove coarse (organic) particles such as leaves and branches, split in two 40x60 cm large high density polyethylene boxes (Nalge Company, USA) that were each filled to a height of 20 cm and incubated under 10 cm water column.

After an incubation time of 34 days 3 pore water depth profiles were sampled (profile 1-3, day -16, -9 and -1; negative numbers indicate times before the mechanical disturbance at day 0) to characterize the initial conditions at a steady state. On day 0 the sediment of both experiments was completely suspended by mixing sediment and water with a stainless steel stirrer (IKA, Germany) driven by a screw driller (Makita, Germany) for 5 minutes.

Aeration of the water column of one of the experiments (Experiment A) was started as soon as the main sediment fraction was settled using a glass air stone (JBL, Germany) and a membrane pump (Sera air 110 plus, Germany). This was meant to support oxygen induced slow "natural" pyrite weathering and subsequent acidification as it would take place after re-connecting the oxbow with the stream. Contrary, the reference Experiment B was left unaerated after the disturbance for the best possible comparison to the field conditions.

Pore water depth profiles across the SWI were sampled on day -16, -9, -1, 1, 9, 19, 27, 43, 69, 85, 110 and 148 as detailed in section 3.3.2 together with redox potential profiles. Subsequent to every sampling profile a micro profile of the parameters oxygen concentration, redox potential and pH was surveyed as detailed in section 3.3.4.

After finishing the last profile, sediment cores were taken using polyethylene terephthalate glycol (PETG) polycarbonate tubes (CT 46.2, ClearTec, Germany) for microwave assisted digestion with reverse *aqua regia* as described in section 2.1, Appendix 2.

3.3.2 Pore water sampling

Profiles of suction based pore water samples were extracted from the experiments as detailed by Schroeder et al. (2017).[13] Basic principle of the sampling process is to move a sampling probe through the SWI in vertical direction by a step motor (Motorized Microprofiling, Unisense A/H, Denmark) while aqueous samples are constantly extracted using a peristaltic pump (REGLO Analog, MS-2/8, ISMATEC, Germany). A fraction collector (Omnicoll, LAMBDA Laboratory Systems, Switzerland), positioned under argon atmosphere to avoid re-oxidation of the samples, is synchronized to gain samples of defined depth intervals. The disturbance of existing gradients is prevented by slow movement of the sampling probe (steps of 100 µm every 270 sec.) and the low pumping speed of ~2 ml/h.

12 profiles à 22 samples were taken during each experiment. Starting the profiles 6 cm above and ending 16 cm below the SWI, every sample represents a depth interval of 1 cm. The horizontal offset between individual profiles was about 10 cm. To meet all analytical demands, 15 ml of sample volume were intended to be sampled by pumping at a rate of ~2 ml/h (equals 165 h (~one week) per profile). Contaminations were prevented by cleaning both the 15 ml centrifuge tubes (VWR catalyst Laboratory Services, USA) used to collect the samples and all pipes and tubes with 1.3% nitric acid for >24 h (HNO_3, 65%, w/w, p.a. purchased by Merck GmbH, Germany and sub-boiled using a dst-1000 Savillex, USA) and rinsing them with ultrapure water (USF ELGA Purelab Plus system, ELGA LabWater, Germany).

Half of the volume sampled was filtered by syringe filters (pore size 0.45 µm, Minisart NML Syringe Filters, surfactant-free cellulose acetate, Sartorius, Germany) before evacuation from the glove box. The filtrate is regarded as the "dissolved" fraction (<0.45) in accordance to the general convention. The

unfiltered fraction (<16 µm) is referred to as total concentration. Until measurement all samples were stored frozen after acidification to a concentration of 1.3% HNO_3. Potential sample contaminations were monitored by methodological blank values as described in section A2.3.2, Appendix 2).

Some samples in the pore water profiles are missing due to different reasons. If insufficient sample volume was obtained to analyze both size fractions, the focus was targeted to the dissolved fraction. In an event of technical difficulties (e.g. malfunction of the fraction collector), samples are missing in both fractions.

The colloidal fraction was calculated as the difference between total and dissolved concentration. Hence, the size fraction addressed in this study is limited by the cut-off of the filter used to obtain the dissolved fraction (<0.45 µm) and the cut-off of the sampling probe used (16 µm). While the dissolved fraction also comprises smaller colloids, bigger colloids and small particles can be present in the "colloidal fraction".

3.3.3 Measurement of the redox potential

Parallel to the sampling process the redox potential was measured with Mansfeldt-type electrodes (ecoTech Umweltmeßsysteme GmbH, Germany) connected to Ag/AgCl-reference electrodes (REF321, Radiometer Analytical, Germany) and stored with an enviLog data logger (ecoTech, Germany).

Large differences in pH occurred in the course of the experiments. As the redox potential is a pH dependent quantity all redox measurements were corrected to pH 7 using the Nernst equation[14] and the pH values detected by microprofiling (section 3.3.4).

3.3.4 Microprofiling

Subsequent to every pore water profile microprofiles of the O_2 concentration, the redox potential and the pH were surveyed using Clark-type O_2 microsensors (Ox 500, Unisense, Denmark) and redox microelectrodes (standard hydrogen potential; RD-500, pH-500 glass electrode, Unisense, Denmark) connected to a Ag/AgCl-reference electrode (REF321, Radiometer Analytical, Germany) and a motorized microprofiling system (Motorized Microprofiling, Unisense A/H, Denmark) operated with the profiling software SensorTrace Suite (Unisense, Denmark).

3.3.5 ICP-QQQ-MS Analyses

ICP-MS is one of the most common and powerful techniques in environmental analytical chemistry of metal(loid)s. The availability of ICP-QQQ-MS allows quantification of analytes that were not possible to measure with classical ICP-MS thanks to the possibility to eliminate polyatomic interferences.[15] Several studies have been published describing the quantification of S and P by ICP-QQQ-MS in oxygen mass-shift mode in the context of different scientific issues.[16-20] Even more unusual and rare is the

application of ICP-QQQ-MS for the detection of C. However the possibility of parallel measurement of metal(loid)s and C was pointed out by Amaral et al. (2015).[21]

Following these recommendations simultaneous quantification of the metal(loid)s and the polyatomic nonmetals C, P and S in the pore water fractions was performed by means of inductively coupled plasma-triple-quadrupole mass spectrometry (ICP-QQQ-MS, Agilent 8800 series; Agilent Technologies, Japan) equipped with an auto sampler (SPS 4, Agilent Technologies, Japan) and a standard sample introduction kit. Information on the isotopes analyzed and the certified reference materials used is given in Appendix 2 (Table A2. 7). For validation purposes, five certified reference materials (CRMs) and three internal standards were included in the measurements (^{72}Ge, ^{103}Rh, ^{185}Re for He mode and ^{74}Ge, ^{103}Rh, ^{185}Re for O_2 mode). Additionally tartaric acid solution was used for the validation of carbon measurements. The recoveries of at least two of the CRMs were in the range of ± 10% of the certified value, the maximum accepted variation of the internal standards were at 20% from the initial value. Maximal accepted analytical instability of the measurements was 10% relative standard deviation (all samples measured 5 times). Further details on the isotopes analyzed and the CRMs used are given in Appendix 2 (section 2.3.1).

3.3.6 Statistics and graphs

Data analyses were performed using R (version 3.3.2; 2016-10-31). The R packages ”outliers” and “PerformanceAnalytics” were used to test for outliers and calculations of correlation coefficients. Since some of the profile data were not normal distributed, bivariate correlation analyses were performed using Spearman’s rank correlation test. Measured concentrations below the limit of detection (<LoD; refer to section 2.3.1, Appendix 2) have been set to half of the respective LoD for the statistical calculations. In order to take into account the changing conditions in the course of the experiment, separate correlation coefficients were calculated for different periods of the experiments: (i) samples of the first 3 profiles (day -16, -9 and-1) representing the initial state, (ii) samples of profile 4 and 5 (day 1 and 9) as mainly influenced by mechanical disturbance and (iii) profiles 6-12 (day 19, 27, 43, 69, 85, 110 and 148) representing the acidification of Experiment A. Origin 2016 has been used to prepare the graphs presented.

3.4. Results and discussion

3.4.1 Oxygen, pH and redox potential

The O_2 saturation, pH value, temperature and redox potential in the water column of both experiments are shown in Figure 3.1.

Experiment A, was aerated subsequent the mechanical disturbance as detailed in section 3.3.1. Accordingly, elevated values of O_2 saturation compared to Experiment B were measured from day 0 on. Only between day 40 and 50, algal growth caused O_2 supersaturation in the water column of Experiment B before a reduction was achieved by not only shadowing of the windows but also of both experiments.

The initially nearly neutral pH in both experiments increased as consequence of the mechanical disturbance. As intended, the aeration of the water column of Experiment A led to increasingly acid conditions. The main pH shift from pH 6.8 to 4.7 took place between day 34 and day 37. The final pH was 3.6. This is in good agreement with a previous study with this sediment [13] and can be related to sulfide weathering as the oxidation of metal sulfides in the presence of oxygen is a well-known process leading to the release of SO_4^{2-}, H^+ and metal cations.[22] Comparably, a reduction of the pH took place in the unaerated Experiment B, but values about pH 5 were only reached during the period of oxygen supersaturation from the short algae bloom. Otherwise the pH varied mostly between 5.5 and 7, displaying the ability of the system to compensate the short term impact. Approximately neutral pH values were found throughout this study below the SWI in Experiment B and below a depth of a few centimeters in the low pH Experiment A (Figure A2. 1-A2. 2, Appendix 2).

After the initial incubation, a steep redox gradient was detected at the SWI of both experiments. As a consequence of the mechanical disturbance and the associated O_2 supply, this gradient was weakened but re-established within approximately 15 days after the sediment settled. In the further course of the experiment, the different conditions caused by the presence and absence of O_2 led to increased redox potentials in Experiment A compared to Experiment B (Figure 3.1).

Redox potential and pH value are two mutually dependent variables. Since a decrease in the pH value means an increase in the H^+ ion concentration, the redox potential generally decreases when the pH increases and vice versa.[14,23] This relationship was detected in both experiments following the mechanical disturbance as well as during the acidification of Experiment A.

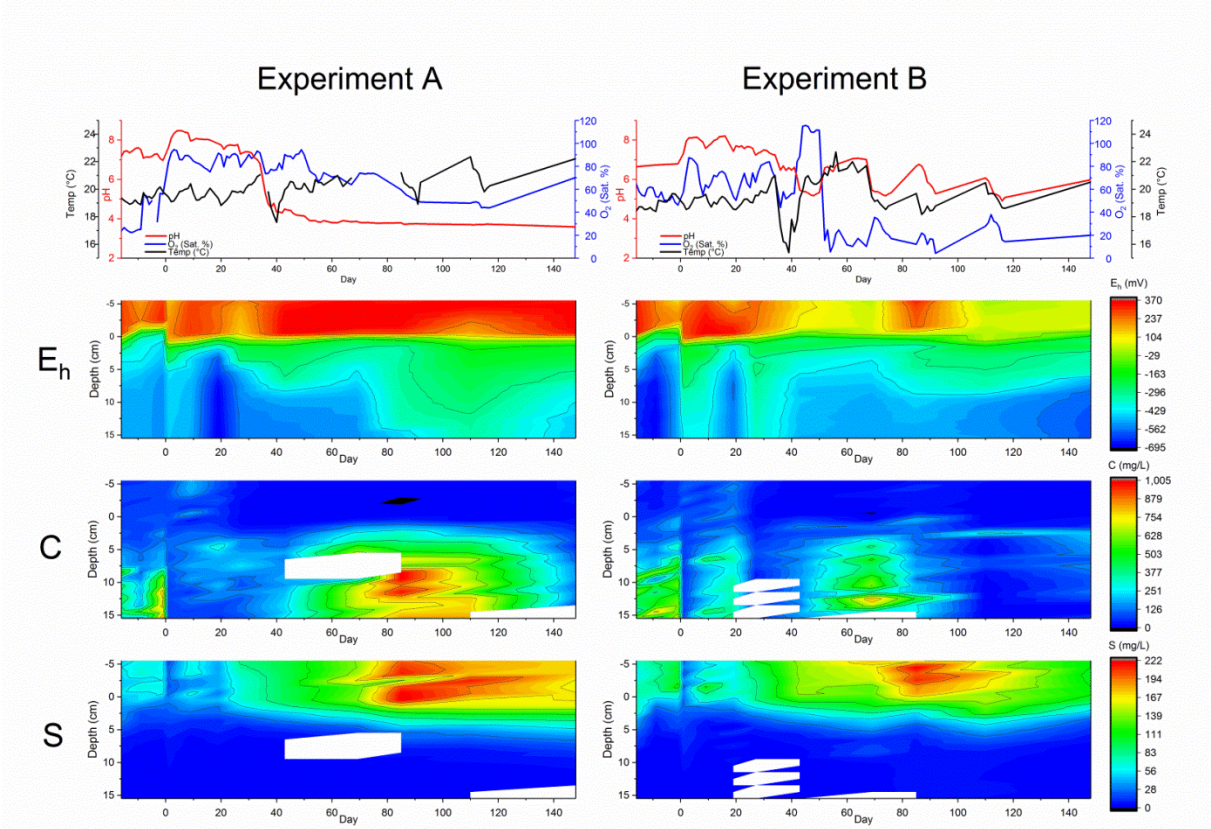


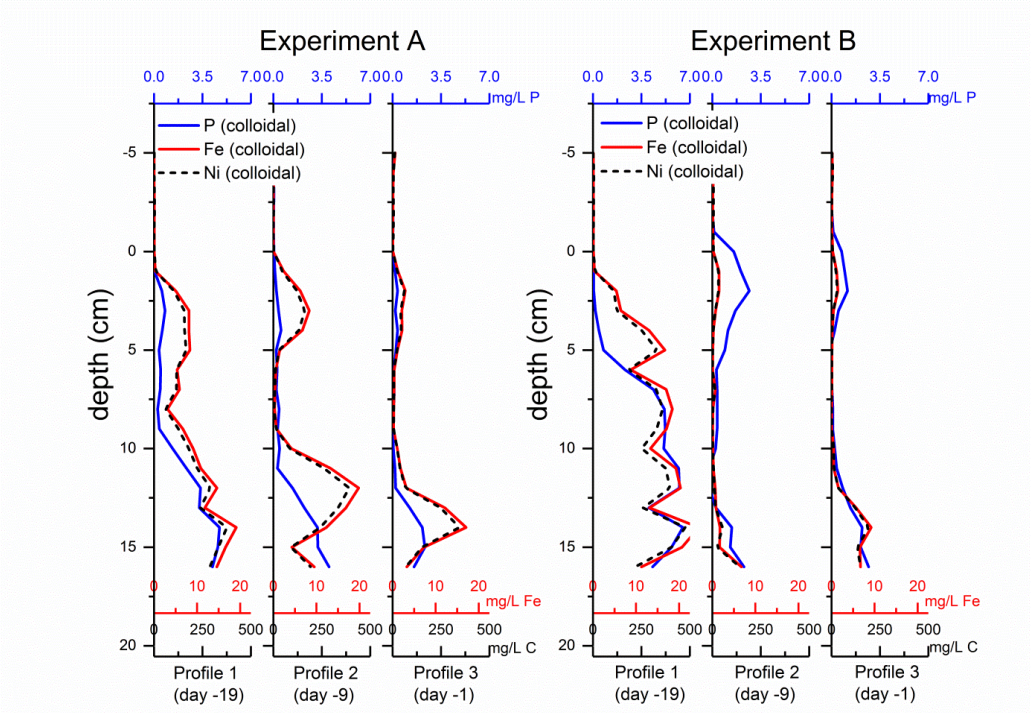
Figure 3.1: *O_2 saturation, pH and temperature in the water columns of Experiment A and B (upper most graphs, missing values for temperature are due to broken sensor) and Eh, C and S heat plots (<0.45µm filtered fraction). Concentrations <LoD were set to zero. Samples missing due to malfunction of the fraction collector are displayed as white spots in the heat plots. The corresponding graph for P is shown in Appendix 2 (Figure A2. 3).*

3.4.2 Colloidal fraction

The colloidal fraction (0.45-16 µm) was calculated as the difference between total (<16 µm) and dissolved concentrations (<0.45 µm). Due to wide concentration ranges of analytes within the same SWI profile, negative values may occur where the concentrations are close to the LoD and are easily biased by slight inaccuracies, not at least because in the case of most analytes the dissolved fraction significantly exceeds the colloidal portion.

For most analytes (As, Cd, Co, Cr, Cu, Fe, Mn, Pb, S, Sb, Tl and V) the concentrations of the dissolved (<0.45 µm) and the total (<16 µm) fraction are almost the same and hence, the colloidal contribution to the total concentration was not relevant with respect to metal(loid) mobilization. High relative proportions of the colloidal fraction for these elements appeared only in samples with total concentrations close to the LoDs. Only Fe, Ni, P, and C were found to be present in the colloidal fraction 0.45-16 µm in larger quantities, especially prior to the mixing of the sediment after 12 weeks of

stabilization. The first three depth profiles were highly comparable for all 4 analytes (Figure 3.2). After the mechanical disturbance, the total concentrations of these elements in the pore water (including the colloidal and dissolved fraction; refer to Tables A2. 17, A2. 19, A2. 41, A2. 43, A2. 49 and A2. 51, Appendix 2) were reduced. But within one or two weeks the concentrations reached the higher initial state again. However, in the further course of the study the colloidal concentrations of these elements decreased again in both experiments. Fe occurs to a large extend as (hydr)oxides in natural waters under oxic conditions which dissolve under anoxic, reducing conditions.[24] The SWI-near concentration peak (refer to Figure 3.2) may point to the formation of colloidal (hydr)oxides due to the oxygen supply by diffusion from the water into the upper layer of the sediment. The increasing colloidal concentrations in the deeper sediment layers can be explained by generally enhanced total concentrations present under the reducing conditions (refer to Table A2. 41, A2. 43, Appendix 2). The association of phosphates with Fe in colloidal and particulate material is well known for decades[25,26] and the composition and physicochemical characteristics of the colloidal iron phosphate species were already studied in detail (e.g., Buffle et al. (1988)[27] and Hyacinthe & Cappellen (2004) [28]). Evidence of the coupled mobilization of both elements was recently presented.[29] Since Fe (hydr)oxides are assumed to be important binding agents for trace metal(loid)s[30] a similar course of the depth profiles of colloidal Fe and metal(loid)s could have been expected, but was only verified for Ni in the



experiments. This might be explained by very high differences in concentration between Fe and all other trace metal(loid)s, “blurring” the effect.

Figure 3.2: *Depth profiles across the SWI of the calculated colloidal fraction of Fe, Ni and P prior the mechanical disturbance of the sediment.*

3.4.3 Dissolved concentrations

3.4.3.1 Polyatomic nonmetals: Carbon, phosphorous and sulfur

Dissolved concentrations (<0.45 µm) of C and S as well as the redox potential and the pH of the water column are shown in Figure 3.1. The corresponding graph for P is shown in the supplementary material (Figure A2. 3, Appendix 2). Until approximately day 40 the concentration gradients across the SWI in both experiments were highly comparable: Prior disturbance, increasing concentrations of dissolved C and P were detected below the SWI followed by a decrease down to values similar to those found in the water column after disturbance. After conditions stabilized, approximately from day 40 on, a markedly increased release of C and P into the pore water took place in the acidifying Experiment A compared to the reference Experiment B. In the water column C concentrations decreased below the LoD in many profiles in both experiments.

The C concentrations measured by ICP-QQQ-MS include both organic and inorganic C species. Considering the low solubility of inorganic C compounds in comparison to the detected quantities of C and the low content of inorganic C in the sediment (refer to Table A2. 4, Appendix 2), the concentration differences measured are most likely determined by the mobility of dissolved organic carbon (DOC). The general increase of dissolved C concentrations with increasing depth below the SWI is also reflected by a negative correlation between C and the redox potential (Table A2. 69, Appendix 2). This agrees well with findings of other authors who reported enhanced mobilization of DOC at low redox potentials.[31,32] Two processes can be considered as an explanation: The release of DOC from reductive dissolution of Fe and Mn (hydr)oxides[33] and the degradation of complex organic matter (OM) to DOC by reductive fermentation and hydrolysis under reducing conditions.[34] A stimulation of microbial activity under the acidic conditions due to the acidophilic properties of some sulfur reducing bacteria[35] explains the increased C release in the acidic Experiment A compared to the reference Experiment B. The fact that the C release to the pore water did not result in increasing concentrations in the water column indicates that either under acidic conditions insoluble species dominate (e.g., humic acids rather than fulvic acids) or enhanced microbial C consumption takes place at higher redox potentials as observed by other authors.[36-38]

The classical paradigm postulates that phosphates adsorb to Fe (hydr)oxides under oxic conditions and are released when Fe is reduced to Fe(II) under anoxic conditions. More recently it has been pointed out that this concept is only valid under circumstances when factors such as dissolution of calcium-bound P and decomposition of OM can influence the fate of the P species.[39,40] In this study, the coupling between Fe (refer to Figure 3.3) and P cycle is reflected by a parallel concentration pattern in the profiles, in both the dissolved and the colloidal fraction until an acidification induced enrichment of Fe occurred in the surface-near pore water in Experiment A. This relationship was additionally proven by

the calculated correlation coefficients between both elements (Tables A2. 68, A2. 69, Appendix 2). The enhanced release of P, accompanied by a C release during the acidification of Experiment A as well as during the short pH drop in Experiment B is a clear marker for the importance of the co-release of P with OM. High correlation coefficients between solute P and solute C in both experiments, taking account of profiles no. 6 to no. 12, equally underline this relationship (Tables A2. 68, A2. 69, Appendix 2).

Dissolved (<0.45 µm) sulfur was originally present in concentrations from 60-100 µg/L in the water column of both experiments. These concentrations decreased to values <40 µg/L following the mechanical disturbance due to S sorption to sediment particles. 6-9 cm below the SWI, the S concentrations dropped to values <10 µg/L before and after the disturbance. In the course of the study S was enriched in the water column as well as the SWI near pore water of both experiments, reaching lasting concentrations >250 µg/L in Experiment A on day 85 and 110 while in the reference Experiment B concentrations of 200 µg/L were only shortly exceeded during profile 10 (day 85). As discussed in section 3.4.1, the enhanced release of S in Experiment A compared to the reference Experiment B is caused by the experimentally intended weathering of sulfides under aerobic conditions.

3.4.3.2 Iron and manganese

Concentrations of Fe and Mn measured in the dissolved fraction (<0.45 µm) during this study are shown in Figure 3.3. Under stable conditions, before mechanical disturbance, dissolved Fe concentrations experienced a subsurface peak in 1-6 cm depth and concentrations increased with depth below 10 cm reaching >10,000 µg/L in 15 cm depth. Dissolved manganese concentrations increased to 600-1500 µg/L below the SWI during the first three profiles (day -16, -9, -1). The mechanical disturbance resulted in small changes in the concentrations of both elements compared to the acidification of Experiment A, with a release of Mn into the water column and lower concentrations of Fe over the entire depth profile (refer to Tables A2. 40-A2. 47, Appendix 2) most likely reasoned in the formation of Fe (hydr)oxides due to oxygen introduced into the sediment pore water. In the course of the sulfide weathering induced acidification, a joint release of Fe, Mn and S has been assumed. But only Mn accumulated progressively in the water column similar to S, while an observed sedimentation of iron ochre explains that high Fe concentrations were limited to the near-surface pore water (between 0 and 3 cm depth). Consequently a positive correlation was found between dissolved Mn and S within the profiles affected by the acidification process (profiles 6-12, days 19-148), while no significant correlation between Fe and S was found (Tables A2. 68-A2. 69, Appendix 2).

The solubility of Fe and Mn generally depends on the redox conditions.[31,41,42] At high redox potentials both elements form (hydr)oxides which are reduced to soluble Fe^{2+} and Mn^{2+} at low redox potentials. In the presence of H_2S the reduced species Fe(II) and Mn(II) may both precipitate as sulfides.[43]

Accordingly, negative correlations between both elements, Fe and Mn, and the redox potential were found (Tables A2. 68-A2. 69, Appendix 2), especially when considering the stable conditions during the first 3 profiles (profiles 1-3, day -16, -9, -1). Positive correlations were found between both elements and C. This is in good agreement with the fact that microorganisms use metals such as Fe and Mn instead of O_2 as terminal electron acceptors during OM degradation under anoxic conditions[44] resulting in their reductive dissolution.[45-49]

3.4.3.3 Trace metal(loid)s

Results for the elements Cu and Sb are exemplary shown in Figure 3.3. Corresponding graphs for the elements As, Cd, Co, Cr, Ni, Pb, Tl and V (Figure A2. 4-A2. 11, Appendix 2) as well as all measured concentrations (Table A2. 20-A2. 67, Appendix 2) are given in the supplementary material. The solubility of metal(loid)s is influenced by a variety of factors including the redox conditions and pH value as well as their interactions with binding agents such as sulfides, Fe and Mn (hydr)oxides and OM. After summarizing the measured results, these various aspects and how they are influenced by mechanical disturbance and acidification are discussed.

During the first 3 profiles the dissolved (<0.45 µm) concentrations of Cd, Cu, Pb and Tl decreased significantly below the SWI compared to the water column. In contrast, the concentrations of dissolved Co, Cr and Ni were higher in the pore water compared to the water column above. After the mechanical disturbance Cd, Ni and Tl were found in lower concentrations than before, while the mixing did not significantly change the concentrations of Co, Cr, Cu and Pb. During the acidification of Experiment A, joint release of the elements Cd, Co, Cr, Cu, Pb, Tl and Ni took place leading to an increase in the dissolved concentrations by the factor 10, 5, 100, 20, 70, 200, and 5, respectively, in the water column between day 27 (last profile before the main pH shift) and day 148 (end of experiment).

In contrast to the aforementioned elements the concentrations of As, Sb and V were more strongly affected by the disturbance than by the acidification process. The mechanical disturbance led to increasing concentrations of all three elements, which in the case of V was limited to the water column. During the acidification of Experiment A dissolved Sb and V were removed from the water column while the concentration of As was rather unaffected. Concentrations of Sb and V also decreased in the reference Experiment B, even though not as strong as in Experiment A.

The solubility of many metal(loid)s is directly influenced by the redox conditions as their speciation can change in consequence of varying redox conditions due to a higher solubility of the reduced species compared to their oxidized counterparts.[50,51] Additionally, their solubility can be indirectly affected by the redox potential as consequence of their association to a range of components such as Fe and Mn

(hydr)oxides and sulfides which solubility is in turn (beside other factors) influenced by the redox potential.[30]

As a result of the mechanical disturbance existing redox gradients were blurred. However, this had only a minor influence on the concentrations of metals Cd, Cu, Ni, Zn, Co, whose solubility had been shown to be redox-dependent in reactor experiments.[34,37,41] However, the calculated correlation coefficients between Cd, Cu, Pb, Tl and Zn and the redox potential were highest when only the profiles under stable conditions were considered before the mechanical disturbance.

Also As, Sb and V are redox sensitive elements with their reduced species being more mobile than their oxidized counterparts.[52-55] The measured concentrations of As and Sb agree with these findings until the pH became the dominant parameter for the release in this study. The concentration of dissolved V did not show a trend that could be explained by the redox conditions.

Frequently it has been shown that the influence of the pH value on the solubility of metal(loid)s exceeds that of the redox potential.[56,57] Low pH values cause a reduction of negative surface charges of OM, clay minerals and Fe and Al oxides, leading to a release of associated metal(loid)s. Additionally, the solubility of compounds such as carbonates and sulfides is increased at low pH values [30]. In agreement with this, a substantial release of metals predominantly present as cations in aqueous solutions was triggered by the acidification of experiment A. As, Sb and V form (oxy)anionic species in aqueous solution.[58,59] As decreasing pH values cause an increase of positive surface charges of different sediment compounds, their adsorption is favored under acid conditions.[60] This explains the decrease of dissolved Sb and V concentrations in the course of the acidification of Experiment A. Surprisingly, a decrease of dissolved As in the course the acidification was not detected.

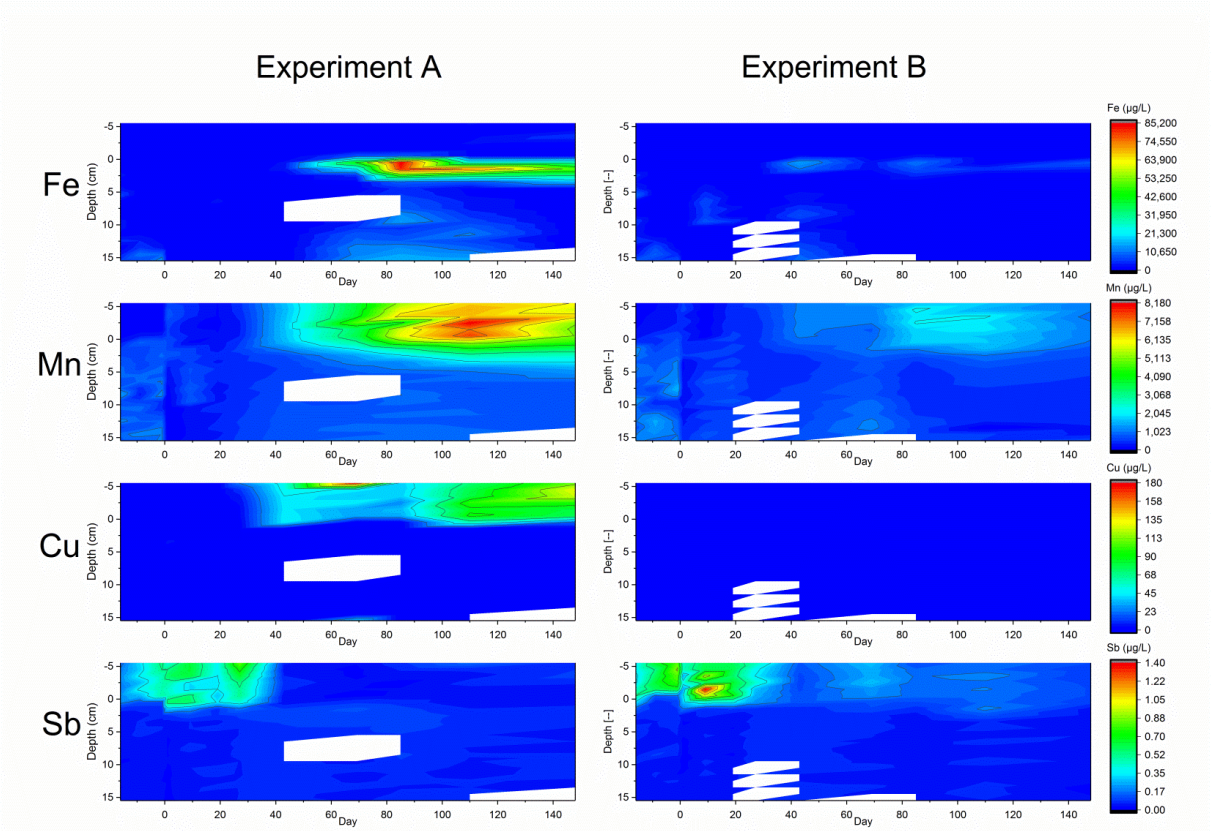


Figure 3.3: *Concentration of iron, manganese, copper and antimony in the <0.45 µm filtered fraction across the sediment water interface of Experiment A and B. Concentrations <LoD were set to zero. Samples missing due to malfunction of the fraction collector are displayed as white spots in the heat plots. The corresponding graphs for As, Cd, Co, Cr, Ni, Pb, Tl, V are shown in Appendix 2 (Figure A2. 4-A2. 11).*

The potential metal sulfide precipitation has already been discussed for Fe and Mn (section 3.3.2). Sulfides are also considered to be the predominant solid phase of many other metal(loid)s in most anoxic sediments.[61] With respect to its high S content (Table A2. 4, Appendix 2), it can be assumed that this is also the case in the present sediment. While usually Fe sulfides are by far the most abundant sulfide minerals, other metal(loid)s can either co-precipitate and adsorb to them or form discrete sulfide minerals.[62,63] Consequently, only very low concentrations of sulfide forming metal(loid)s should be found in the pore water samples. The latter was the case for the elements Cd, Cu, Tl and Pb. But, in contrast, the dissolved concentrations of Co, Ni and Cr increased below the SWI compared to the water column. This is in good agreement with the findings of Morse & Luther (1999)[63] that metals such as Cd, Pb and Zn that have faster water exchange kinetics than Fe, precipitate as sulfides prior to it, whereas Cu forms a variety of sulfide species with and without Fe.

As the weathering of sulfides was identified to be the process causing the oxygen induced acidification of Experiment A (refer to section 3.3.1) a joint release of metal(loid)s with S was expected. This explains

the release from the sediment of Cd, Co, Cr, Cu, Pb, Tl, Ni into the water column of Experiment A and is also reflected by high correlations between the metals and S (Table A2. 68-A2. 69, Appendix 2). But it does not necessarily imply that the released metals were present as sulfides in all cases. As an example, Cr does not form sulfide minerals. Furthermore, several processes initiated by the acidic conditions, as discussed above, can contribute to the release of the metals. Among the anion forming metal(loid)s Sb was reported to be associated with sulfides in sediments.[64] This delivers an additional explanation for the low solubility of Sb under low redox potential conditions in the anoxic sediment. This hypothesis is supported by a positive correlation found between Sb and S (Table A2. 68-A2. 69, Appendix 2).

Under oxic conditions Fe and Mn (hydr)oxides are important binding agents for metal(loid)s which can be released or scavenged as consequence of (hydr)oxide dissolution or precipitation. The decreasing dissolved concentrations of Cd, Ni and Tl during the mechanical disturbance can thus be explained by the precipitation of Fe (hydr)oxides caused by oxygen introduction. Low pH conditions are reported to generally lead to a low adsorption capacity of Fe (hydr)oxides for metal(loid)s.[65] Nevertheless, in contrast to most other elements, the solubility of As during this study seems to be strongly correlated to Fe. Co-precipitation with Fe (hydr)oxides limited the release of As in Experiment A while this was not observed in Experiment B. This is in good agreement with results from a similar experiment published earlier showing that the formation of Fe (hydr)oxides acts as an effective SWI barrier, hindering As release to the water column.[13]

Organic C fractions are known to have a strong impact on the solubility of metal(loid)s.[32] Consisting of a complex, heterogeneous mixture of molecules covering a wide range of molecular weight, size and solubility, OM is represented by both, the dissolved and the particulate phase. Having a large quantity of negatively charged groups and, hence, a high capacity to complex and adsorb cations,[66] OM might scavenge metal(loid)s from solution or promote their solubility by complexation. Co and V were released to the pore water together with increasing concentrations of dissolved C in both experiments between day 50 and day 90, resulting in positive correlation coefficients between both elements and C (Table A2. 68-A2. 69, Appendix 2). In the case of V this is an additional proof with findings that associated to the OM fraction the element can be transferred to the DOC fraction as a consequence of partial OM degradation.[67,68]

As a result of the interplay of the various factors determining the solubility of metals, the mobility of the metalloids As, Sb, and V was strongly affected by the mechanical disturbance and the concomitant changes in redox conditions, while metals were released from the various processes associated with sulfide weathering and acidification.

3.5 Conclusions

Observing the influence of mechanical and chemical disturbance on the release of metal(loid)s from sediment to the aqueous phase using the *messy*-setup showed that the mobility of the (oxy)anion forming elements As, Sb, and V was promoted mainly by the mechanical disturbance, while sulfide weathering and concomitant acidification caused the release of Cd, Co, Cr, Cu, Ni, Pb, Tl and Zn across the SWI, resulting in a diffusion based contamination of the overlying water. With respect to best management practice the results of this study must be taken into account, when measures are envisaged (e.g., reconnection of the oxbow) that may result in an increase in oxygen availability in the waterbody, or that foster the resuspension of the sediment. The high spatial resolution of the *messy* sampling technique also enabled the localization of hot spots of dissolved concentrations of individual analytes, spatial as well as in time. The chance to include C, S and P in the same run with the metal(loid)s delivered by the ICP-QQQ-MS delivered mechanistic explanations for the processes observed without a significant increase of the required sample volume or the analytical effort. ICP-QQQ-MS thereby opens a door to extend in the future our knowledge in SWI studies with no additional resources needed. Applying a robust size fractionation approach throughout the study to address the colloidal fraction (0.45 – 16 µm) made visible that for most metal(loid)s the colloidal fraction was from little significance for their mobility, but for Ni the results clearly indicate an incorporation into the colloidal Fe-phosphate phase.

The presented method enables the generation of very comprehensive data sets that cover existing gradients at the SWI under different and changing environmental conditions with a very satisfying spatial resolution. Further insight in the complex interplay of nutrient and metal(loid) chemistry at the SWI calls for adding in the future more frequently questions on element speciation, on nutrient and on metal(loid)s.

Not least the *messy* setup - thanks to the materials used and the possibility of combining the sampling process with different analytical techniques - offers the possibility to be used in the future in different study designs, including the fate of organic pollutants and their degradation at the SWI, to evaluate the “services” provided by sediments in this respect. Hence, the estimation of ecosystem performances with regard to degradation of certain organic pollutants in incubation experiments, next to sink/source estimations, is a promising perspective for future *messy*- setup applications.

3.6 References

1. Santschi, P.; Höhener, P.; Benoit, G.; Buchholtz-ten Brink, M., Chemical processes at the sediment-water interface. *Marine Chemistry* **1990,** *30*, 269-315.
2. Eggleton, J.; Thomas, K. V., A review of factors affecting the release and bioavailability of contaminants during sediment disturbance events. *Environment International* **2004,** *30*, (7), 973-980.
3. Stockdale, A.; Davison, W.; Zhang, H., Micro-scale biogeochemical heterogeneity in sediments: A review of available technology and observed evidence. *Earth-Science Reviews* **2009,** *92*, (1-2), 81-97.
4. Lourino-Cabana, B.; Lesven, L.; Billon, G.; Denis, L.; Ouddane, B.; Boughriet, A., Benthic exchange of sedimentary metals (Cd, Cu, Fe, Mn, Ni and Zn) in the Deûle River (Northern France). *Environmental Chemistry* **2012,** *9*, (5), 485.
5. Scholz, F.; Hensen, C.; Noffke, A.; Rohde, A.; Liebetrau, V.; Wallmann, K., Early diagenesis of redox-sensitive trace metals in the Peru upwelling area – response to ENSO-related oxygen fluctuations in the water column. *Geochimica et Cosmochimica Acta* **2011,** *75*, (22), 7257-7276.
6. Lewandowski, J.; Rüter, K.; Hupfer, M., Two-Dimensional Small-Scale Variability of Pore Water Phosphate in Freshwater Lakes: Results from a Novel Dialysis Sampler. *Environmental Science & Technology* **2002,** *36*, (9), 2039-2047.
7. Rigaud, S.; Radakovitch, O.; Couture, R.-M.; Deflandre, B.; Cossa, D.; Garnier, C.; Garnier, J.-M., Mobility and fluxes of trace elements and nutrients at the sediment–water interface of a lagoon under contrasting water column oxygenation conditions. *Applied Geochemistry* **2013,** *31*, 35-51.
8. Zhang, C.; Ding, S.; Xu, D.; Tang, Y.; Wong, M. H., Bioavailability assessment of phosphorus and metals in soils and sediments: a review of diffusive gradients in thin films (DGT). *Environ Monit Assess* **2014,** *186*, (11), 7367-78.
9. Duester, L.; Prasse, C.; Vogel, J. V.; Vink, J. P. M.; Schaumann, G. E., Translocation of Sb and Ti in an undisturbed floodplain soil after application of Sb2O3 and TiO2 nanoparticles to the surface. *Journal of Environmental Monitoring* **2011,** *13*, (5), 1204.
10. Seeberg-Elverfeldt, J.; Schlüter, M.; Feseker, T.; Kölling, M., Rhizon sampling of porewaters near the sediment-water interface of aquatic systems: Rhizon porewater sampling. *Limnology and Oceanography: Methods* **2005,** *3*, (8), 361-371.
11. Vink, J. P. M., Measurement of Heavy Metal Speciation over Redox Gradients in Natural Water−Sediment Interfaces and Implications for Uptake by Benthic Organisms. *Environmental Science & Technology* **2002,** *36*, (23), 5130-5138.

12. Fabricius, A.-L.; Duester, L.; Ecker, D.; Ternes, T. A., New Microprofiling and Micro Sampling System for Water Saturated Environmental Boundary Layers. *Environmental Science & Technology* **2014,** *48*, (14), 8053-8061.
13. Schroeder, H.; Fabricius, A. L.; Ecker, D.; Ternes, T. A.; Duester, L., Metal(loid) speciation and size fractionation in sediment pore water depth profiles examined with a new meso profiling system. *Chemosphere* **2017,** *179*, 185-193.
14. DeLaune, R. D.; Reddy, K. R., Redox Potential. In *Encyclopedia of Soils in the Environment*, Hillel, D., Ed. Academic Press: 2005; pp 366-371.
15. Profrock, D.; Prange, A., Inductively coupled plasma-mass spectrometry (ICP-MS) for quantitative analysis in environmental and life sciences: a review of challenges, solutions, and trends. *Appl Spectrosc* **2012,** *66*, (8), 843-68.
16. Diez Fernandez, S.; Sugishama, N.; Ruiz Encinar, J.; Sanz-Medel, A., Triple quad ICPMS (ICPQQQ) as a new tool for absolute quantitative proteomics and phosphoproteomics. *Anal Chem* **2012,** *84*, (14), 5851-7.
17. Gong, J.; Solivio, M. J.; Merino, E. J.; Caruso, J. A.; Landero-Figueroa, J. A., Developing ICP-MS/MS for the detection and determination of synthetic DNA-protein crosslink models via phosphorus and sulfur detection. *Anal Bioanal Chem* **2015,** *407*, (9), 2433-7.
18. Kroepfl, N.; Marschall, T. A.; Francesconi, K. A.; Schwerdtle, T.; Kuehnelt, D., Quantitative determination of the sulfur-containing antioxidant ergothioneine by HPLC/ICP-QQQ-MS. *Journal of Analytical Atomic Spectrometry* **2017,** *32*, (8), 1571-1581.
19. Møller, L. H.; Macherius, A.; Hansen, T. H.; Nielsen, H. M.; Cornett, C.; Østergaard, J.; Stürup, S.; Gammelgaard, B., Quantification of pharmaceutical peptides in human plasma by LC-ICP-MS sulfur detection. *Journal of Analytical Atomic Spectrometry* **2016,** *31*, (9), 1877-1884.
20. Zhu, Y.; Kitamaki, Y.; Kato, M.; Kinumi, T.; Hioki, A.; Chiba, K., Determination of Sulfur in Bio-Samples by ICP-QMS/QMS with an ORC. *Journal of Analytical & Bioanalytical Techniques* **2015,** *6*, (6).
21. Amaral, C. D. B.; Amais, R. S.; Fialho, L. L.; Schiavo, D.; Nogueira, A. R. A.; Nóbrega, J. A., Determination of carbon in digested samples and amino acids by inductively coupled plasma tandem mass spectrometry. *Microchemical Journal* **2015,** *122*, 29-32.
22. Schippers, A., Biogeochemistry of metal sulfide oxidation in mining environments, sediments, and soils. In *Special Paper 379: Sulfur Biogeochemistry - Past and Present*, Geological Society of America: 2004; Vol. 379, pp 49-62.
23. *Redox: Fundamentals, Processes and Applications*. Springer: Heidelberg, 2000.
24. Ponnamperuma, F. N., The Chemistry of Submerged Soils. *Advances in Agronomy* **1972,** *24*, 29-96.

25. Mortimer, C. H., The Exchange of Dissolved Substances between Mud and Water in Lakes. *Journal of Ecology* **1942,** *30*, (1), 147-201.
26. Mortimer, C. H., *The Exchange of Dissolved Substances Between Mud and Water in Lakes: Pt. III and IV, Summary and References*. Cambridge University Press: 1942.
27. Buffle, J.; Vitre, R. R.; Perret, D.; Leppard, G. G., Physico-chemical characteristics of a colloidal iron phosphate species formed at the oxic-anoxic interface of a eutrophic lake. *Geochimica et Cosmochimica Acta* **1988,** *53*, 399-408.
28. Hyacinthe, C.; Van Cappellen, P., An authigenic iron phosphate phase in estuarine sediments: composition, formation and chemical reactivity. *Marine Chemistry* **2004,** *91*, (1-4), 227-251.
29. Ding, S.; Wang, Y.; Wang, D.; Li, Y. Y.; Gong, M.; Zhang, C., In situ, high-resolution evidence for iron-coupled mobilization of phosphorus in sediments. *Scientific Reports* **2016,** *6*, 24341.
30. Du Laing, G.; Rinklebe, J.; Vandecasteele, B.; Meers, E.; Tack, F. M., Trace metal behaviour in estuarine and riverine floodplain soils and sediments: a review. *Sci Total Environ* **2009,** *407*, (13), 3972-85.
31. Antić-Mladenović, S.; Rinklebe, J.; Frohne, T.; Stärk, H.-J.; Wennrich, R.; Tomić, Z.; Ličina, V., Impact of controlled redox conditions on nickel in a serpentine soil. *Journal of Soils and Sediments* **2010,** *11*, (3), 406-415.
32. Grybos, M.; Davranche, M.; Gruau, G.; Petitjean, P.; Pédrot, M., Increasing pH drives organic matter solubilization from wetland soils under reducing conditions. *Geoderma* **2009,** *154*, (1-2), 13-19.
33. Pan, W.; Kan, J.; Inamdar, S.; Chen, C.; Sparks, D., Dissimilatory microbial iron reduction release DOC (dissolved organic carbon) from carbon-ferrihydrite association. *Soil Biology and Biochemistry* **2016,** *103*, 232-240.
34. Frohne, T.; Rinklebe, J.; Diaz-Bone, R. A., Contamination of Floodplain Soils along the Wupper River, Germany, with As, Co, Cu, Ni, Sb, and Zn and the Impact of Pre-definite Redox Variations on the Mobility of These Elements. *Soil and Sediment Contamination: An International Journal* **2014,** *23*, (7), 779-799.
35. Muyzer, G.; Stams, A. J., The ecology and biotechnology of sulphate-reducing bacteria. *Nat Rev Microbiol* **2008,** *6*, (6), 441-54.
36. Abel, C. D. T.; Sharma, S. K.; Malolo, Y. N.; Maeng, S. K.; Kennedy, M. D.; Amy, G. L., Attenuation of Bulk Organic Matter, Nutrients (N and P), and Pathogen Indicators During Soil Passage: Effect of Temperature and Redox Conditions in Simulated Soil Aquifer Treatment (SAT). *Water, Air, & Soil Pollution* **2012,** *223*, (8), 5205-5220.

37. Shaheen, S. M.; Rinklebe, J.; Frohne, T.; White, J. R.; DeLaune, R. D., Redox effects on release kinetics of arsenic, cadmium, cobalt, and vanadium in Wax Lake Deltaic freshwater marsh soils. *Chemosphere* **2016,** *150*, 740-748.
38. Yu, K.; Böhme, F.; Rinklebe, J.; Neue, H.-U.; DeLaune, R. D., Major Biogeochemical Processes in Soils-A Microcosm Incubation from Reducing to Oxidizing Conditions. *Soil Science Society of America Journal* **2007,** *71*, (4), 1406.
39. Gächter, R.; Meyer, J. S.; Mares, A., Contribution of bacteria to release and fixation of phosphorus in lake sediments. *Limnology and Oceanography* **1988,** *33*, (6_part_2), 1542-1558.
40. Hupfer, M.; Lewandowski, J., Oxygen Controls the Phosphorus Release from Lake Sediments - a Long-Lasting Paradigm in Limnology. *International Review of Hydrobiology* **2008,** *93*, (4-5), 415-432.
41. Frohne, T.; Rinklebe, J.; Diaz-Bone, R. A.; Du Laing, G., Controlled variation of redox conditions in a floodplain soil: Impact on metal mobilization and biomethylation of arsenic and antimony. *Geoderma* **2011,** *160*, (3-4), 414-424.
42. Ramesh Reddy, K.; DeLaune, R., Biogeochemistry of Wetlands. . *Boca Raton: CRC Press.* **2008**.
43. Lewis, A. E., Review of metal sulphide precipitation. *Hydrometallurgy* **2010,** *104*, (2), 222-234.
44. Stumm, W.; Sulzberger, B., The cycling of iron in natural environments: Considerations based on laboratory studies of heterogeneous redox processes. *Geochimica et Cosmochimica Acta* **1992,** *56*, (8), 3233-3257.
45. Davranche, M.; Bollinger, J.-C., A Desorption–Dissolution Model for Metal Release from Polluted Soil under Reductive Conditions. *Journal of Environment Quality* **2001,** *30*, (5), 1581.
46. Davranche, M.; Bollinger, J. C., Heavy Metals Desorption from Synthesized and Natural Iron and Manganese Oxyhydroxides: Effect of Reductive Conditions. *J Colloid Interface Sci* **2000,** *227*, (2), 531-539.
47. Davranche, M.; Bollinger, J. C., Release of Metals from Iron Oxyhydroxides under Reductive Conditions: Effect of Metal/Solid Interactions. *J Colloid Interface Sci* **2000,** *232*, (1), 165-173.
48. Quantin, C.; Becquer, T.; Rouiller, J. H.; Berthelin, J., Oxide weathering and trace metal release by bacterial reduction in a New Caledonia Ferralsol. *Biogeochemistry* **2001,** *53*, (3), 323-340.
49. Zachara, J. M. F., James K.; Smith, Steven C.; Gassman, Paul L., Solubilization of Fe(III) oxide-bound trace metalsby a dissimilatory Fe(III) reducing bacterium. *Geochimica et Cosmochimica Acta* **2001,** *65*, (1), 75-93.
50. Cappuyns, V.; Swennen, R., Kinetics of element release during combined oxidation and pHstat leaching of anoxic river sediments. *Applied Geochemistry* **2005,** *20*, (6), 1169-1179.

51. Du Laing, G.; Meers, E.; Dewispelaere, M.; Vandecasteele, B.; Rinklebe, J.; Tack, F. M.; Verloo, M. G., Heavy metal mobility in intertidal sediments of the Scheldt estuary: Field monitoring. *Sci Total Environ* **2009,** *407*, (8), 2919-30.
52. Amrhein, C.; Mosher, P. A.; Brown, A. D., THE EFFECTS OF REDOX ON Mo, U, B, V, AND As SOLUBILITY IN EVAPORATION POND SOILS. *Soil Science* **1993,** *155*, (4), 249-255.
53. Masscheleyn, P. H.; Delaune, R. D.; Patrick, W. H., Arsenic and Selenium Chemistry as Affected by Sediment Redox Potential and pH. *Journal of Environmental Quality* **1991,** *20*, (3), 522-527.
54. Masscheleyn, P. H.; Delaune, R. D.; Patrick, W. H., Effect of redox potential and pH on arsenic speciation and solubility in a contaminated soil. *Environmental Science & Technology* **1991,** *25*, (8), 1414-1419.
55. Ilgen, A. G.; Foster, A. L.; Trainor, T. P., Role of structural Fe in nontronite NAu-1 and dissolved Fe(II) in redox transformations of arsenic and antimony. *Geochimica et Cosmochimica Acta* **2012,** *94*, 128-145.
56. Calmano, W.; Hong, J.; Förstner, U., Binding and Mobilization of Heavy Metals in Contaminated Sediments Affected by pH and Redox Potential. *Water Science and Technology* **1993,** *28*, (8-9), 223-235.
57. Chuan, M. C.; Shu, G. Y.; Liu, J. C., Solubility of heavy metals in a contaminated soil: Effects of redox potential and pH. *Water, Air, and Soil Pollution* **1996,** *90*, (3), 543-556.
58. Filella, M.; Belzile, N.; Chen, Y.-W., Antimony in the environment: a review focused on natural waters. *Earth-Science Reviews* **2002,** *57*, (1-2), 125-176.
59. Takeno, N., National Institute of Advanced Industrial Science and Technology. *Atlas of Eh-pH Diagrams. Geological Survey of Japan Open File Report* **2005,** *409*, 1.
60. Xi, J.; He, M.; Lin, C., Adsorption of antimony(V) on kaolinite as a function of pH, ionic strength and humic acid. *Environmental Earth Sciences* **2009,** *60*, (4), 715-722.
61. Simpson, S. L.; Apte, S. C.; Batley, G. E., Effect of Short-Term Resuspension Events on Trace Metal Speciation in Polluted Anoxic Sediments. *Environmental Science & Technology* **1998,** *32*, (5), 620-625.
62. Huerta-Diaz, M. A.; Tessier, A.; Carignan, R., Geochemistry of trace metals associated with reduced sulfur in freshwater sediments. *Applied Geochemistry* **1998,** *13*, (2), 213-233.
63. Morse, J. W.; Luther, G. W., Chemical influences on trace metal-sulfide interactions in anoxic sediments. *Geochimica et Cosmochimica Acta* **1999,** *63*, (19-20), 3373-3378.
64. Wilson, N.; Webster-Brown, J., The fate of antimony in a major lowland river system, the Waikato River, New Zealand. *Applied Geochemistry* **2009,** *24*, (12), 2283-2292.
65. Schulz-Zunkel, C.; Krueger, F., Trace metal dynamics in floodplain soils of the river Elbe: a review. *J Environ Qual* **2009,** *38*, (4), 1349-62.

66. Laveuf, C.; Cornu, S., A review on the potentiality of Rare Earth Elements to trace pedogenetic processes. *Geoderma* **2009,** *154*, (1-2), 1-12.
67. Shaheen, S. M.; Rinklebe, J.; Rupp, H.; Meissner, R., Lysimeter trials to assess the impact of different flood–dry-cycles on the dynamics of pore water concentrations of As, Cr, Mo and V in a contaminated floodplain soil. *Geoderma* **2014,** *228-229*, 5-13.
68. Shaheen, S. M.; Rinklebe, J.; Frohne, T.; White, J. R.; DeLaune, R. D., Biogeochemical Factors Governing Cobalt, Nickel, Selenium, and Vanadium Dynamics in Periodically Flooded Egyptian North Nile Delta Rice Soils. *Soil Science Society of America Journal* **2014,** *78*, (3), 1065-1078.

4

Sediment water (interface) mobility of metal(loid)s and nutrients under undisturbed conditions and during resuspension

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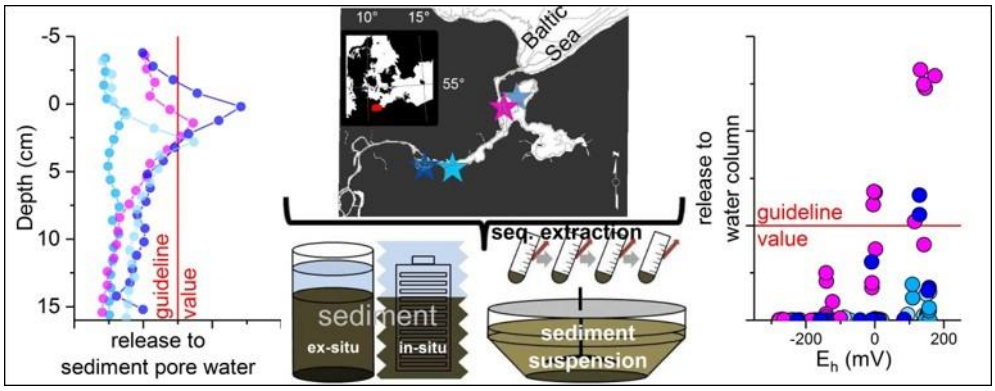

4.1 Abstract

The contribution of the release from sediments to the overall river Trave budget was evaluated with respect to 16 metal(loid)s, three non-metals and the ions PO_4^{3-} and NH_4^+. To consider undisturbed conditions and sediment resuspension *in-situ* dialyses-based and *ex-situ* suction-based pore water sampling was complemented by sequential extraction and suspension reactor experiments. In the investigated sediments, representative for the study area, metal(loid) partitioning between the different geochemical fractions was very similar despite some higher contaminated spots. Pore water investigations emphasis that profiling and peeper based analyses are comparable and deliver an indication that sediment dwelling organisms are exposed to elevated metal(loid) concentrations. However, higher toxicity of the contaminated sediments compared to the sediment treated as background reference was not revealed. During resuspension only few metal(loid)s exceeded specified guideline values. The maximum amounts released, were only between 10^{-5} and 10^{-1}% of the average daily load of the river Trave per ton of suspended sediment. Overall the "most pristine sediments" and not the potentially hazardous materials in the study area are found to be from highest concern. The results support requests to better include fractionation and speciation demands in legal assessments of sediments.

4.2 Introduction

The environmental risk posed by contaminated soils and sediments remains to be often estimated by methods based on the total contaminant content. However, many elements are only partially bioavailable due to their specific chemical properties and prevailing environmental parameters.[1,2] Therefore, it is generally accepted that mobile fractions <0.45 µm operationally defined as dissolved provide a more significant measure to describe potential adverse environmental effects for many contaminants including metal(loid)s.[3,4] In this context mechanical disturbance of sediments by human activities (e.g., construction and maintenance activities in waterways) or from natural causes (sediment dwelling or sediment slides) are of interest. Thus, the availability and release of pollutants both from deposited and from suspended sediment needs to be considered. Approaches that evaluate sediments, based on mobile concentrations (dissolved in pore water) have been developed for a limited number of contaminants.[5] However, steep gradients of environmental parameters prevailing at the sediment water interface (SWI) and the typically resulting steep concentration gradients of metal(loid)s in particular in the dissolved fraction are usually not (sufficiently) considered. This is partly due to constraints associated with different available sampling techniques such as the affection of sample properties and analytes speciation, missing spatial information (e.g. squeezing and centrifugation) or the need of long exposure times (e.g. diffusive gradients/equilibration in thin film (DGT/DET)). With the mesoprofiling and mesosampling system (*messy*) the authors recently

introduced techniques for low-invasive, high spatially resolved pore water sampling[6,7] capable to overcome some of these limitations. When working with disturbed samples, the release remains to be often estimated based on fractionation concepts by (sequential) extractions, which are also used in regulation worldwide. With respect to the changing conditions, "dynamic" bio-geochemical microcosm experiments,[8,9] offer additionally to the "static" (sequential) extractions, the opportunity to study the release of metal(loid)s from sediment suspensions, while manipulating environmental key parameters such as redox potential (E_h) and pH value.

State of the art analytical techniques deliver the opportunity to easier expand the set of analytes beyond the few potentially toxic elements (next to organic pollutants) considered in standardized risk assessment procedures. Further potentially toxic elements as well as elements acting as important sorbents or reactants can nowadays be included in a single analytical run.

To describe the potential contribution of the sediment release to the overall metal(loid) and nutrient mobility the Trave estuary (German Baltic Sea coast) was chosen as study area, owning an intensive history of pollution and strongly impacted by the management (water way maintenance). Four different approaches were combined to address the mobile fraction from four sampling sites investigated. The sites were chosen by feature, characteristic for the estuary with respect to physicochemical properties and the relocation potential. Operationally defined as dissolved concentrations of the 16 metal(loid)s Ag, As, Cd, Co, Cr, Cu, Fe, Mn, Mo, Ni, Pb, Sb, Se, Sn, V, Zn, the non-metals C, P and S as well as the ions NH_4^+, PO_4^{3-} and SO_4^{2-} were examined. Therefore, the mobility of the analytes at the SWI *ex-situ* using a high resolution suction-based pore water sampling, was compared to peeper based *in-situ* sampling (all sampling and installations were undertaken by scuba divers), complemented by sequential extraction following the BCR (Community Bureau of Reference, European Commission)[10] scheme and by information obtained from incubating the sediments in a bio-geochemical microcosm.

4.3 Materials and methods

4.3.1 Study area and field sampling

The entire course of the river Trave is located in a landscape, the subsoil of which forms the terminal moraine of the Weichselian glacial period. Its lower reaches nowadays form the entrance to one of the most important German Baltic ports. As in many estuaries, navigability in this area can only be guaranteed by maintenance work. In this context, the river bed of the Trave has been deepened, straightened and shortened through breakthroughs several times in the past centuries. At the same time wide (shore) areas are subject to special protection (e.g. Habitats and Birds Directive).

The German Federal Institute of Hydrology provides an information system of results from physical, chemical, and ecotoxicological investigations of sediments and suspended matter for the German Federal Waterways and Shipping Administration (SedKat). Based on this data set, by means of hierarchical cluster analysis, taking into account the physicochemical parameters fine grain content, TOC, DOC and the contents of As, Pb, Cd, Cr, Cu, Ni, Hg, Zn, S, P and N in bulk sediments and eluates, five characteristic sediment types were identified in the study area: (i) highly compacted marls with low metal and nutrient contents; (ii) a small area with sediments with high contents of N and P in the city Lübeck; (iii) organic silts with lower metal(loid) contents; (iv) organic silts with elevated metal(loid) contents; and (v) sandy sediments of the mouth of the river Trave (refer to Figure 4.1).

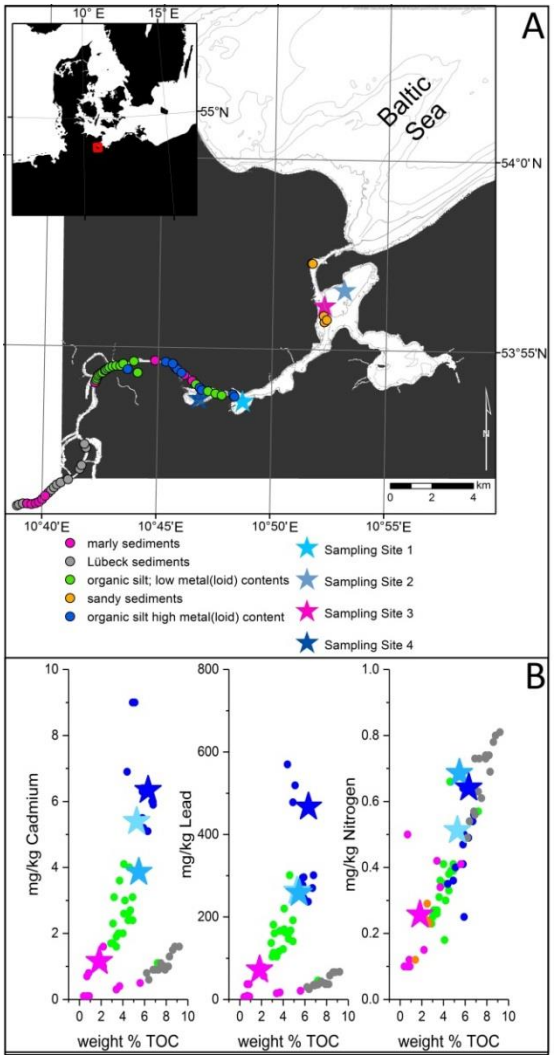

Figure 4.1: *Sediments of the Trave estuary and examined sampling sites. a) Location of sediment samples provided in SedKat and examined sampling sites in the Trave estuary. The coloring represents the results of hierarchical cluster analysis. b) Cadmium, lead, and nitrogen of samples located in SedKat and examined sediments plotted against their TOC content. The coloring represents again the results of the cluster analysis.*

For this study, four sites were chosen to be investigated (refer to Figure 4.1) based on the key parameter organic carbon and contaminants. Three spots represent organic silt sediments with increased metal(loid) contents. The fourth spot represents reworked Pleistocene material (sampling site 3) as it is found in clearly defined areas where the Pleistocene underground protrudes through the recent sediments. It serves as a reference for the geochemical background most pristine with respect to manmade pollution. Information on sediment properties is given in Appendix 3 (section A3.1.1-A3.1.3).

At all four locations three sediment cores with an inner diameter of 15.5 cm were taken and three dialyses samplers were applied by scuba divers on 05-10-2016 (sampling site 1 and 2) and 10-18-2016 (sampling site 3 and 4). The water depth was between 4.5 and 8 m. After sampling the sediment cores were immediately placed in tanks (PP, Auer Packaging, Germany) filled with surface water sampled at the same location for transportation and storage. In the laboratory, the cores were stored at 10°C (similar to measured temperatures at the sites) in darkness. The oxygen concentration of the tank water was monitored and maintained close to the values measured at the sampling sites by bubbling air via a glass air stone (JBL, Germany) and a membrane pump (Sera air 110 plus, Germany) when necessary.

4.3.2 Chemicals and materials

Ultrapure water was produced with a USF ELGA Purelab Plus system (ELGA LabWater, Germany). Nitric acid (HNO_3, 65% w/w, for analysis) was purchased from Merck GmbH (Germany) and re-distilled using a DST-1000 (Savillex, USA).

All samples for inductively coupled plasma-triple-quadrupole mass spectrometry (ICP-QQQ-MS, Agilent 8800 series; Agilent Technologies, Germany) analysis were collected in 15 mL centrifuge tubes (VWR catalyst Laboratory Services, USA, cleaned in 1.3% nitric acid for >24 h rinsed with ultrapure water), acidified to a concentration of 1.3% HNO_3 and stored frozen till measurement.

Prior to acidification aliquots of 0.5 mL of every sample were separated in 1.5 mL microcentrifuge tubes (StarLab, Germany) and stored frozen for ion chromatography measurements (Metrohm 881, Metrohm, Switzerland; Dionex ICS 1100, Thermo Fisher Scientific, USA).

4.3.3 Ex-situ suction-based pore water sampling

Three profiles of suction-based pore water across the SWI were sampled from each sediment core in the lab using the meso profiling and sampling system (*messy*).[6] In this process aqueous samples are constantly extracted by a peristaltic pump (REGLO Analog, MS-2/8, ISMATEC, Germany), while a sampling probe is moved across the SWI with a step motor (Motorized Microprofiling, Unisense,

Denmark). The synchronization of a fraction collector (Omnicoll, LAMBDA Laboratory Systems, Switzerland) enabled the sampling of defined depth intervals. It is positioned in a glovebox using Argon to prevent re-oxidation of the samples. From 4 cm above sediment surface to 16 cm depth samples were taken with a spatial resolution of 1 cm. Prior to evacuation, samples were filtered with syringe filters (pore size 0.45 µm, Minisart NML Syringe Filters, surfactant-free cellulose acetate, Sartorius, Germany) to obtain the fraction <0.45 µm.

Profiles of the E_h and the O_2 saturation were measured in parallel to the sampling process with Mansfeldt-type electrodes (ecoTech Umweltmeßsysteme GmbH, Germany) connected to an Ag/AgCl-reference electrode (REF321, Radiometer Analytical, Germany) and a Multi-channel Fiber Optic Oxygen Meter (OXY-3 SMA) equipped with optical oxygen sensors (Oxygen Dipping Probe DP-PSt3) and temperature probes (Pt 100, all PreSens, Germany).

4.3.4 In-situ dialyses-based pore water sampling

In-situ pore water samples were obtained using acrylic modified Hesslein *in-situ* pore water samplers (Rickly Hydrological CO, USA), called pore water peepers, with cavity volumes of 10 ml, equipped with 0.45 µm polyether sulfone membranes (Pall Laboratory, Germany). Prior to use, the acrylic sampling devices and the membranes were cleaned in 1.3% nitric acid for >24 h, rinsed with ultrapure water to remove contaminations and subsequently stored in ultrapure water, treated with N_2 for >14 days to remove dissolved oxygen traces. Two days before deployment the peepers were mounted, with special care being taken to ensure that all cavities were completely filled with ultrapure water. For the transport to the sampling sites the mounted peepers were stored in ultrapure water previously treated with N_2 to limit the diffusion of O_2 in the acrylic parts.

Three peepers per sampling site were deployed for 14 days with a distance of approximately 0.5 m by scuba divers. To protect the membranes the peepers were covered by butyl rubber mats during transfer from aboard the ship to the sediment and back. Samples were extracted from the peepers immediately after their sampling on board ship by perforating the membranes with pipette tips and transfer in acid cleaned 15 ml centrifuge tubes (VWR catalyst Laboratory Services, USA). After removing a 0.5 ml aliquot for IC measurements, samples were immediately acidified for ICP-QQQ-MS measurements (cf. Appendix 3, paragraph A3. 2).

4.3.5 Suspension experiments

After sampling of pore water was finished 500g wet weight of a pooled sample from each sediment core and 1 L of natural water (same sampling site as the respective sediment) were fed to a biogeochemical microcosm system (slurry reactor, Mikrokosmossystem MRE2, UIT Umweltleistungen, Germany). It consists of a glass vessel that can be hermetically sealed with an airtight lid equipped with

a stirrer to keep the sediment in suspension and electrodes to measure the E_h (EMC 133, Meinsberger Elektroden, Germany) and the pH value (EGA 142, Meinsberger Elektroden, Germany). Data was stored with a logger (MRE2 Datenloggereinheit, UIT Umweltleistungen, Germany). An automatic-valve gas regulation system enables automatic control of the E_h by adding N_2 or O_2 (to lower or increase the E_h, respectively). The sediment was left in suspension untreated to equilibrate at its "natural" E_h. Thereafter, the E_h was forced to -150 mV, 0 mV and 150 mV and kept within E_h windows of approximately 20 mV. At every redox state two samples (5 mL) were extracted through a PES porous hollow fiber (Pijpker Laboratorium Technik, Netherlands, 0.45 µm) using a peristaltic pump (Preciflow, LAMBDA Laboratory Systems, Switzerland). The extracted volume was replaced with ultrapure water to keep the sediment/water ratio, resulting in a dilution of <10% over the course of the experiment.

4.3.6 Sequential extraction

To create a basic understanding on the release to be expected, the binding forms of the metal(loid)s were examined following a modified BCR scheme.[10] Even though the fractions of a sequential extraction procedure are necessarily operationally defined, they are considered to represent the amount of an element that is easily exchangeable or carbonate bound (exchangeable), associated with amorphous Fe and Mn oxides (reducible), sulfides and organic material (oxidizable) or the crystalline structures of sedimentary minerals (residual).[11] These fractions were determined in exact 0.5 g of freeze dried (Christ Gefriertrocknungsanlagen GmbH, Germany) and milled (planetary mill pulverisette, Fritsch, Germany) sub-samples taken at 4-5 cm depth from the sediment cores. The exchangeable fraction was extracted with 20 ml 0.11 M acetic acid, the reducible fraction with 0.1 M hydroxylamine hydrochloride. The oxidizable fraction was extracted with ammonium acetate after organic substance removal by repeated addition of hydrogen peroxide. In all cases the extraction included 16 h overhead shaking (ELMI Ltd., Latvia), subsequent centrifugation (20 min, 1700 rpm) and decanting. After each extraction step, the residues were purified by rinsing with ultrapure water and centrifugation. Finally, residual fractions were calculated as the difference between pseudo total content, determined after microwave assisted digestion in reverse *aqua regia* (2,5 mL 30% HCl + 7,5 mL 65% HNO_3, refer to Appendix 3, section A3.1.2 for details) and the sum of the three fractions.

4.3.7 Analysis

The metal(loid)s and the nonmetals C, P and S in the pore water, microcosm samples and the sequential extracts were quantified by means of ICP-QQQ-MS. To measure the non-metals simultaneously with the metal(loid)s, the metal(loid)s and nonmetals were calibrated separately. Additionally, a matrix matching was performed by adding NaCl to a concentration of 10‰ to all standards used for calibration and to quality control samples to account for the salinity. Details on the

isotopes analyzed and the reference materials used for measurement validation can be found in Appendix 3 (Table A3. 5).

To quantify PO_4^{3-}, SO_4^{2-} and NH_4^+ by ion chromatography despite the salt concentration of ~10 PSU 40 µl of non-acidified samples were diluted 1:50 and standard addition by 0.1 mg/L was applied to exceed the respective limit of quantification.

The anionic species were quantified with a Metrohm 881 compact IC Pro equipped with a Metrosep A Sup 5 Guard 4.0 guard column and a Metrosep A Supp7 separation column (all Metrohm, Switzerland). 3.6 mM sodium carbonate solution was used as eluent and 100 mM sulfuric acid as regenerating acid.

The parallel quantification of the cation NH_4^+ was performed by a Dionex ICS 1100 equipped with an IonPac CG16-4µm RFICTM 4*50 mm guard column and an IonPac CS16-4µm 4*250 mm separation column (all Thermo Fisher Scientific, USA) with 25 mM methyl sulfonic acid as eluent.

4.3.8 Statistics and graphs

Data analyses were performed using R (version 3.3.2; 2016-10-31). Outliers in the measured concentrations and correlation coefficients were identified/calculated using the R packages “outliers” and “PerformanceAnalytics”. Concentrations below the limit of detection (<LoD) were set to half of the respective LoD for statistical calculations. The presented graphs were prepared using Origin 2017 G (OriginLab, USA).

4.4 Results and discussion

4.4.1 Metal(loid)s fractionation

Despite differences in total content, the metal(loid)s are partitioned very comparable in the four fractions addressed by the modified BCR scheme in the four sampling sites investigated. Ag, As, Cr, Fe, Mo, Sn, Pb and V remain in the residual fraction to a large extent (>80%), Cd, Mn and Zn are available predominantly in the acid-soluble fraction and Ni, Co, Cu, Sb and Se predominantly in the oxidizable fraction (refer to Figure 4.2 and Figure A3. 2, Appendix 3). Thus, the metal contaminations of the studied sediments are not reflected in a changed distribution between the binding forms, which contradicts a frequently expressed assumption.[12, 13]

The release of the different geochemical fractions to the environment can be expected if conditions become more acidic (acid-soluble), more reductive (reducible) or more oxic (oxidizable), while the residual fraction is regarded as immobile.[11] Thus, the release of the reducible fraction into the pore water of undisturbed sediments with increasing depth is to be expected, while the release of predominantly oxidizable bound elements is likely to occur during sediment resuspension events.

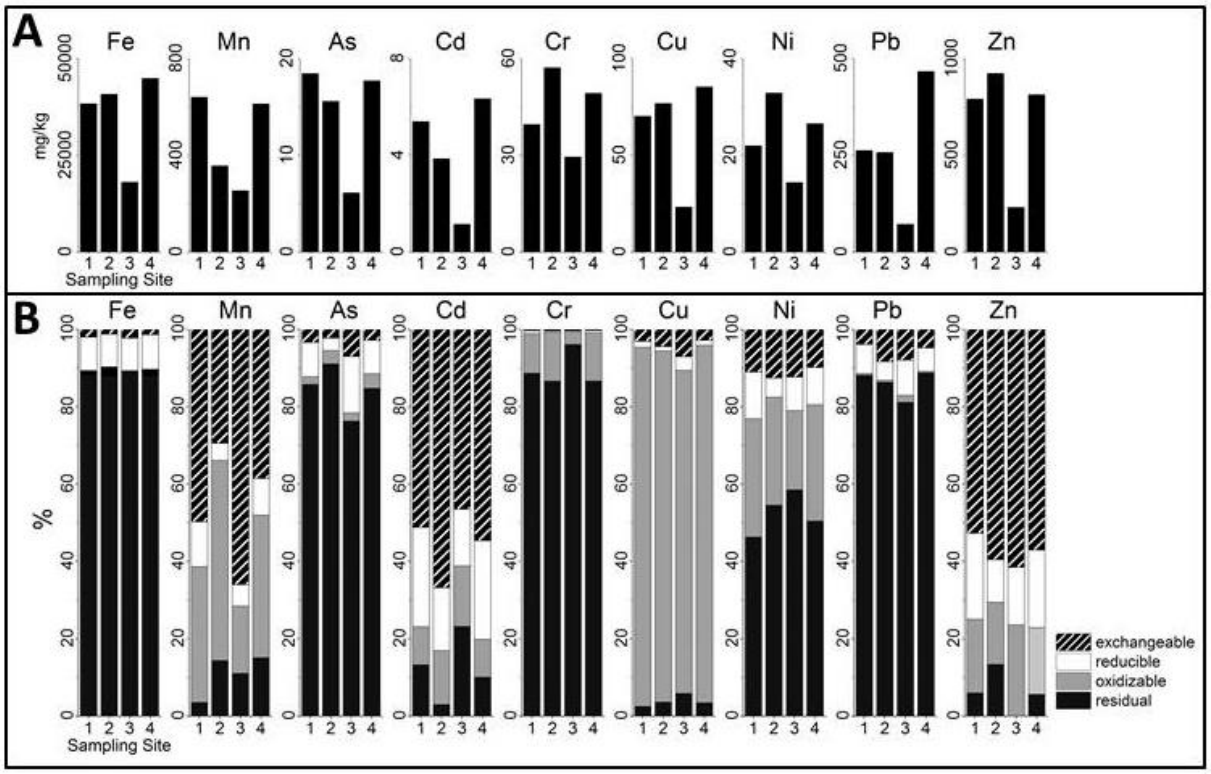

Figure 4.2: *Total content (A) and binding form (B) of Fe, Mn, As, Cd, Cr, Cu, Ni, Pb and Zn in the sediments of sampling site 1 to 4. Data is presented as average value of the sediments of a sampling site. Corresponding graphs for Ag, Co, Mo, Sb, Se, Sn and V are given in Appendix 3 (Figure A3. 2).*

4.4.2 O2-concentration and Eh during ex-situ suction-based pore water sampling

The O_2 concentration profiles measured in parallel to *ex-situ* suction-based pore water sampling in the laboratory show that oxygen penetration depth in the sediment cores of sampling sites 1-3 is less than 1 mm. It is slightly larger in the cores from sampling site 4 where the values vary between <1mm and up to and up to 3 mm. Additionally, the values confirm that the oxygen concentrations measured during sampling on site (data not shown) were successfully maintained in the laboratory. Profiles of the O_2 concentration are given in Appendix 3 (Figure A3. 3).

The E_h-profiles measured in parallel to *ex-situ* suction-based pore water sampling display a rapid change from oxic (>100 mV) to anaerobic (<-100 mV) conditions within in the first 2-5 mm below the SWI in the sediment cores of sampling site 1, 2 and 4, while the E_h in the depth profiles of sampling site 3 fluctuates around -100 mV (refer to Figure 4. 2 and Figure A3. 4, Appendix 3).

4.4.3 Pore water depth profiles

Results of individual measurements are given in Appendix 3 (Tables A3. 11-A3. 143). In both the *in-situ* dialyses-based and the *ex-situ* suction-based samples maximum concentrations measured were in the range of 0.1-1 µg/L for Cd, Sb, Sc and Tl, in the range of 1-10 µg/L for As, Cr, Cu, V, Pb, Mo, Ni, Se, Sn

and Ti, in the range of 10-100 µg/L for Zn, in the range of 1-10 mg/L for C and Mn, in the range of 10-100 mg/L for Fe, P, PO_4^{3-} and NH_4^+ and in the range of 100-2000 mg/L for S and SO_4^{2-}.

The concentrations measured in the different *in-situ* dialysis-based pore water depth profiles of the individual sampling sites are very similar. Significantly higher differences were found repeating the *ex-situ* suction-based pore water depth profiles of the individual sampling sites. This effect can be ascribed in non-homogenized "living sediments" to the visible macro-biota and bioturbation activity and the resulting sediment heterogeneities.[14,15] Whereas the temporal and spatial "smoothing" over exposure time (~14 days) and cavity width (up to 10 cm) of the *in-situ* dialyses based pore water sampling explains the lower variation of the these profiles. However, comparing averaged pore water depth profiles obtained with the two completely different sampling techniques as shown in Figure 4.3 and 4.4, results remain remarkably comparable for most of the analytes. Taking into account the different sampling principles (passive *vs.* active) and the capability of *messy* to make sediment heterogeneities visible, it seems possible to generate sediment pore water samples in the laboratory that represent field conditions. This is especially from interest when not scuba diver, but only sediment corer based sampling is possible due to, e.g. economic reasons or water depth.

Next to profiles of the E_h the dissolved concentrations of C, P and PO_4^{3-}, NH_4^+, S and SO_4^{2-}, Fe and Mn in *ex-situ* suction-based and *in-situ* dialyses-based pore water depth profiles are shown in Figure 4.3. In the pore water depth profiles of all sediments the concentrations of C, P, PO_4^{3-} and NH_4^+ increase with depth, while the concentrations of dissolved S and SO_4^{2-} decrease. The concentrations of dissolved Fe and Mn experience pronounced peaks below SWI with Fe concentrations being the most variable between the individual *ex-situ* suction-based depth profiles of all analytes in the mg/L range. Also the averaged depth profiles obtained for Fe *in-situ* show larger variations than most other analytes.

The release of NH_4^+ and PO_4^{3-} can be attributed to a large extent to organic matter (OM) decomposition. Accordingly, significantly higher concentrations of both analytes are reached in the organic-rich sediments of sampling sites 1, 2 and 4 than in the reworked Pleistocene material of sampling site 3. On the other hand a relevant difference between total dissolved P and dissolved PO_4^{3-}-P that increases with increasing concentrations of dissolved C in this organic-rich sediments indicates that the amount of dissolved organic matter (DOM) increases with depth. Since for H_2S no analytical method was available, the total S concentrations determined by ICP-QQQ-MS represent essentially SO_4^{2-}-S. This is confirmed by the good agreement between total-S concentrations and SO_4^{2-}-S concentrations determined by IC. However, S is also incorporated in DOM[16] explaining the total S concentrations being slightly above the SO_4^{2-}-S concentrations.

The depth profiles of Fe and Mn are in good agreement with the measured redox profiles and reflect the rapid transition from oxic to anaerobic conditions in organic-rich sediments. The release of both elements by reductive dissolution of their (hydr)oxides as well as Fe and Mn precipitation by the formation of sulfides with increasing sulfate reduction are well studied diagenetic processes.[17]

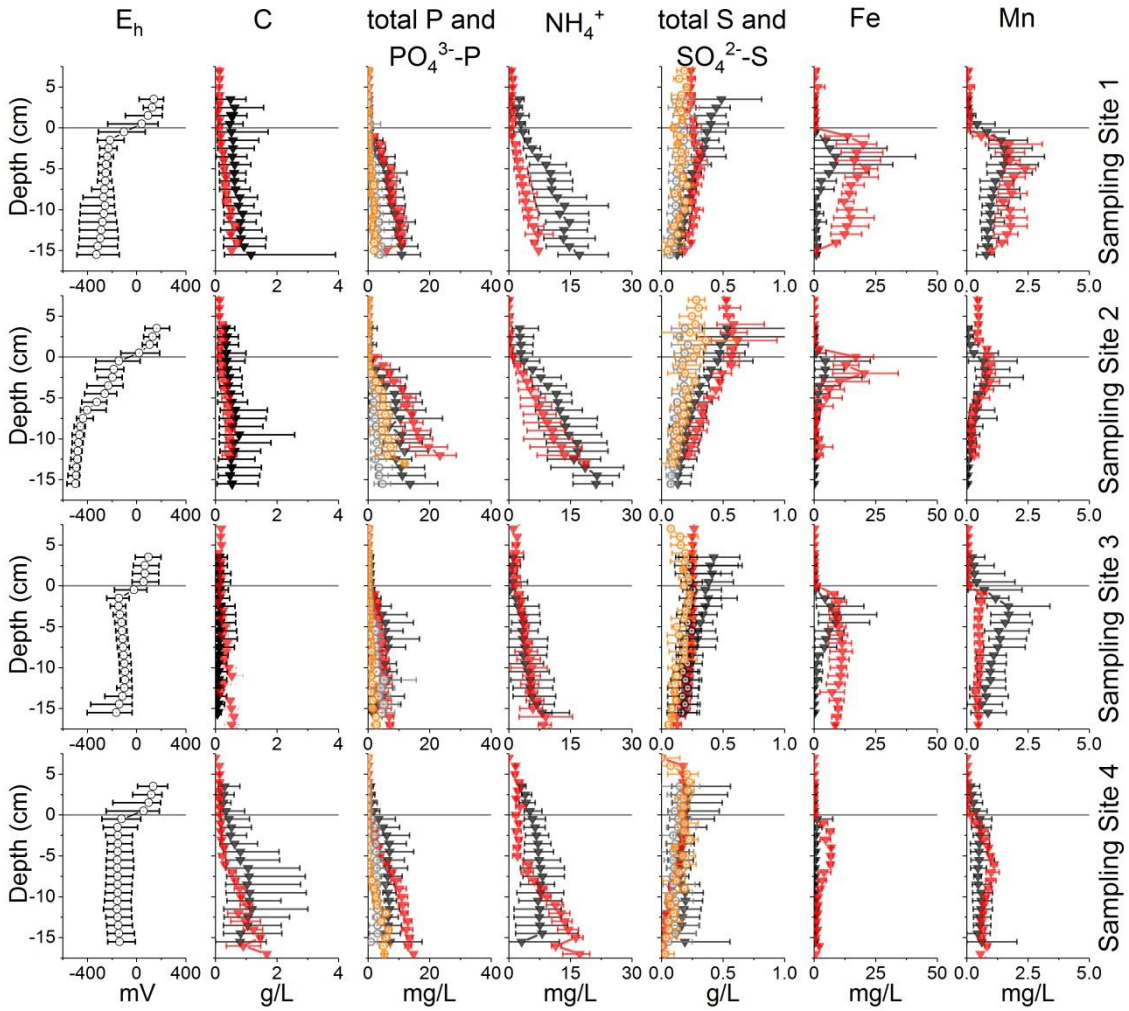

Figure 4.3: *E_h (○) and laterally averaged dissolved concentrations of C, total P, NH_4^+, total S, Fe and Mn in ex-situ suction-based (n=9, black) and in-situ dialyses-based (n=3, red) pore water samples at the four sampling sites. With total P and total S also PO_4^{3-}-P and SO_4^{2-}-S are given in the ex-situ suction based (grey) and in-situ dialyses based (orange) samples. Error bars represent the minimum and maximum value / concentration measured at the respective depth. Grey lines represent the SWI.*

Pore water depth profiles of the trace metal(loid)s As, Cd, Cr, Cu, Ni, Pb and Zn are shown in Figure 4.4. Corresponding graphs for Ag, Co, Mo, Sb, Se, Sn and V are given in Appendix 3 (Figure A3. 5). The concentrations of the metal(loid)s were either approximately constant from the water column to maximum sampling depth (Ag, Pb, Zn), decreased to values near the respective limit of detection within the first centimeters below the SWI (Cu, Mo, Ni, Sb) or increased with depth (Cr, Se, Sn, V). Pronounced concentration peaks below the SWI characterize the depth profiles of As, Cd, and Co. In addition, their concentrations show the greatest variability in the first 3-4 cm below the SWI both, in *ex-situ* suction-based and *in-situ* dialyses-based samples. Hence, with respect to the similarities to major elements grouping of the metal(loid)s addressed in this study based on the shape of their pore water depth profiles in Fe/Mn-type (As, Cd, Co, Zn), C/P/ NH_4^+-type (Cr, Se, Sn, V) and S-type (Cu, Mo, Sb) appears appropriate and reflects important processes controlling their solubility. The essential control of Fe and Mn (hydroxides) on the mobility of As and Co, as shown in the Trave sediments, has been described before.[18-22] However, their reductive dissolution contributes to increased concentrations only in the uppermost 2-3 cm of the sediments. With depth increasing concentrations of the elements Cr, Se, Sn and V indicate their release during OM degradation. The decreasing concentrations and limited availability in the pore water of Cd, Cu, Mo, Ni and Sb are explainable by their affinity for sorption to binding sites of particulate OM or caused by sulfide precipitation.[23-25] Based on the elements which were present in significant proportions (>5%) in the reducible fraction of sequential extraction (As, Cd, Co, Sb V, Zn), only V was continuously or increasingly released into the pore water with increasing depth.

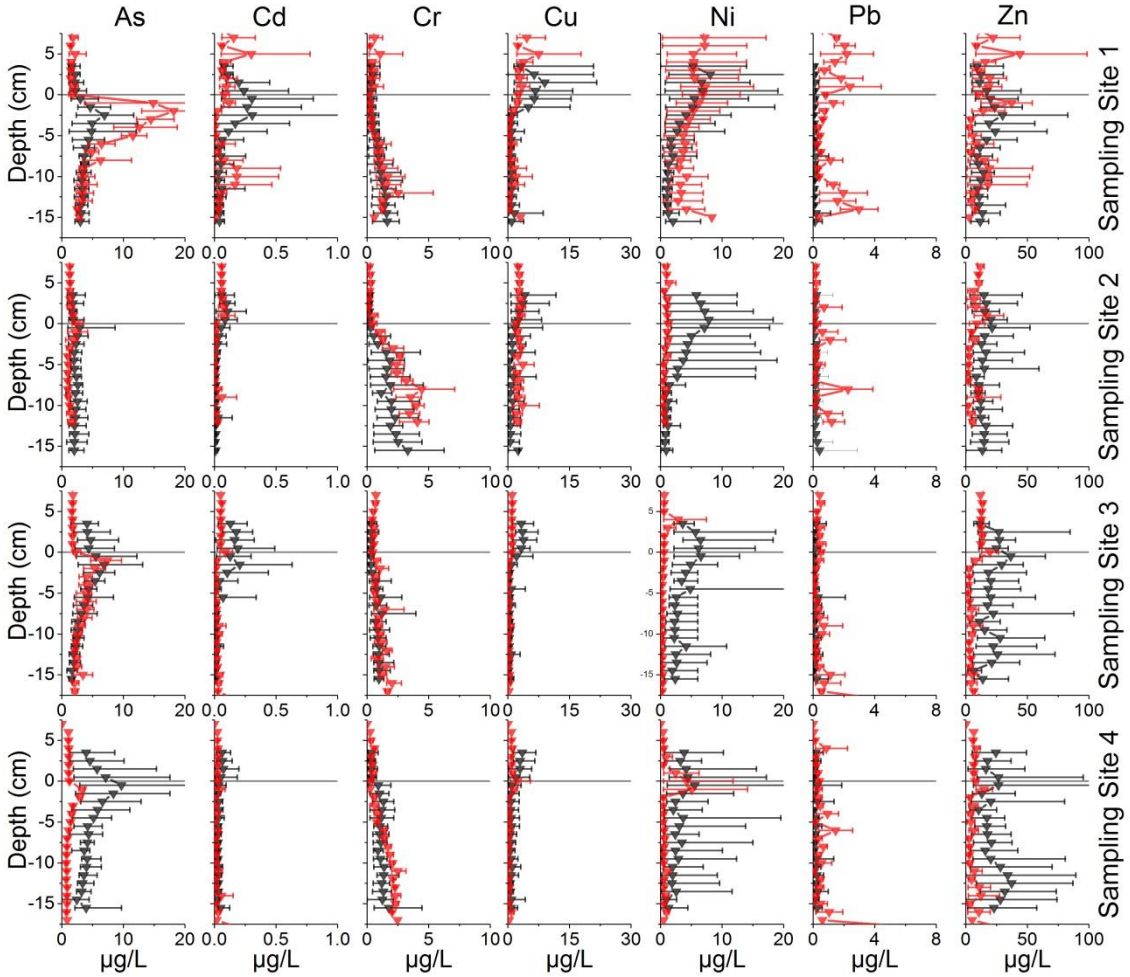

Figure 4.4: *Laterally averaged dissolved concentrations of As, Cd, Cr, Cu, Ni, Pb and Zn in ex-situ suction-based (n=9, black) and in-situ dialyses-based (n=3, red) pore water samples at the four sampling sites. Error bars represent the minimum and maximum value/concentration measured at the respective depth. Grey lines represent the SWI.*

4.4.4 Suspension experiments

The measured concentrations of S, Fe, As, Cd, Ni and Pb are shown in Figure 4.5 as a function of E_h. Corresponding graphs for C, P, Mn, Ag, Co, Cr, Cu, Mo, Sb, Se, Sn, V, Zn and changes of E_h and pH value during the individual experiments are given in Appendix 3 (Figure A3. 6-A3. 7). The "natural" E_h that occurred in the sediment suspensions before the E_h was forced to defined values of -150 mV, 0 mV and +150 mV reached mostly values between -100 mV and -300 mV. The pH value and E_h are two interdependent measures in the way that an increase in E_h leads to a decrease in pH as consequence of H+ ion formation during oxidation and vice versa.[26] Corresponding changes in pH also occurred during the redox manipulations in the mesocosm. However, all measured pH values were between 7.5 and 9.5.

Regarding the metal(loid)s, maximum concentrations across all experiments were <1 µg/L for Cr, Sc, Sn, Ti and Tl, 1-10 µg/L for Ag, Cd, Cu, Pb, Sb and Se, 10-100 µg/L for As, Co, Ni and V and 100-1000 µg/L for Mo and Zn. Maximum concentrations of Fe and Mn were about 50 and 6 mg/L respectively. An increase in concentrations in the liquid phase <0.45 µm with increasing E_h can be found for S and the metal(loid)s Cd, Co, Cu, Ni, Sb and Zn with largest amounts of all 6 metal(loid)s being released from the reworked Pleistocene material of sampling site 3. In addition, the increase in release starts at lower E_h values than in the organic-rich sediments of the other sampling sites. A similar redox behavior of these elements was observed in comparable experiments with different soils and sediments by several authors.[27-30] The reason for the increased metal(loid) release with rising E_h can be the oxidative dissolution of sulfide minerals[24,31] while the constant C and P concentrations in the course of the experiment indicate that aerobic degradation of OM was of minor importance.[32] On the other hand, the increase in metal(loid) concentrations is limited by their re-sorption on existing surfaces and the co-precipitation with Fe and Mn (hydr)oxides[33] leading to significant alteration of metal(loid) binding forms during resuspension.[34]

The increasing release of Cd, Co, Cu, Ni, Sb and Zn with increasing E_h agrees well with the results of the sequential extraction where all these elements were found in the oxidizable fraction in significant proportions (>10%) in all four sediments. However, only small proportions of the oxidizable bound fraction were released to the aqueous phase. The proportion of the metalloids Cr and Mo in the oxidizable fraction was as well more than 10% without being released at increasing E_h. The latter may be caused by the affinity of both elements to OM or by the lower solubility of their oxidized species (Cr(VI), Mo(VI)) compared to their reduced species (Cr(III), Mo(IV)).[35,36]

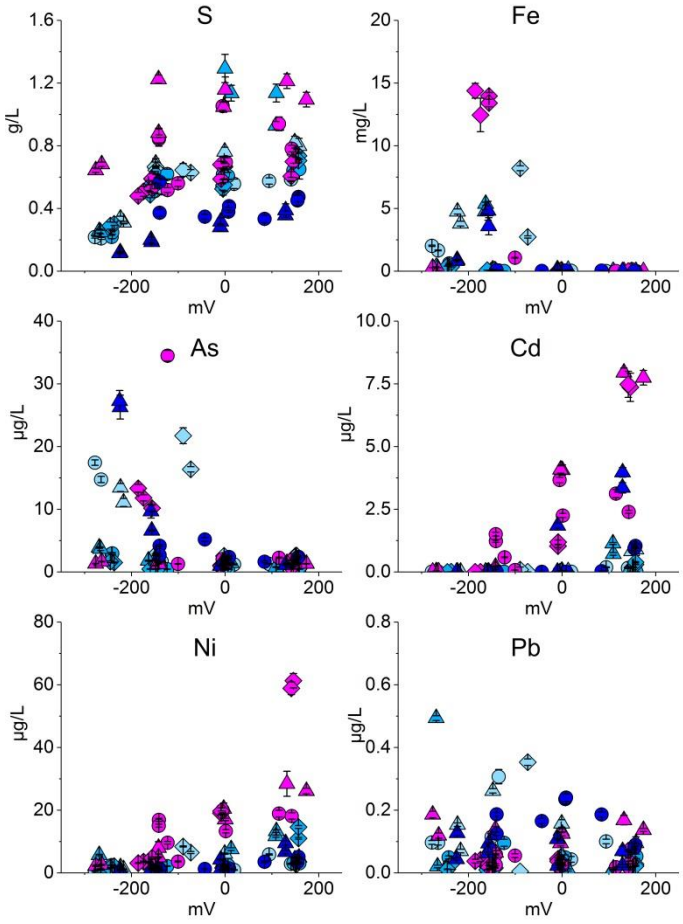

Figure 4.5: *Concentrations of S, Fe, As, Cd, Ni and Pb as a function of E_h (●, ●, ●, ● for sampling site 1, 2, 3 and 4; ●, ▲, ♦ representing the different sediment cores). Error bars represent analytical standard deviation.*

4.4.5 Data evaluation with respect to dredging and reuse

Results of sequential extraction are frequently evaluated by application of concepts such as enrichment factor (EF),[37] geoaccumulation index (Igeo),[38] individual or global contamination factor (ICF or GCF)[39] and risk assessment code (RAC).[40] The application of EF and Igeo (refer to Appendix 3, section 3.7) indicate that next to Cd, Pb and Zn, that exceed the German threshold values for dredged material, also As, Ag, Se and Sn are severely enriched in the sediment samples of sampling site 1, 2 and 4 (refer to Appendix 3, Table A3. 7). Application of the ICF and RAC (refer to Appendix 3, section A3. 7) predicts the highest risk of release into the aqueous environment for Cd and Zn or Cd, Cu, Sb and Zn, respectively. The risk of release for all elements is estimated to be the lowest for sediments of sampling site 3.

Assessment of dissolved concentrations can be conducted by comparison with predicted no effect concentrations or other (eco-)toxicity measures.[4] However, such values delivering sufficient reliability

are not available for all elements addressed in this study. Stricter threshold values for the dissolved concentrations of more elements (As, Cd, Cr, Cu, Fe, Ni, Pb, Sb, Se, Zn) than in other regulations are specified in the European Drinking Water Directive.[41] Regarding the pore water of the undisturbed sediments these values, developed for human consumption not ecological issues, delivering here a very conservative reference value, are only exceeded by Fe and As in some of the near-surface samples. Assessment criteria for dissolved metal mixtures in sediment pore water taking into account the metals Cd, Cu, Pb, Ni and Zn were developed by USEPA (refer to Appendix 3, section A3. 8).[5] In the *ex-situ* suction-based pore water samples the assessment criteria is exceeded by most of the samples of the first 1-2 cm below SWI, by individual samples from all four sampling sites and in each case almost a complete depth profile of the locations 2 and 4 (refer to Appendix 3, Table A3. 9). This delivers an indication that sediment dwelling organisms are exposed to elevated metal(loid) concentrations. Although this underlines the heterogeneity of the sediment surfaces, it does not reveal any higher toxicity of the contaminated sediments compared to the sediment treated as background reference.

With regard to the suspension experiments, the metal(loid)s released per dry mass of sediment can be calculated. The maximum amounts released per kg sediment are computed to be <0.1 µmol for Ag, Cr, Se, Sn, and Pb, between 0.1 and 1 µmol for Cd, Cu and Sb, 1-10 µmol for As, Co, Mo, Ni and V and approximately 50, 450 and 3500 µmol for Zn, Mn and Fe, respectively. This corresponds to a maximum expected release of the order of 10^{-1}% of the average daily load from river Trave (calculated from data of the surface water monitoring of the federal state Schleswig-Holstein in the years 2005-2014; data not shown) per ton sediment suspended for Cd, 10^{-2}% for As, Ni and Zn, 10^{-3}% for Cu and PO_4^{3-} and 10^{-4}% for Cr and Pb.

This indicates that a singular, time-limited resuspension event significantly affects the budget of only few analytes, compared to the continuous load of the Trave, even if quantities typically relocated during a single dredging campaign are considered.

However, the European Water Framework Directive specifies maximum permissible concentrations for dissolved Cd, Ni and Pb (0.45 – 1.5 depending on water hardness, 34 and 14 µg/L, respectively). These values are exceeded for Cd and Ni in the sediment suspensions by up to ~16 and ~2 times, respectively. This suggests that, depending on the hydrological conditions, a spatial and temporal impairment of water quality is to be expected in case of dumping of the examined sediments as dredged material. However, the expected impairment is largest for the most “pristine” sediment of sampling site 3, initially treated as reference.

4.5 Conclusions

During dredging the investigated sediments, the dissolved metal(loid) fractions of the sediment pore waters contribute only to a minor extent to the water column content, while this release path may be crucial for NH_4^+. From the results of the resuspension experiments and the application of RAC to the sequential extraction findings, a risk of release for the elements Cd, Cu, Sb and Zn can be derived. On the other hand, application of the RAC did not predict the observed release of Ni and Co, and the lower predicted risk for sampling site 3 did not match the observations of the resuspension experiment.

The results suggest that despite the visible enrichment, from anthropogenic causes, for most of the sediments studied, only minor metal(loid) release must be expected, which is in good agreement with observations during monitoring of dredging operations.[42-44] Nevertheless, metal(loid)s and nutrients are among the key substances when it comes to improvement of the ecological state of the Baltic Sea[45] and next to their release into the water phase bio-methylation, ingestion or dermal uptake cause environmentally harmful effects. However, the results emphasis once again, that dredged sediments have to be seen as a potential secondary resource in, e.g. recreation efforts. Therefore, miss matching evaluation criteria, neglecting the onsite fractionation and speciation of the potentially hazardous substances may cause a significant loss of management opportunities and may bear in themselves the risk to create ecologically unnecessary cost increases.

4.6 References

1. Eggleton, J.; Thomas, K. V., A review of factors affecting the release and bioavailability of contaminants during sediment disturbance events. *Environ Int* **2004,** *30*, (7), 973-80.
2. Vink, J. P., The origin of speciation: trace metal kinetics over natural water/sediment interfaces and the consequences for bioaccumulation. *Environ Pollut* **2009,** *157*, (2), 519-27.
3. Schafer, S.; Buchmeier, G.; Claus, E.; Duester, L.; Heininger, P.; Korner, A.; Mayer, P.; Paschke, A.; Rauert, C.; Reifferscheid, G.; Rudel, H.; Schlechtriem, C.; Schroter-Kermani, C.; Schudoma, D.; Smedes, F.; Steffen, D.; Vietoris, F., Bioaccumulation in aquatic systems: methodological approaches, monitoring and assessment. *Environ Sci Eur* **2015,** *27*, (1), 5.
4. Mayer, P.; Parkerton, T. F.; Adams, R. G.; Cargill, J. G.; Gan, J.; Gouin, T.; Gschwend, P. M.; Hawthorne, S. B.; Helm, P.; Witt, G.; You, J.; Escher, B. I., Passive sampling methods for contaminated sediments: scientific rationale supporting use of freely dissolved concentrations. *Integr Environ Assess Manag* **2014,** *10*, (2), 197-209.
5. EPA, U. S. *Procedures for the Derivation of Equilibrium Partitioning Sediment Benchmarks (ESBs) for the Protection of Benthic Organisms: Metal Mixtures (Cadmium, Copper, Lead, Nickel, Silver, and Zinc)*; Environmental Protection Agency, Washington, DC. Office of Water: Washington, DC, Tuesday, July 21, 2015 4:24:06 PM, 2005; p 121
6. Schroeder, H.; Fabricius, A. L.; Ecker, D.; Ternes, T. A.; Duester, L., Metal(loid) speciation and size fractionation in sediment pore water depth profiles examined with a new meso profiling system. *Chemosphere* **2017,** *179*, 185-193.
7. Schroeder, H.; Fabricius, A. L.; Ecker, D.; Ternes, T. A.; Duester, L., Impact of mechanical disturbance and acidification on the metal(loid) and C, P, S mobility at the sediment water interface examined using a fractionation meso profiling ICP-QQQ-MS approach. *Sci Total Environ* **2019,** *651*, (Pt 2), 2130-2138.
8. Yu, K. D., RD, A brief history on soil microcosms as an experimental apparatus for biogeochemical research. In *Microcosms: Ecology, Biological Implications and Environmental Impact*, Harris, C. C., Ed. 2013; pp 169-177.
9. Yu, K.; Rinklebe, J., Advancement in soil microcosm apparatus for biogeochemical research. *Ecological Engineering* **2011,** *37*, (12), 2071-2075.
10. Ure, A. M.; Quevauviller, P.; Muntau, H.; Griepink, B., Speciation of Heavy Metals in Soils and Sediments. An Account of the Improvement and Harmonization of Extraction Techniques Undertaken Under the Auspices of the BCR of the Commission of the European Communities. *International Journal of Environmental Analytical Chemistry* **1993,** *51*, (1-4), 135-151.
11. Tessier, A.; Campbell, P. G. C.; Bisson, M., Sequential extraction procedure for the speciation of particulate trace metals. *Analytical Chemistry* **1979,** *51*, (7), 844-851.

12. Cao, L.; Tian, H.; Yang, J.; Shi, P.; Lou, Q.; Waxi, L.; Ni, Z.; Peng, X., Multivariate Analyses and Evaluation of Heavy Metals by Chemometric BCR Sequential Extraction Method in Surface Sediments from Lingdingyang Bay, South China. *Sustainability* **2015,** *7*, (5), 4938-4951.
13. Saleem, M.; Iqbal, J.; Shah, M. H., Geochemical speciation, anthropogenic contamination, risk assessment and source identification of selected metals in freshwater sediments—A case study from Mangla Lake, Pakistan. *Environmental Nanotechnology, Monitoring & Management* **2015,** *4*, 27-36.
14. Teal, L. R.; Parker, E. R.; Solan, M., Coupling bioturbation activity to metal (Fe and Mn) profiles in situ. *Biogeosciences* **2013,** *10*, (4), 2365-2378.
15. Stockdale, A.; Davison, W.; Zhang, H., Micro-scale biogeochemical heterogeneity in sediments: A review of available technology and observed evidence. *Earth-Science Reviews* **2009,** *92*, (1-2), 81-97.
16. Ksionzek, K. B.; Lechtenfeld, O. J.; McCallister, S. L.; Schmitt-Kopplin, P.; Geuer, J. K.; Geibert, W.; Koch, B. P., Dissolved organic sulfur in the ocean: Biogeochemistry of a petagram inventory. *Science* **2016,** *354*, (6311), 456-459.
17. Du Laing, G.; Rinklebe, J.; Vandecasteele, B.; Meers, E.; Tack, F. M., Trace metal behaviour in estuarine and riverine floodplain soils and sediments: a review. *Sci Total Environ* **2009,** *407*, (13), 3972-85.
18. Mitsunobu, S.; Harada, T.; Takahashi, Y., Comparison of Antimony Behavior with that of Arsenic under Various Soil Redox Conditions. *Environmental Science & Technology* **2006,** *40*, (23), 7270-7276.
19. Dang, D. H.; Lenoble, V.; Durrieu, G.; Omanovic, D.; Mullot, J. U.; Mounier, S.; Garnier, C., Seasonal variations of coastal sedimentary trace metals cycling: insight on the effect of manganese and iron (oxy)hydroxides, sulphide and organic matter. *Mar Pollut Bull* **2015,** *92*, (1-2), 113-124.
20. Heggie, D.; Lewis, T., Cobalt in pore waters of marine sediments. *Nature* **1984,** *311*, (5985), 453-455.
21. Stockdale, A.; Davison, W.; Zhang, H.; Hamilton-Taylor, J., The Association of Cobalt with Iron and Manganese (Oxyhydr)oxides in Marine Sediment. *Aquatic Geochemistry* **2010,** *16*, (4), 575-585.
22. Gorny, J.; Billon, G.; Lesven, L.; Dumoulin, D.; Made, B.; Noiriel, C., Arsenic behavior in river sediments under redox gradient: a review. *Sci Total Environ* **2015,** *505*, 423-34.
23. Huerta-Diaz, M. A.; Morse, J. W., Pyritization of trace metals in anoxic marine sediments. *Geochimica et Cosmochimica Acta* **1992,** *56*, (7), 2681-2702.
24. Morse, J. W., Interactions of trace metals with authigenic sulfide minerals: implications for their bioavailability. *Marine Chemistry* **1994,** *46*, (1-2), 1-6.

25. Morse, J. W.; Luther, G. W., Chemical influences on trace metal-sulfide interactions in anoxic sediments. *Geochimica et Cosmochimica Acta* **1999,** *63*, (19-20), 3373-3378.
26. Yu, K.; Böhme, F.; Rinklebe, J.; Neue, H.-U.; DeLaune, R. D., Major Biogeochemical Processes in Soils-A Microcosm Incubation from Reducing to Oxidizing Conditions. *Soil Science Society of America Journal* **2007,** *71*, (4).
27. Shaheen, S. M.; Rinklebe, J.; Frohne, T.; White, J. R.; DeLaune, R. D., Redox effects on release kinetics of arsenic, cadmium, cobalt, and vanadium in Wax Lake Deltaic freshwater marsh soils. *Chemosphere* **2016,** *150*, 740-748.
28. Shaheen, S. M.; Rinklebe, J.; Frohne, T.; White, J. R.; DeLaune, R. D., Biogeochemical Factors Governing Cobalt, Nickel, Selenium, and Vanadium Dynamics in Periodically Flooded Egyptian North Nile Delta Rice Soils. *Soil Science Society of America Journal* **2014,** *78*, (3), 1065-1078.
29. Frohne, T.; Rinklebe, J.; Diaz-Bone, R. A.; Du Laing, G., Controlled variation of redox conditions in a floodplain soil: Impact on metal mobilization and biomethylation of arsenic and antimony. *Geoderma* **2011,** *160*, (3-4), 414-424.
30. Frohne, T.; Rinklebe, J.; Diaz-Bone, R. A., Contamination of Floodplain Soils along the Wupper River, Germany, with As, Co, Cu, Ni, Sb, and Zn and the Impact of Pre-definite Redox Variations on the Mobility of These Elements. *Soil and Sediment Contamination: An International Journal* **2014,** *23*, (7), 779-799.
31. Schippers, A., Biogeochemistry of metal sulfide oxidation in mining environments, sediments, and soils. In *Special Paper 379: Sulfur Biogeochemistry - Past and Present*, 2004; pp 49-62.
32. Gerringa, L. J. A., Aerobic degradation of organic matter and the mobility of Cu, Cd, Ni, Pb, Zn, Fe and Mn in marine sediment slurries. *Marine Chemistry* **1990,** *29*, 355-374.
33. Calmano, W.; Förstner, U.; Hong, J., Mobilization and Scavenging of Heavy Metals Following Resuspension of Anoxic Sediments from the Elbe River. In *Environmental Geochemistry of Sulfide Oxidation*, American Chemical Society: 1993; Vol. 550, pp 298-321.
34. Xie, M.; Alsina, M. A.; Yuen, J.; Packman, A. I.; Gaillard, J. F., Effects of resuspension on the mobility and chemical speciation of zinc in contaminated sediments. *J Hazard Mater* **2019,** *364*, 300-308.
35. Gorny, J.; Billon, G.; Noiriel, C.; Dumoulin, D.; Lesven, L.; Madé, B., Chromium behavior in aquatic environments: a review. *Environmental Reviews* **2016,** *24*, (4), 503-516.
36. Smedley, P. L.; Kinniburgh, D. G., Molybdenum in natural waters: A review of occurrence, distributions and controls. *Applied Geochemistry* **2017,** *84*, 387-432.
37. Abrahim, G. M.; Parker, R. J., Assessment of heavy metal enrichment factors and the degree of contamination in marine sediments from Tamaki Estuary, Auckland, New Zealand. *Environ Monit Assess* **2008,** *136*, (1-3), 227-38.

38. Iqbal, J.; Shah, M. H., Distribution, correlation and risk assessment of selected metals in urban soils from Islamabad, Pakistan. *J Hazard Mater* **2011,** *192*, (2), 887-98.
39. Zhao, S.; Feng, C.; Yang, Y.; Niu, J.; Shen, Z., Risk assessment of sedimentary metals in the Yangtze Estuary: new evidence of the relationships between two typical index methods. *J Hazard Mater* **2012,** *241-242*, 164-72.
40. Jain, C. K., Metal fractionation study on bed sediments of River Yamuna, India. *Water Res* **2004,** *38*, (3), 569-78.
41. EC, Council Directive 98/83/EC of 3 November 1998 on the quality of water intended for human consumption. In Off J Commun L 330:32-54, 1998; Vol. L 330, pp 32-54.
42. De Groote, J. D., G.; Vangheluwe, M.;, Environmental monitoring of dredging operations in the Belgian nearshore zone. *Aqua et Terra* **1998,** *70*, 21-25.
43. Pieters, A. V. P., M.; Dumon, G.;, Speelers, L., Chemical monitoring of maintenance dredging operations at Zeebrugge. *Aqua et Terra* **2002,** *86*, 3-10.
44. Morgan, B.; Rate, A. W.; Burton, E. D., Water chemistry and nutrient release during the resuspension of FeS-rich sediments in a eutrophic estuarine system. *Sci Total Environ* **2012,** *432*, 47-56.
45. HELCOM, Hazardous substances in the Baltic Sea – An integrated thematic assessment of hazardous substances in the Baltic Sea. *Balt. Sea Environ. Proc. No. 120* **2010**.

5

Final Conclusion

This thesis outlines the development and application of an approach for the investigation of processes at the sediment water interface (SWI) and the impact of changing environmental conditions such as mechanical or chemical disturbances on the mobility of metal(loid)s, non-metals and nutrition ions. With the meso profiling and sampling system (*messy)* a setup is presented that enables automated, minimal-invasive sampling of sediment pore water from undisturbed or manipulated sediments down to 20 cm depth. Additionally, the setup enables the detection of sediment parameters such as O_2-concentratoion, redox potential and pH-value in parallel to the sampling process. By investigating metal(loid)s size fractionation as well as the As(III/V) and Sb(III/V) speciation, it is demonstrated that the system offers a multitude of options to combine different sample preparation and analytical techniques. It opens a door to a variety of potential future applications in inorganic and organic environmental analytical chemistry and beyond. For example, the combination of the microbial status and speciation analyses of individual metal(loid)s may improve the understanding of their biogeochemical cycles, or the combination of ecotoxicological effects with metal mobility may enable new approaches for sediment risk assessments. However, one challenge is to further develop and optimize the system, to extend its application from metals, non-metals and nutrient ions, to trace organic compounds, in order to make potential ecosystem services of the SWI visible.

The so far missing comparison, between a suction based *ex-situ* sampling system (here *messy*) with a dialyses driven sampling system (here peeper arrays) has proven, from the best of the author's knowledge, for the first time the ability to reproduce field conditions in detail in the laboratory. This strikes the path to investigate geochemical cycles of metal(loid)s, e.g. at sampling sites where the installation of dialyses based devices is prevented by poor accessibility. It also provides an option to combine spatially high-resolution examinations of sediment pore water with additional investigations (e.g. measurement of bulk concentrations). Potential future applications will be significantly extended by autonomous in-situ operations of *messy*. The basis for such a system is delivered in this thesis and due to the modular setup, this platform can be implemented with a manageable additional technical effort.

In this work a compromise was found between spatial resolution of the pore water sampling and the obtained sample volume needed for the parallel detection of a large number of elements, so far impossible for other close to low impact approaches. An ICP-QQQ-MS method is expanded to simultaneously quantify various metal(loid)s and important non-metals in the complex matrix sediment pore water, including the steep concentration gradients at the SWI. This approach is worth

further development. ICP-QQQ-MS delivers the unique opportunity to quantify up to 70 elements within the same analytical run. Not only with regard to pore water analysis, but also to monitor and understand the chemical status of surface waters, the quantification of a wide spectrum of inorganic analytes is of great importance, e.g. to better understand the trace element contribution of river to the ocean budgets. The application and further development of ICP-QQQ-MS multi-element approaches therefore delivers a significant potential to better describe global element cycles and this thesis is another contribution to deliver the methodological backbone.

Finally, the sampling system has been applied in the context of sediment risk assessment. Therefore, the analytical approach was extended to samples with strong matrix effects from brackish water bodies. The results confirm, a rather “pristine” sediment with low total contents may pose a higher risk regarding the release of metal(loid)s and nutrients compared to contaminated sites. This emphasizes once again the need to better include fractionation and speciation in legal evaluations. Environmental quality standards for metal(loid)s are specified for the dissolved fraction, the total sample or the suspended solids in several environmental regulations, e.g. the European water framework direction. Unfortunately, methods that enable a prediction of release and speciation of most of the elements studied in this thesis is missing. The complementary study of sediments from the Trave estuary with the slurry reactor enabled an estimation of the impact of sediment re-suspension on metal(loid) mobility. This setup may not be suitable for routine analysis within public authorities, but it strikes a path towards sediment risk assessment methods that include fractionation and speciation under changing close to environmental conditions. Additionally, the application of the bio-geochemical microcosm appears promising as a complementary method in the context of sediment risk assessment, not only for the water and shipping administration.

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Appendix I

Supporting Information Chapter 2:

Metal(loid) speciation and size fractionation in sediment pore water depth profiles examined with a new meso profiling system

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AI.I Experimental setup

Table A1. 1: Experimental setup and time line.

profile / event	parameter and sample preservation	day
profile 1	EDTA: total content and III/V speciation As and Sb <16 µm	-10
profile 2	EDTA: total content and III/V speciation As and Sb <16 µm	-5
profile 3/Sb_2O_3 spike/oxygen	EDTA: total content and III/V speciation As and Sb <16 µm	0
profile 4/oxygen	EDTA: total content and III/V speciation As and Sb <16 µm	5
profile 5/oxygen	EDTA: total content and III/V speciation As and Sb <16 µm	10
profile 6/oxygen	EDTA: total content and III/V speciation As and Sb <16 µm	15
profile 7/oxygen	EDTA: total content and III/V speciation As and Sb <16 µm	20
profile 8/oxygen	EDTA: total content and III/V speciation As and Sb <16 µm	57
profile 9/oxygen	EDTA: III/V speciation As and Sb, HNO_3: total content <16 µm and <0.45 µm	65
profile 10/oxygen	EDTA: III/V speciation As and Sb, HNO_3: total content <16 µm and <0.45 µm	77
profile 11/oxygen	EDTA: III/V speciation As and Sb, HNO_3: total content <16 µm and <0.45 µm	141

AI.II Sediment sampling

The sediment was sampled 06/2015 at an oxbow of the river Lahn in Germany (50°18'56.87"N; 7°37'41.25"E). The surrounding of the water body is strongly vegetated leading to an impact of fallen leaves, forming a 20 – 40 cm organic layer on top of the older sediment layers. The older layers are strongly affected by former lead and silver mining activities displaying increasing metal(loid) concentrations down to 2 m depth (data not shown). After removing the organic layer, mainly containing less degraded leaves, the upper 40 cm of the sediment were sampled in a disturbed manner with a snow shovel (Randschaufel, Hornbach, DE). Water from the river was sampled the same day (3 times 30 L) and stored in the dark at 4°C. The sediment was transferred into a rectangular tank (Nalgene, polypropylene, 42 L, USA). 22 L of the sediment were incubated with 10 cm overlaying water and let at rest for two month with the floating cover of the tank closed to allow the formation of stable SWI conditions. The water column was maintained constant by refilling evaporated river water on weakly basis.

Figure A1. 1: Sampling area in winter 2015. The sediment is impacted from former mining activities and the input of organic material from the surrounding vegetation. Fresh water is introduced at flood events (2 – 3 times per year).

AI.III Sediment characteristic

Subsequently to the experiment, a sediment core was sampled in the laboratory, frozen and cut with ceramic knife into 1 cm slices. The sediment samples were freeze dried (Christ Gefriertrocknungsanlagen GmbH, Germany), milled (planetary mill pulverisette, Fritsch, Germany) and digested by application of a microwave assisted procedure. Therefore, 1 g of the sediment was mixed with 10 mL of reverse *aqua regia* (2,5 mL 30% HCl + 7,5 mL 65% HNO_3) an digested in a five-step power-controlled program (refer to table A1. 2) using a Multiwave PRO (Anton Paar, Austria). After digestion, samples were diluted to 100 mL and analysed by means of ICP-OES (Optima 8300, Perkin Elmer,) and ICP-QQQ-MS (Agilent 8800, Agilent Technologies, Japan).

Table A1. 2: Micro wave program.

Step	Program	Power	Time
		W	mm:ss
1	Power ramp	600	11:00
2	Power ramp	1500	3:00
3	Power hold	1500	13:00
4	Power ramp	860	9:30
5	Power hold	750	13:30

To determine the total content of carbon, nitrogen and sulphur, 100 mg of the freeze-dried and milled sediment samples were analysed by means of a total content analyser (Vario Macro, Elementar, Germany). For the analyses sulphur measurements, 120 mg of tungsten oxide (WO_3) were added to support the combustion process. Calibration was performed using sulphanilamide and verified by measurements of acetanilide. Two certified reference materials were included in the measurements (Leco 308, Leco 309). Results are presented in table A1. 3 and A1. 4.

Table A1. 3: Total CNS content of the sediment at the end of the experiment.

depth [cm]	C [%]	TOC [%]	N [%]	S [%]	C/N	C/S
0-1	12.5	12.4	0.9	5.5	13.4	2.3
1-2	13.1	13.1	0.9	6.1	15.1	2.2
2-3	13.4	13.3	0.8	6.0	16.2	2.2
3-4	13.3	13.1	0.8	6.1	16.2	2.2
4-5	13.4	13.3	0.8	6.1	16.2	2.2
5-6	13.2	13.2	0.8	6.2	15.8	2.1
6-7	13.4	13.3	0.8	6.3	15.9	2.1
7-8	13.7	13.7	0.8	6.1	16.3	2.2
8-9	13.2	13.2	0.8	6.2	15.8	2.1
9-10	13.3	13.3	0.8	6.1	16.0	2.2

Table A1. 4: Metal(loid)s content of the sediment at the end of the experiment. All values in mg/kg.

depth cm	V	SD	Cr	SD	Ni	SD	Cu	SD
0-1	55.54	1.52	152.4	5.3	137.0	5.0	6,108	35
1-2	50.86	1.81	128.9	5.4	129.4	2.6	5,358	117
2-3	49.91	1.41	129.0	5.7	131.8	1.8	5,497	22
3-4	47.78	0.25	133.1	2.8	130.2	3.2	5,337	33
4-5	46.47	1.05	121.8	3.8	123.7	2.2	5,421	29
5-6	42.56	1.97	110.9	5.7	130.4	2.8	5,549	111
6-7	46.53	1.07	122.3	1.9	126.2	3.0	5,423	21
7-8	50.17	0.54	124.8	1.0	126.2	2.5	5,608	14
8-9	46.85	2.00	121.4	6.4	126.1	1.7	5,522	76
9-10	48.61	2.89	129.2	5.9	124.3	2.7	5,506	93
10-11	49.63	0.69	132.5	3.6	126.5	4.0	5,405	142
11-12	44.94	2.19	119.0	4.5	125.1	2.1	5,507	34
>12	44.16	1.30	118.4	3.6	124.8	3.1	5,532	31
depth cm	Co	SD	As	SD	Mo	SD	Ag	SD
0-1	24.11	0.17	36.04	0.71	23.28	0.74	2.748	0.067
1-2	24.44	0.32	31.28	1.53	18.64	0.83	1.656	0.064
2-3	25.34	0.48	30.58	0.58	19.83	0.17	2.030	0.011
3-4	24.85	0.39	28.79	0.66	17.57	0.33	1.785	0.034
4-5	25.44	0.35	29.06	0.43	19.52	0.55	1.818	0.027
5-6	23.29	1.37	27.41	1.76	18.38	1.43	1.587	0.129
6-7	26.11	0.08	29.20	1.02	18.89	0.53	1.759	0.028
7-8	23.87	0.15	30.91	0.67	18.68	0.37	1.798	0.017
8-9	25.47	0.25	29.38	1.37	20.59	0.50	2.533	0.045
9-10	25.05	0.42	29.65	1.35	20.22	1.45	1.945	0.113
10-11	24.90	0.34	30.53	0.74	17.96	0.07	1.805	0.036
11-12	25.76	0.16	28.11	0.99	19.01	0.96	1.698	0.096
>12	26.50	0.12	28.78	1.23	19.45	0.34	2.027	0.018
depth cm	Cd	SD	Sb	SD	U	SD	Fe	SD
0-1	7.221	0.196	36.85	0.43	3.489	0.101	89,452	120
1-2	5.651	0.173	21.34	0.44	2.801	0.047	84,423	1211
2-3	6.420	0.040	28.33	0.59	2.992	0.091	85,594	1131
3-4	5.673	0.130	19.97	0.46	2.919	0.016	85,194	443
4-5	5.813	0.047	23.82	0.10	2.823	0.055	85,800	1811
5-6	5.362	0.412	24.47	1.53	2.948	0.065	87,994	744
6-7	5.777	0.132	28.04	0.14	2.731	0.114	86,368	229
7-8	5.720	0.097	24.09	0.19	2.627	0.140	84,872	769
8-9	5.839	0.113	28.01	0.75	2.671	0.165	85,616	627
9-10	5.819	0.305	25.68	0.61	2.690	0.175	84,766	2013
10-11	5.692	0.122	23.57	0.83	2.713	0.164	84,439	643
11-12	5.533	0.356	25.64	0.64	2.648	0.103	85,192	257
>12	5.542	0.020	26.35	0.31	2.943	0.035	85,890	664

Table A1. 4 continued.

depth cm	Mn	SD	Zn	SD	S	SD
0-1	513.8	6.6	3,544	34	34,919	815
1-2	734.4	2.2	2,663	9	38,235	569
2-3	692.4	9.7	3,044	54	34,792	513
3-4	756.1	5.0	2,814	11	37,970	365
4-5	715.4	2.8	2,873	20	41,777	78
5-6	718.4	1.7	2,905	20	39,938	7792
6-7	705.8	3.9	2,886	13	40,553	1278
7-8	711.6	10.8	2,874	37	41,746	5877
8-9	705.1	0.8	2,884	1	38,664	525
9-10	680.0	4.9	2,847	18	39,574	489
10-11	725.2	4.9	2,814	8	39,890	854
11-12	697.2	5.1	2,834	25	36,555	95
>12	689.0	4.3	2,884	21	38,712	290

AI.IV ICP-MS Analyses of sediment pore water samples

The information about the measurements of the total metal(loid) concentrations in the pore water samples and the different size fractions are given in Table A1. 8-A1. 19. Most of the elements were measured by application of a collision cell (He) with a He gas flow of 5 ml/min, only Mo and Ag were analysed in the standard measurement modus. For validation purposes three certified reference materials (CRMs) and three internal standards (^{72}Ge, ^{103}Rh, ^{185}Re) were included in the measurements. The recoveries of at least two of the CRMs were in the range of ± 10% of the certified value, the maximum accepted variation of the internal standards were at 20% from the initial value. Maximal accepted analytical instability of the measurements were 10% RSD (all samples measured 5 times). Limits of detection (LoD) and limits of quantification (LoQ) are given together with the results.

Table A1. 5: Information about ICP-QMS analyses of sediment pore water samples

Isotope	^{51}V	^{52}Cr	^{55}Mn	^{56}Fe	^{59}Co	^{60}Ni	^{63}Cu	^{66}Zn	^{75}As	^{95}Mo	^{107}Ag	^{111}Cd	^{121}Sb	^{238}U
Modus	He	He	He	He	He	He	He	He	He	He	No gas	He	He	No gas
CRM	Certified value [µg/L]													
TM 23.4 **	1.93	6.8	8.75	14.4	7.09	4.95	8.51	2.47	8.16	4.23	4.8	2.92	3.27	5.01
TM 25.4 **	27.4	24.0	25.1	31.0	27.5	16.2	26.7	44.5	27.1	27.5	22.0	23.5	23.8	27.3
TMDA 64.2**	289	290	295	306	254	263	275	310	162	290	13	266	128	142

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AI.V As and Sb speciation in sediment pore water samples

Details on the As and Sb speciation measurements are summarized in Table A. 21, A1. 22 and A.1 24. All calibration standards, references and samples contained 20 mM EDTA. The solubility of EDTA in the stock solution was supported by adding NH_4OH (Sigma Aldrich, TraceSelect ultra). In order to avoid biases of the results of As(V), plastic vials were used instead of glass vials which might contain arsenate used as an additive in the production process.

Table A1. 6: ICP-MS /HPLC parameters and retention times of the As an Sb species

ICP-QMS / HPLC parameters			Retention times		
RF	1550	W	As (III)	2.047	min
Sample depth	7.0	mm	As (V)	3.625	min
Carrier Gas	0.97	L/min	Sb (III)	8.361	min
Make Up Gas	0.1	L/min	Sb (V)	2.865	min
Flow rate (HPLC)	15	ml/min			
Runtime	14	min			
Injection volume	100	µl			
Isotope	^{75}As,	^{121}Sb			

Table A1. 7: HPLC gradients

Time		Eluent	
t_1	t_2	A	B
min	**min**	**%**	**%**
0.0	4.5	100	0
4.5	5.0	66.7	33.3
5.0	5.5	33.3	66.7
5.5	11.0	0	100
11.0	11.5	33.3	66.7
11.5	12.0	66.7	33.3
12.0	14.0	100	0

Table A1. 8: Species standards used for analyses

Species	Name	Manufacturer
Sb(III)	Potassmium antimonyltatratetrihydrate	Merck, p.A.
Sb(V)	Potassmium hexahydroxoantimonate(V)	Sigma Aldrich p.A
As(III)	Arsenic (III) speciation standard	Spex, CertiPrep
As(V)	Arsenic (V) speciation standard	Spex, CertiPrep

AI.VI Sediment parameters

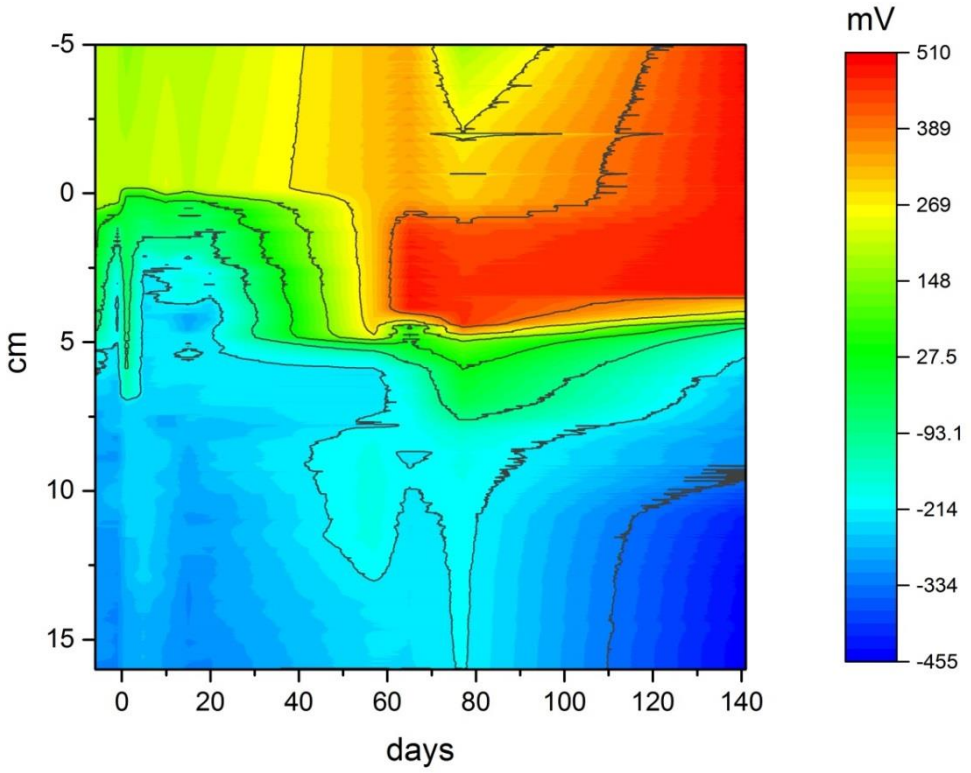


Figure A1. 2: Redox heatplot across the SWI.

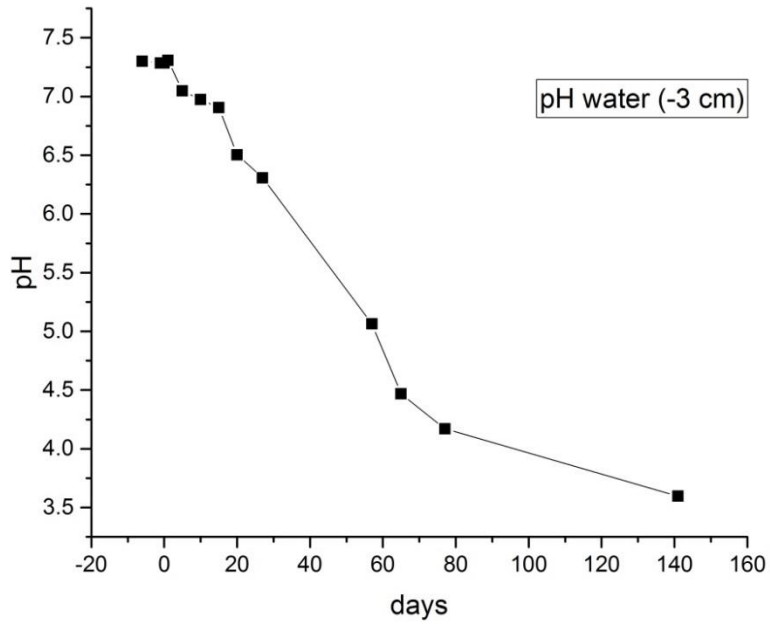


Figure A1. 3: pH in the overlying water body.

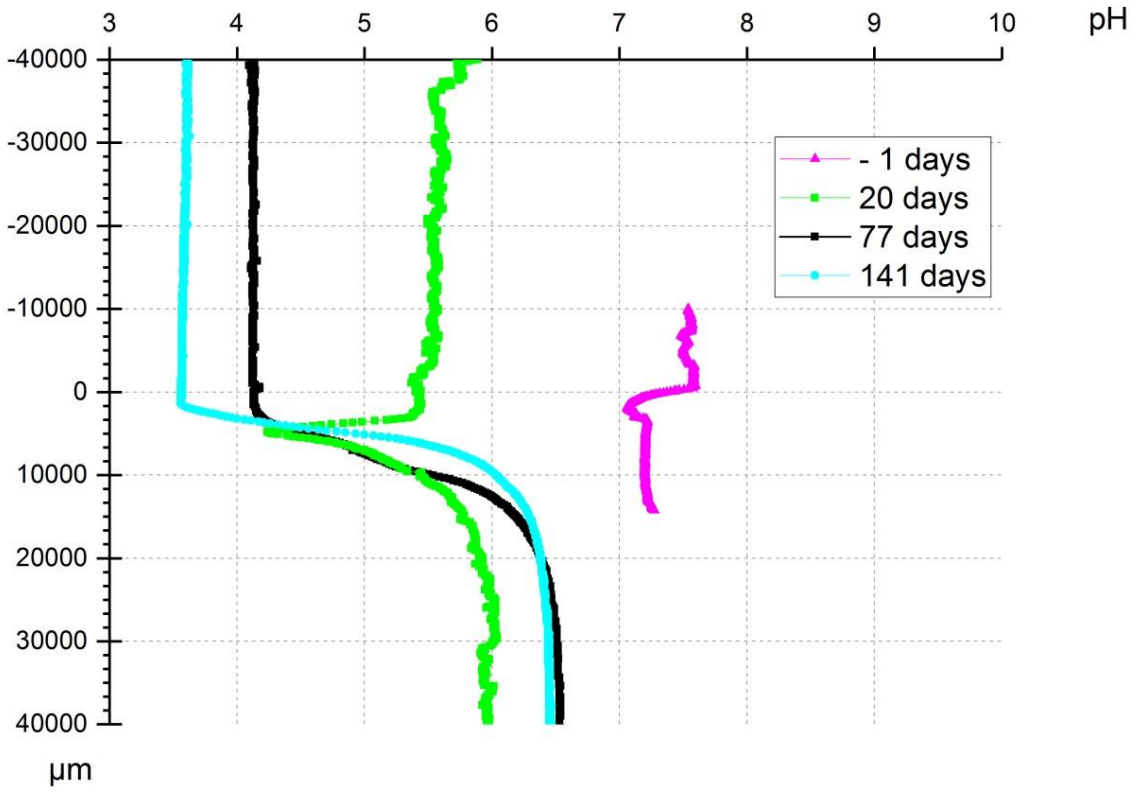


Figure A1. 4: pH profiles in between the respective *messy* profiles. In the first profile the microsensor was broken at 1.425 cm depth and as a consequence the profile was aborted.

AI.VII Metal(loid) concentrations in pore water samples

Table A1. 9: Iron concentration across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth \ day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**150**	2,7	**15**	8,6	**250**	0,5	**7,2**	0,2	**8,3**	0,3	**8,5**	0,2	**58**	1,6	**10**	0,2	**42**	0,3	**26**	0,8	**329**	4,6
-4	**160**	5,5	**8,1**	4,7	**140**	0,2	**9,2**	0,2	**13**	0,5	**10**	0,4	**59**	1,9	**9,1**	0,4	**6,9**	0,1	**15**	0,9	**326**	10,1
-3	**147**	12	**7,0**	0,5	**16**	0,2	**17**	0,8	**28**	1,1	**12**	0,5	**65**	1,4	**9,3**	0,3	**18**	0,3	**20**	0,8	**316**	4,9
-2	**120**	5,2	**7,9**	0,2	**6,8**	0,2	**41**	1,3	**34**	0,9	**21**	0,6	**62**	1,4	**10**	0,3	**28**	0,3	**41**	1,2	**295**	4,8
-1	**111**	2,3	**7,7**	0,2	**5,0**	0,2	**66**	1,0	**31**	0,9	**37**	1,5	**62**	1,5	**11**	0,2	**38**	0,3	**28**	0,6	**287**	7,3
0	**114**	5,5	**20**	0,3	**4,1**	0,3	**54**	1,4	**32**	0,6	**32**	1,1	**69**	2,0	**12**	0,3	**89**	0,7	**34**	1,1	**959**	7,7
1	**93**	1,1	**1619**	31	**480**	43	**81**	2,4	**803**	32	**904**	29	**2056**	59	**282**	10	**1058**	10	**7585**	143	**19572**	458
2	**399**	16	**3849**	84	**1190**	71	**753**	27	**3587**	103	**4104**	59	**6559**	108	**3240**	70	**7509**	42	**12490**	501	**24471**	341
3	**1316**	61	**4051**	6,4	**905**	43	**3059**	69	**3336**	125	**4001**	115	**6046**	147	**2402**	84	**8474**	50	**3557**	109	**676**	68
4	**1996**	70	**4386**	28	**1173**	64	**3055**	56	**3637**	94	**3170**	67	**5518**	133	**49**	2,3	**4331**	26	**329**	24	**10108**	285
5	**2271**	72	**4951**	2,4	**89**	259	**3480**	110	**4986**	144	**2708**	87	**5838**	47	**43**	0,9	**250**	1,4	**3867**	85	**177**	2,0
6	**2012**	101	**4926**	1,6	**44**	140	**4390**	107	**5790**	142	**4063**	108	**6787**	143	**31**	0,8	**126**	1,2	**6574**	158	**92**	3,5
7	**420**	21	**4569**	1,3	**43**	120	**5835**	203	**7047**	611	**5865**	240	**7696**	140	**30**	0,9	**80**	0,5	**9269**	550	**64**	2,2
8	**82**	3,6	**4120**	1,9	**45**	174	**6035**	147	**7474**	330	**6859**	176	**8449**	280	**29**	1,2	**91**	0,3	**8043**	182	**60**	1,6
9	**84**	1,9	**5413**	1,3	**47**	84	**6604**	153	**7958**	208	**7558**	348	**9255**	183	**503**	11	**3061**	34	**8397**	133	**3304**	0,9
10	**1393**	65	**6353**	1,5	**47**	210	**7443**	99	**8191**	119	**8361**	259	**9752**	132	**3764**	59	**8997**	77	**9885**	244	**90**	3,3
11	**3943**	110	**6895**	1,0	**51**	129	**8047**	463	**8184**	136	**8920**	229	**10047**	188	**7017**	204	**7659**	60	**15945**	453	**116**	2,0
12	**5644**	229	**7456**	1,0	**56**	193	**7954**	173	**8203**	368	**9291**	175	**10577**	949	**8345**	61	**7529**	52	**14729**	282	**253**	4,7
13	**7178**	200	**7916**	0,9	**54**	233	**7603**	93	**8400**	313	**9578**	146	**10175**	226	**9033**	281	**7852**	64	**12790**	440	**2834**	120
14	**7750**	138	**8150**	0,7	**60**	220	**7775**	143	**8688**	153	**9567**	154	**10530**	285	**9620**	236	**13878**	988	**12980**	456	**7062**	148
15	**8005**	147	**8630**	4,1	**77**	674	**7814**	149	**8794**	217	**9925**	106	**10542**	285	**9312**	286	**11519**	79	**17812**	353	**9611**	333
16	**7983**	118	**8634**	3,7	**147**	148	**8088**	68	**9003**	343	**9672**	506	**10929**	274	**10068**	167	**14883**	1411	**13332**	498	**8899**	123
LoD	0,2		0,8		0,8		0,4		0,4		0,4		0,2		0,5		1,0		0,8		1,3	
LoQ	0,5		1,1		1,1		0,9		0,9		0,9		0,4		1,1		2,6		1,3		3,0	

Table A1. 10: Manganese concentration across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth \ day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**174**	3	**106**	4	**630**	21	**395**	8	**267**	9	**229**	4	**265**	7	**1354**	23	**1507**	58	**1379**	43	**2470**	31
-4	**188**	7	**102**	3	**660**	15	**348**	9	**272**	9	**228**	8	**274**	8	**1340**	35	**1501**	60	**1464**	88	**2482**	70
-3	**162**	13	**99**	3	**634**	14	**325**	12	**260**	10	**228**	8	**270**	6	**1336**	34	**1501**	52	**1450**	64	**2481**	37
-2	**126**	6	**94**	4	**632**	15	**311**	9	**267**	7	**227**	7	**263**	5	**1363**	30	**1494**	24	**1454**	43	**2477**	42
-1	**114**	1	**91**	2	**636**	19	**336**	5	**257**	7	**227**	9	**265**	7	**1396**	27	**1539**	27	**1484**	32	**2628**	55
0	**123**	6	**86**	6	**661**	8	**325**	9	**270**	26	**229**	8	**255**	7	**1408**	36	**1548**	61	**1470**	42	**2539**	14
1	**130**	3	**300**	20	**799**	27	**329**	9	**413**	16	**363**	12	**333**	10	**1355**	47	**1489**	24	**1420**	28	**2210**	48
2	**449**	17	**474**	31	**694**	12	**532**	20	**574**	15	**521**	7	**498**	72	**1099**	23	**1179**	23	**1204**	41	**1851**	25
3	**452**	21	**500**	3	**672**	6	**550**	13	**574**	21	**575**	17	**563**	13	**826**	29	**920**	11	**883**	27	**1220**	35
4	**422**	18	**490**	12	**686**	12	**544**	10	**588**	17	**597**	13	**574**	15	**692**	32	**815**	29	**764**	56	**1617**	41
5	**479**	17	**492**	14	**691**	35	**558**	17	**614**	17	**590**	20	**595**	5	**637**	14	**701**	13	**751**	16	**1094**	16
6	**544**	34	**535**	18	**662**	19	**603**	15	**616**	15	**607**	17	**635**	12	**624**	14	**658**	16	**744**	18	**931**	34
7	**492**	34	**576**	14	**661**	17	**659**	24	**653**	57	**634**	26	**666**	12	**623**	18	**636**	6	**818**	47	**856**	30
8	**546**	22	**631**	27	**650**	27	**560**	15	**639**	29	**632**	16	**663**	20	**625**	27	**656**	11	**759**	16	**787**	25
9	**573**	13	**652**	17	**650**	9	**546**	13	**650**	16	**663**	64	**711**	17	**672**	12	**680**	15	**751**	12	**980**	13
10	**678**	29	**663**	23	**654**	21	**592**	8	**649**	9	**671**	21	**731**	13	**687**	12	**690**	14	**801**	19	**976**	35
11	**603**	15	**684**	13	**643**	10	**627**	38	**641**	12	**690**	18	**746**	13	**689**	19	**620**	14	**1090**	28	**978**	18
12	**573**	23	**701**	11	**671**	16	**603**	13	**634**	27	**697**	13	**783**	71	**698**	6	**638**	28	**960**	18	**853**	18
13	**638**	19	**676**	9	**672**	21	**551**	6	**638**	25	**701**	10	**750**	15	**703**	23	**611**	20	**834**	33	**837**	35
14	**663**	15	**698**	8	**671**	18	**551**	9	**649**	12	**694**	12	**773**	21	**718**	15	**726**	62	**890**	30	**757**	17
15	**648**	13	**740**	44	**704**	52	**550**	8	**648**	15	**717**	7	**762**	21	**702**	21	**709**	22	**993**	19	**810**	28
16	**636**	11	**719**	17	**681**	12	**582**	4	**665**	27	**698**	35	**785**	20	**727**	12	**808**	63	**884**	33	**746**	12
LoD	0,1		0,1		0,1		0,1		0,1		0,1		0,0		0,2		0,0		0,1		0,1	
LoQ	0,2		0,3		0,3		0,2		0,2		0,2		0,0		0,6		0,1		0,1		0,3	

Table A1. 11: Arsenic concentration in across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth \ day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**0,807**	0,02	**1,139**	0,05	**2,300**	0,08	**1,124**	0,03	**0,762**	0,04	**0,757**	0,03	**0,622**	0,03	**0,345**	0,02	**0,558**	0,04	**0,487**	0,03	**0,481**	0,02
-4	**0,913**	0,04	**1,061**	0,03	**2,170**	0,07	**1,064**	0,07	**0,767**	0,02	**0,710**	0,03	**0,626**	0,05	**0,319**	0,02	**0,480**	0,03	**0,416**	0,04	**0,461**	0,02
-3	**0,884**	0,09	**0,924**	0,02	**1,881**	0,08	**0,920**	0,04	**0,706**	0,02	**0,697**	0,03	**0,637**	0,02	**0,257**	0,02	**0,390**	0,02	**0,374**	0,03	**0,513**	0,02
-2	**0,839**	0,05	**0,913**	0,05	**1,776**	0,04	**0,917**	0,04	**0,778**	0,04	**0,610**	0,04	**0,614**	0,01	**0,267**	0,01	**0,338**	0,03	**0,308**	0,02	**0,465**	0,03
-1	**0,857**	0,03	**0,922**	0,03	**1,725**	0,06	**0,948**	0,02	**0,729**	0,05	**0,643**	0,03	**0,593**	0,03	**0,253**	0,01	**0,294**	0,01	**0,282**	0,04	**0,496**	0,04
0	**0,958**	0,02	**0,857**	0,04	**1,572**	0,05	**0,903**	0,04	**0,712**	0,02	**0,651**	0,04	**0,563**	0,02	**0,316**	0,01	**0,285**	0,02	**0,267**	0,03	**0,532**	0,03
1	**0,911**	0,02	**1,103**	0,05	**2,592**	0,04	**0,913**	0,05	**1,321**	0,04	**0,986**	0,08	**1,158**	0,06	**0,298**	0,02	**0,218**	0,02	**0,586**	0,03	**0,798**	0,03
2	**1,089**	0,05	**1,454**	0,11	**3,297**	0,04	**1,482**	0,05	**2,470**	0,08	**2,522**	0,03	**2,799**	0,07	**0,284**	0,02	**0,448**	0,03	**1,204**	0,05	**0,612**	0,01
3	**1,529**	0,07	**1,832**	0,04	**3,170**	0,54	**2,928**	0,04	**2,140**	0,07	**2,752**	0,11	**2,692**	0,09	**0,894**	0,05	**1,133**	0,04	**1,900**	0,08	**0,786**	0,04
4	**1,708**	0,07	**1,978**	0,06	**2,638**	0,08	**2,697**	0,04	**1,948**	0,04	**2,540**	0,06	**2,408**	0,06	**1,089**	0,07	**1,262**	0,03	**2,051**	0,15	**0,600**	0,03
5	**1,675**	0,04	**1,941**	0,07	**2,320**	0,14	**2,462**	0,09	**1,793**	0,08	**2,365**	0,06	**2,093**	0,04	**1,257**	0,02	**1,318**	0,05	**2,277**	0,11	**1,035**	0,06
6	**0,995**	0,06	**1,871**	0,06	**2,170**	0,04	**2,239**	0,09	**1,699**	0,06	**2,317**	0,08	**1,932**	0,04	**1,302**	0,05	**1,304**	0,05	**2,304**	0,07	**1,159**	0,05
7	**0,866**	0,06	**1,823**	0,07	**2,310**	0,05	**2,204**	0,07	**1,753**	0,15	**2,138**	0,09	**1,835**	0,05	**1,305**	0,05	**1,287**	0,00	**2,156**	0,15	**1,148**	0,07
8	**0,867**	0,05	**1,545**	0,06	**2,784**	0,11	**2,015**	0,03	**1,638**	0,07	**1,969**	0,08	**1,620**	0,05	**1,283**	0,09	**1,304**	0,02	**2,035**	0,09	**1,101**	0,05
9	**0,779**	0,03	**1,463**	0,02	**2,704**	0,06	**1,819**	0,05	**1,593**	0,05	**1,776**	0,11	**1,531**	0,07	**1,217**	0,03	**1,287**	0,05	**1,848**	0,02	**1,031**	0,02
10	**0,788**	0,05	**1,394**	0,06	**2,696**	0,11	**1,793**	0,06	**1,546**	0,02	**1,770**	0,08	**1,493**	0,05	**1,188**	0,04	**1,201**	0,01	**1,734**	0,10	**0,946**	0,04
11	**0,711**	0,02	**1,316**	0,02	**2,477**	0,03	**1,850**	0,12	**1,473**	0,03	**1,785**	0,06	**1,360**	0,04	**1,110**	0,03	**1,114**	0,01	**1,719**	0,05	**0,860**	0,01
12	**0,652**	0,03	**1,318**	0,03	**2,157**	0,04	**1,761**	0,07	**1,505**	0,21	**1,723**	0,06	**1,366**	0,12	**1,081**	0,03	**1,110**	0,08	**1,544**	0,06	**0,858**	0,02
13	**0,681**	0,02	**1,209**	0,05	**2,033**	0,07	**1,684**	0,04	**1,425**	0,07	**1,736**	0,07	**1,151**	0,03	**1,015**	0,05	**1,042**	0,05	**1,278**	0,05	**0,880**	0,04
14	**0,588**	0,01	**1,208**	0,03	**1,873**	0,07	**1,644**	0,04	**1,391**	0,03	**1,654**	0,09	**1,122**	0,04	**1,033**	0,03	**1,062**	0,09	**1,358**	0,05	**0,803**	0,03
15	**0,570**	0,02	**1,215**	0,07	**1,908**	0,14	**1,673**	0,02	**1,351**	0,06	**1,624**	0,04	**1,049**	0,04	**0,982**	0,03	**1,044**	0,04	**1,259**	0,04	**0,797**	0,04
16	**0,568**	0,04	**1,123**	0,04	**2,250**	0,08	**1,630**	0,04	**1,307**	0,06	**1,559**	0,08	**1,061**	0,04	**0,929**	0,03	**1,030**	0,08	**1,306**	0,05	**0,724**	0,02
LoD	0,103		0,027		0,027		0,044		0,044		0,044		0,017		0,189		0,017		0,037		0,011	
LoQ	0,198		0,072		0,072		0,124		0,124		0,124		0,044		0,510		0,042		0,104		0,029	

Table A1. 12: Cobalt concentration across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth \ day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**0,738**	0,01	**0,725**	0,02	**0,804**	0,03	**0,885**	0,01	**0,696**	0,03	**0,707**	0,02	**0,877**	0,02	**3,590**	0,07	**4,935**	0,04	**4,729**	0,11	**8,040**	0,04
-4	**0,793**	0,03	**0,701**	0,02	**0,983**	0,02	**0,828**	0,02	**0,703**	0,02	**0,675**	0,02	**0,900**	0,03	**3,638**	0,14	**4,860**	0,03	**4,812**	0,08	**8,108**	0,06
-3	**0,688**	0,07	**0,684**	0,02	**0,992**	0,02	**0,751**	0,02	**0,683**	0,03	**0,676**	0,04	**0,874**	0,02	**3,623**	0,13	**4,844**	0,10	**4,954**	0,03	**8,250**	0,12
-2	**0,525**	0,03	**0,698**	0,02	**1,013**	0,02	**0,723**	0,02	**0,710**	0,01	**0,704**	0,02	**0,860**	0,01	**3,731**	0,08	**4,782**	0,06	**5,000**	0,03	**8,327**	0,08
-1	**0,454**	0,01	**0,682**	0,02	**1,031**	0,03	**0,778**	0,01	**0,689**	0,02	**0,722**	0,04	**0,877**	0,02	**3,842**	0,07	**4,790**	0,05	**5,366**	0,07	**8,495**	0,09
0	**0,471**	0,03	**0,647**	0,02	**1,162**	0,02	**0,753**	0,02	**0,708**	0,02	**0,736**	0,02	**0,855**	0,02	**3,863**	0,07	**4,811**	0,04	**5,541**	0,07	**8,529**	0,12
1	**0,490**	0,01	**1,782**	0,05	**1,462**	0,01	**0,751**	0,03	**1,160**	0,05	**1,355**	0,05	**1,216**	0,04	**3,697**	0,12	**4,561**	0,04	**4,888**	0,04	**5,451**	0,05
2	**1,839**	0,08	**1,980**	0,10	**0,989**	0,03	**1,343**	0,04	**1,015**	0,02	**1,214**	0,03	**0,907**	0,01	**1,621**	0,03	**1,871**	0,02	**1,631**	0,05	**0,966**	0,02
3	**1,212**	0,06	**1,315**	0,03	**0,725**	0,03	**1,002**	0,02	**0,803**	0,03	**0,950**	0,03	**0,818**	0,02	**0,585**	0,01	**0,745**	0,01	**0,762**	0,02	**0,467**	0,01
4	**0,836**	0,04	**1,147**	0,01	**0,668**	0,01	**0,774**	0,01	**0,797**	0,03	**0,911**	0,01	**0,829**	0,03	**0,585**	0,03	**0,667**	0,02	**0,923**	0,07	**0,412**	0,01
5	**0,584**	0,03	**1,061**	0,02	**0,687**	0,02	**0,704**	0,01	**0,830**	0,02	**0,906**	0,03	**0,864**	0,01	**0,697**	0,03	**0,837**	0,01	**1,065**	0,03	**0,888**	0,00
6	**0,606**	0,05	**1,002**	0,05	**0,699**	0,02	**0,762**	0,02	**0,827**	0,03	**0,908**	0,02	**0,918**	0,01	**0,809**	0,02	**0,945**	0,03	**1,176**	0,01	**1,074**	0,02
7	**0,522**	0,04	**0,976**	0,02	**0,622**	0,01	**0,791**	0,04	**0,854**	0,07	**0,917**	0,05	**0,915**	0,01	**0,837**	0,02	**1,060**	0,01	**1,218**	0,02	**1,169**	0,01
8	**0,539**	0,03	**0,996**	0,05	**0,464**	0,01	**0,615**	0,02	**0,828**	0,04	**0,885**	0,03	**0,899**	0,03	**0,884**	0,03	**1,145**	0,01	**1,271**	0,02	**1,246**	0,02
9	**0,541**	0,01	**1,020**	0,03	**0,506**	0,01	**0,570**	0,02	**0,827**	0,02	**0,861**	0,04	**0,921**	0,02	**0,898**	0,01	**1,227**	0,02	**1,237**	0,02	**1,354**	0,01
10	**0,612**	0,04	**1,034**	0,02	**0,511**	0,01	**0,633**	0,01	**0,831**	0,00	**0,889**	0,03	**0,911**	0,02	**0,895**	0,02	**1,282**	0,01	**1,273**	0,02	**1,421**	0,01
11	**0,541**	0,02	**1,051**	0,01	**0,547**	0,01	**0,680**	0,04	**0,811**	0,02	**0,900**	0,03	**0,920**	0,02	**0,855**	0,02	**1,307**	0,01	**1,366**	0,02	**1,421**	0,01
12	**0,506**	0,02	**1,037**	0,04	**0,754**	0,01	**0,667**	0,01	**0,803**	0,04	**0,894**	0,02	**0,937**	0,08	**0,875**	0,01	**1,311**	0,01	**1,329**	0,02	**1,387**	0,03
13	**0,591**	0,02	**0,992**	0,03	**0,810**	0,01	**0,583**	0,01	**0,812**	0,04	**0,896**	0,01	**0,883**	0,02	**0,851**	0,03	**1,275**	0,02	**1,135**	0,02	**1,372**	0,02
14	**0,628**	0,02	**1,035**	0,02	**0,827**	0,01	**0,590**	0,01	**0,810**	0,01	**0,859**	0,02	**0,906**	0,03	**0,871**	0,02	**1,359**	0,10	**1,329**	0,02	**1,462**	0,01
15	**0,613**	0,02	**1,066**	0,04	**0,853**	0,01	**0,596**	0,01	**0,817**	0,03	**0,891**	0,02	**0,895**	0,02	**0,885**	0,03	**1,293**	0,01	**1,255**	0,02	**1,540**	0,03
16	**0,593**	0,02	**1,032**	0,02	**0,669**	0,02	**0,648**	0,01	**0,829**	0,03	**0,872**	0,05	**0,924**	0,03	**0,917**	0,01	**1,338**	0,12	**1,286**	0,03	**1,550**	0,01
LoD	0,033		0,018		0,018		0,012		0,012		0,012		0,009		0,014		0,001		0,001		0,003	
LoQ	0,035		0,052		0,052		0,032		0,032		0,032		0,021		0,038		0,003		0,003		0,007	

Table A1. 13: Copper concentration across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth / day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**4,66**	0,10	**2,44**	0,12	**0,70**	0,03	**2,43**	0,03	**1,19**	0,02	**1,24**	0,02	**2,21**	0,02	**188,56**	0,60	**4,56**	0,03	**11,60**	0,13	**159,54**	1,11
-4	**6,27**	0,12	**2,02**	0,05	**0,50**	0,02	**2,53**	0,02	**1,23**	0,02	**1,12**	0,02	**2,25**	0,03	**220,84**	1,31	**8,82**	0,12	**83,54**	0,64	**160,32**	4,56
-3	**6,43**	0,46	**1,80**	0,07	**0,63**	0,01	**1,74**	0,03	**1,39**	0,03	**1,17**	0,02	**2,32**	0,04	**232,56**	1,47	**40,08**	0,68	**150,21**	2,00	**168,29**	2,62
-2	**5,76**	0,20	**2,23**	0,05	**0,99**	0,03	**1,85**	0,04	**1,52**	0,02	**1,26**	0,02	**2,30**	0,11	**240,88**	0,53	**118,76**	0,61	**174,15**	0,53	**176,11**	2,42
-1	**5,66**	0,10	**2,74**	0,06	**1,40**	0,04	**2,26**	0,05	**1,62**	0,03	**1,37**	0,04	**2,25**	0,03	**252,15**	1,96	**177,96**	1,37	**206,79**	1,69	**191,89**	5,75
0	**6,71**	0,37	**3,15**	0,11	**1,68**	0,03	**2,50**	0,02	**1,80**	0,16	**1,47**	0,06	**2,43**	0,03	**258,35**	2,35	**199,52**	0,68	**226,33**	1,29	**203,16**	1,94
1	**6,64**	0,16	**2,90**	0,10	**0,95**	0,07	**2,82**	0,05	**1,16**	0,03	**1,11**	0,02	**1,66**	0,02	**288,76**	3,92	**179,94**	1,08	**153,30**	0,71	**79,83**	1,66
2	**3,79**	0,07	**1,33**	0,08	**0,33**	0,01	**1,91**	0,03	**0,45**	0,01	**0,73**	0,02	**0,57**	0,02	**53,30**	0,22	**24,41**	0,40	**39,59**	1,06	**2,02**	0,04
3	**0,71**	0,03	**0,47**	0,04	**0,19**	0,00	**0,70**	0,01	**0,18**	0,01	**0,37**	0,02	**0,25**	0,02	**2,44**	0,03	**12,01**	0,06	**8,09**	0,11	**0,67**	0,02
4	**0,31**	0,01	**0,23**	0,01	0,11	0,00	**0,42**	0,02	<LoD		**0,24**	0,01	**0,17**	0,01	**1,21**	0,01	**2,77**	0,05	**2,48**	0,16	**1,13**	0,02
5	**0,52**	0,08	**0,20**	0,02	0,10	0,01	**0,32**	0,02	<LoD		**0,19**	0,01	**0,12**	0,00	**0,64**	0,01	**1,29**	0,02	**2,67**	0,04	**0,70**	0,00
6	**0,14**	0,03	**0,29**	0,02	0,12	0,01	**0,26**	0,01	<LoD		**0,34**	0,01	**0,09**	0,00	0,30	0,01	**1,08**	0,01	**1,77**	0,02	**0,48**	0,01
7	**0,16**	0,05	0,09	0,01	0,12	0,01	**0,32**	0,01	<LoD		**0,17**	0,02	**0,08**	0,01	<LoD		**0,96**	0,01	**1,55**	0,03	**0,42**	0,02
8	**0,11**	0,02	<LoD		0,10	0,00	**0,16**	0,01	<LoD		**0,12**	0,01	**0,08**	0,00	<LoD		**0,60**	0,02	**0,71**	0,01	**0,31**	0,01
9	**0,09**	0,01	<LoD		**0,13**	0,00	**0,14**	0,01	<LoD		**0,13**	0,01	**0,08**	0,00	0,28	0,01	**0,46**	0,01	**0,54**	0,02	**0,33**	0,01
10	**0,09**	0,02	<LoD		0,08	0,00	**0,11**	0,01	<LoD		**0,13**	0,01	**0,09**	0,00	**0,84**	0,03	**0,52**	0,01	**0,47**	0,03	**0,25**	0,01
11	**0,11**	0,01	<LoD		**0,13**	0,00	**0,14**	0,01	<LoD		**0,13**	0,01	**0,10**	0,01	0,28	0,00	**0,16**	0,00	**0,80**	0,02	**0,20**	0,01
12	**0,08**	0,01	<LoD		0,11	0,00	**0,12**	0,00	<LoD		**0,11**	0,01	**0,08**	0,01	<LoD		**0,15**	0,00	**0,73**	0,02	**0,16**	0,01
13	**0,06**	0,00	<LoD	0,11	0,00	<LoD			<LoD		**0,12**	0,01	**0,07**	0,00	<LoD		**0,18**	0,01	**0,38**	0,02	**0,24**	0,02
14	**0,07**	0,01	<LoD		0,07	0,00	**0,11**	0,01	<LoD		**0,13**	0,01	**0,07**	0,00	<LoD		**0,40**	0,02	**0,34**	0,01	**0,56**	0,03
15	**0,07**	0,01	<LoD		0,07	0,00	**0,13**	0,01	<LoD		**0,14**	0,01	**0,07**	0,00	<LoD		**0,20**	0,01	**3,56**	0,11	**0,29**	0,02
16	**0,06**	0,01	<LoD		0,09	0,00	**0,11**	0,00	<LoD		**0,15**	0,01	**0,07**	0,00	<LoD		**0,25**	0,03	**0,39**	0,01	**0,15**	0,01
LoD	0,02		0,04		0,04		0,05		0,05		0,05		0,01		0,17		0,02		0,01		0,02	
LoQ	0,04		0,13		0,13		0,11		0,11		0,11		0,02		0,47		0,04		0,02		0,05	

Table A1. 14: Zink concentration across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth / day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**118,3**	2,36	**61,39**	1,97	**8,85**	0,28	**21,21**	0,50	**36,81**	1,23	**53,51**	0,90	**103,1**	2,50	**368,9**	6,70	**478,3**	2,10	**462,9**	6,67	**596,2**	7,90
-4	**144,9**	5,62	**69,71**	2,36	**10,66**	0,29	**22,13**	0,61	**52,84**	2,04	**63,91**	2,29	**120,6**	4,05	**361,8**	9,93	**512,7**	4,02	**480,5**	4,44	**611,2**	20,24
-3	**136,0**	10,92	**70,94**	1,91	**5,67**	0,16	**25,42**	0,72	**58,01**	2,34	**67,87**	2,18	**122,7**	2,27	**357,1**	9,37	**527,3**	8,05	**485,1**	6,69	**631,6**	9,50
-2	**114,2**	5,86	**71,56**	2,25	**8,28**	0,16	**26,10**	0,75	**59,35**	1,45	**68,92**	2,08	**123,3**	2,21	**356,1**	7,67	**533,5**	3,30	**495,4**	1,15	**639,3**	9,12
-1	**105,6**	1,15	**77,17**	1,89	**11,03**	0,26	**32,56**	0,46	**59,04**	1,41	**72,05**	2,80	**126,5**	3,31	**366,1**	6,95	**553,2**	64,03	**529,6**	4,84	**680,4**	17,00
0	**120,9**	6,29	**84,21**	5,93	**14,83**	0,32	**33,46**	1,03	**65,43**	6,25	**77,46**	2,85	**125,3**	3,04	**364,4**	9,19	**515,5**	3,46	**556,5**	4,80	**682,0**	6,18
1	**130,2**	3,68	**129,97**	8,27	**31,20**	0,95	**39,64**	1,18	**91,90**	3,70	**102,5**	4,02	**146,8**	4,18	**401,8**	13,68	**486,3**	3,63	**486,8**	2,49	**365,8**	7,81
2	**144,3**	4,22	**87,64**	5,42	**16,76**	0,31	**61,73**	2,47	**43,02**	1,19	**46,36**	0,57	**47,27**	0,79	**139,2**	2,81	**147,0**	0,94	**193,0**	4,05	**34,0**	0,70
3	**58,58**	2,25	**28,67**	0,22	**6,88**	0,15	**22,09**	0,39	**11,51**	0,39	**9,32**	0,30	**9,71**	0,21	**9,71**	0,27	**9,20**	0,13	**8,74**	0,17	**85,03**	3,03
4	**25,32**	0,95	**16,32**	0,39	**2,19**	0,03	**4,15**	0,09	**6,76**	0,13	**2,08**	0,06	**3,72**	0,08	**3,32**	0,19	**2,31**	0,03	<LoD		**3,17**	0,09
5	**13,99**	0,41	**8,74**	0,16	**3,07**	0,11	**0,76**	0,02	**8,32**	0,24	**1,59**	0,06	**2,16**	0,05	**3,54**	0,10	<LoD		**15,29**	0,20	**2,88**	0,06
6	**6,68**	0,38	**6,52**	0,29	**10,22**	0,26	**0,05**	0,02	**3,95**	0,08	**0,36**	0,01	**2,41**	0,06	**4,51**	0,13	<LoD		**0,92**	0,04	**1,95**	0,08
7	**2,93**	0,24	**3,48**	0,08	**4,05**	0,13	**8,15**	0,34	**1,14**	0,10	**0,97**	0,07	**1,44**	0,04	**3,31**	0,11	**1,00**	0,02	**11,07**	0,17	**8,86**	0,28
8	**1,85**	0,09	**2,71**	0,12	**5,19**	0,25	<LoD		**4,55**	0,23	**0,75**	0,01	**1,76**	0,05	**0,88**	0,03	<LoD		**4,69**	0,08	**0,76**	0,03
9	**1,81**	0,08	**5,13**	0,18	**4,30**	0,12	<LoD		**2,45**	0,07	**3,88**	0,15	**2,56**	0,11	**48,08**	0,81	**5,94**	0,16	**1,65**	0,03	**0,29**	0,01
10	**1,19**	0,07	**0,49**	0,02	**1,36**	0,03	<LoD		**2,35**	0,06	**1,95**	0,10	**1,79**	0,05	**17,01**	0,30	<LoD		**1,10**	0,01	<LoD	
11	**0,66**	0,03	<LoD		**3,45**	0,07	**0,11**	0,01	**0,68**	0,02	**2,27**	0,06	**2,51**	0,07	**1,14**	0,04	<LoD		**18,83**	0,30	**6,27**	0,17
12	**0,37**	0,02	<LoD		**5,51**	0,13	<LoD		**1,85**	0,10	**0,70**	0,03	**1,65**	0,10	**0,96**	0,02	<LoD		**13,42**	0,13	**0,33**	0,01
13	**0,32**	0,01	<LoD		**2,79**	0,08	<LoD		**2,51**	0,11	**1,01**	0,02	**2,09**	0,07	**1,67**	0,09	**33,47**	0,38	<LoD		**3,45**	0,15
14	**0,32**	0,01	**1,10**	0,03	**0,47**	0,01	<LoD		**0,89**	0,02	**2,44**	0,05	**1,46**	0,06	**0,83**	0,02	**31,06**	2,45	<LoD		**2,69**	0,07
15	**0,34**	0,01	<LoD		**2,13**	0,16	<LoD		**3,03**	0,04	**1,28**	0,02	**1,21**	0,04	**1,75**	0,06	**17,84**	0,16	**11,80**	0,20	**0,79**	0,03
16	**1,44**	0,05	<LoD		**3,27**	0,10	<LoD		**1,74**	0,05	**1,48**	0,06	**1,39**	0,04	**2,41**	0,05	<LoD		**16,71**	0,43	**1,81**	0,04
LoD	0,13		0,03		0,03		0,02		0,02		0,02		0,04		0,30		0,69		0,02		0,04	
LoQ	0,23		0,09		0,09		0,05		0,05		0,05		0,09		0,79		1,33		0,06		0,11	

Table A1. 15: Molybdenum concentration across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth / day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**3,808**	0,039	**3,683**	0,059	**2,792**	0,157	**4,189**	0,052	**3,891**	0,079	**3,564**	0,042	**2,446**	0,015	<LoD		**0,491**	0,021	<LoD		<LoD	
-4	**4,497**	0,060	**3,668**	0,052	**2,846**	0,068	**3,342**	0,071	**3,911**	0,078	**3,447**	0,022	**2,421**	0,041	<LoD		**0,223**	0,014	<LoD		<LoD	
-3	**3,816**	0,239	**3,655**	0,125	**2,833**	0,029	**3,222**	0,041	**4,091**	0,380	**3,383**	0,039	**2,396**	0,071	<LoD		**0,150**	0,014	<LoD		<LoD	
-2	**3,052**	0,155	**3,742**	0,076	**2,898**	0,058	**3,110**	0,069	**3,898**	0,036	**3,268**	0,052	**2,335**	0,133	<LoD		**0,083**	0,009	<LoD		<LoD	
-1	**2,760**	0,038	**3,758**	0,080	**2,936**	0,096	**3,510**	0,076	**3,889**	0,130	**3,279**	0,049	**2,301**	0,031	<LoD		**0,000**		<LoD		<LoD	
0	**3,341**	0,195	**3,817**	0,157	**2,945**	0,039	**3,607**	0,062	**3,910**	0,325	**3,239**	0,064	**2,289**	0,049	<LoD		**0,217**	0,011	<LoD		<LoD	
1	**3,185**	0,111	**3,595**	0,121	**2,104**	0,049	**3,687**	0,047	**3,092**	0,078	**2,963**	0,060	**2,265**	0,041	<LoD		**0,074**	0,006	**0,314**	0,027	<LoD	
2	**2,188**	0,050	**2,015**	0,088	**0,757**	0,014	**2,997**	0,055	**1,176**	0,023	**1,482**	0,018	**1,352**	0,051	<LoD		**0,606**	0,013	**1,100**	0,057	**0,452**	0,017
3	**0,658**	0,015	**0,455**	0,012	**0,331**	0,013	**1,166**	0,047	**0,494**	0,013	**0,545**	0,026	**0,491**	0,017	<LoD		**0,595**	0,026	**0,832**	0,057	**0,530**	0,025
4	0,175	0,008	0,145	0,008	0,185	0,005	**0,445**	0,018	**0,259**	0,012	**0,283**	0,012	**0,258**	0,009	<LoD		**0,370**	0,007	**0,571**	0,067	**0,657**	0,032
5	**0,277**	0,009	<LoD	0,005	0,144	0,005	**0,232**	0,010	**0,176**	0,013	**0,224**	0,016	**0,140**	0,008	<LoD		**0,190**	0,009	**0,422**	0,021	**0,415**	0,021
6	<LoD	0,011	<LoD	0,006	0,133	0,004	**0,193**	0,014	<LoD		**0,198**	0,008	**0,101**	0,005	<LoD		**0,483**	0,015	**0,358**	0,018	<LoD	
7	<LoD	0,004	<LoD	0,004	**0,593**	0,021	<LoD		<LoD		**0,178**	0,004	**0,086**	0,004	<LoD		**0,370**	0,023	**0,346**	0,018	<LoD	
8	<LoD	0,002	<LoD	0,004	**0,728**	0,016	<LoD		<LoD		0,170	0,006	**0,075**	0,002	<LoD		**0,273**	0,009	**0,310**	0,021	<LoD	
9	<LoD	0,001	<LoD	0,002	**0,618**	0,025	<LoD		<LoD		<LoD		**0,081**	0,005	<LoD		**0,193**	0,012	**0,291**	0,020	<LoD	
10	<LoD	0,010	<LoD	0,002	**0,646**	0,020	<LoD		<LoD		<LoD		**0,079**	0,004	<LoD		**0,167**	0,006	<LoD		<LoD	
11	<LoD	0,003	<LoD	0,004	**0,590**	0,015	<LoD		<LoD		<LoD		**0,062**	0,005	<LoD		**0,202**	0,009	<LoD		<LoD	
12	<LoD	0,002	<LoD	0,003	0,204	0,007	<LoD		<LoD		<LoD		**0,055**	0,002	<LoD		**0,297**	0,013	<LoD		<LoD	
13	<LoD	0,002	<LoD	0,003	0,122	0,006	<LoD		<LoD		<LoD		**0,060**	0,003	<LoD		**0,171**	0,016	<LoD		<LoD	
14	<LoD	0,002	<LoD	0,003	0,116	0,003	<LoD		<LoD		<LoD		**0,047**	0,003	<LoD		**0,186**	0,014	<LoD		<LoD	
15	<LoD	0,003	<LoD	0,004	0,118	0,007	<LoD		<LoD		<LoD		0,034	0,001	<LoD		**0,187**	0,010	<LoD		<LoD	
16	<LoD	0,003	<LoD	0,002	0,556	0,020	<LoD		<LoD		<LoD		**0,046**	0,002	<LoD		**0,195**	0,020	<LoD		<LoD	
LoD	0,072		0,095		0,095		0,063		0,063		0,063		0,014		0,228		0,028		0,053		0,122	
LoQ	0,198		0,272		0,272		0,174		0,174		0,174		0,036		0,620		0,080		0,148		0,329	

Table A1. 16: Uranium concentration across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth / day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**0,438**	0,017	**0,366**	0,018	**0,535**	0,008	**0,439**	0,005	**0,187**	0,004	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
-4	**0,492**	0,003	**0,376**	0,004	**0,585**	0,007	**0,330**	0,002	**0,214**	0,001	<LoD		**0,024**	0,000	<LoD		<LoD		**0,012**	0,024	0,012	0,002
-3	**0,385**	0,003	**0,377**	0,014	**0,595**	0,024	**0,347**	0,004	**0,201**	0,003	<LoD		**0,030**	0,000	<LoD		<LoD		<LoD		<LoD	
-2	**0,368**	0,012	**0,371**	0,004	**0,624**	0,005	**0,289**	0,001	**0,190**	0,003	<LoD		**0,034**	0,005	<LoD		<LoD		<LoD		<LoD	
-1	**0,383**	0,006	**0,400**	0,021	**0,650**	0,005	**0,326**	0,003	**0,187**	0,003	<LoD		**0,032**	0,001	<LoD		<LoD		<LoD		<LoD	
0	**0,388**	0,006	**0,382**	0,022	**0,613**	0,017	**0,349**	0,007	**0,172**	0,002	<LoD		**0,032**	0,000	<LoD		<LoD		**0,017**	0,000	0,017	0,001
1	**0,348**	0,004	**0,293**	0,008	**0,309**	0,009	**0,337**	0,002	**0,162**	0,002	<LoD		**0,048**	0,001	<LoD		<LoD		**0,021**	0,002	**0,021**	0,002
2	**0,221**	0,003	**0,194**	0,007	**0,112**	0,003	**0,272**	0,001	**0,167**	0,003	**0,233**	0,001	**0,153**	0,003	**0,050**	0,001	**0,075**	0,002	**0,101**	0,003	**0,101**	0,003
3	**0,098**	0,002	**0,131**	0,005	**0,069**	0,002	**0,166**	0,003	**0,139**	0,005	**0,238**	0,005	**0,173**	0,002	**0,136**	0,002	**0,155**	0,002	**0,161**	0,003	**0,161**	0,003
4	**0,075**	0,002	**0,103**	0,002	<LoD		**0,141**	0,003	**0,111**	0,001	**0,214**	0,002	**0,165**	0,002	**0,157**	0,002	**0,116**	0,003	**0,183**	0,004	**0,183**	0,004
5	**0,039**	0,001	**0,079**	0,001	<LoD		**0,119**	0,003	<LoD		**0,164**	0,002	**0,120**	0,003	**0,132**	0,001	**0,091**	0,001	**0,177**	0,003	**0,177**	0,003
6	0,018	0,001	**0,066**	0,001	<LoD		<LoD		<LoD		**0,130**	0,002	**0,099**	0,001	**0,111**	0,002	**0,073**	0,001	**0,171**	0,004	**0,171**	0,004
7	0,013	0,001	<LoD		<LoD		<LoD		<LoD		**0,103**	0,001	**0,086**	0,000	**0,089**	0,001	**0,064**	0,001	**0,150**	0,004	**0,150**	0,004
8	0,013	0,000	<LoD		<LoD		<LoD		<LoD		<LoD		**0,072**	0,002	**0,067**	0,002	**0,056**	0,001	**0,131**	0,001	**0,131**	0,001
9	0,013	0,000	<LoD		<LoD		<LoD		<LoD		<LoD		**0,063**	0,000	**0,059**	0,002	**0,050**	0,002	**0,113**	0,002	**0,113**	0,002
10	0,015	0,000	<LoD		<LoD		<LoD		<LoD		<LoD		**0,049**	0,001	**0,117**	0,124	**0,045**	0,001	**0,100**	0,002	**0,100**	0,002
11	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,042**	0,001	0,046	0,001	**0,041**	0,001	**0,093**	0,002	**0,093**	0,002
12	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,035**	0,001	0,038	0,001	**0,036**	0,001	**0,080**	0,002	**0,080**	0,002
13	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,033**	0,001	0,032	0,001	**0,007**	0,005	**0,061**	0,002	**0,061**	0,002
14	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,031**	0,001	0,028	0,000	**0,021**	0,014	**0,065**	0,001	**0,065**	0,001
15	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,027**	0,000	<LoD		<LoD		**0,059**	0,000	**0,059**	0,002
16	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,027**	0,001	<LoD		**0,019**		**0,055**		**0,055**	0,002
LoD	0,012		0,020		0,020		0,034		0,034		0,034		**0,004**		0,018		0,002		0,002		0,007	
LoQ	0,035		0,061		0,061		0,102		0,102		0,102		0,009		0,048		0,004		0,006		0,019	

Table A1. 17: Vanadium concentration in across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth / day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**0,224**	0,004	**0,324**	0,010	**0,397**	0,017	**0,344**	0,006	**0,180**	0,010	**0,184**	0,007	**0,096**	0,006	<LoD		**0,021**	0,003	**0,026**	0,004	**0,020**	0,002
-4	**0,263**	0,006	**0,278**	0,011	**0,274**	0,013	**0,228**	0,009	**0,177**	0,007	**0,168**	0,006	**0,101**	0,005	<LoD		**0,048**	0,005	**0,025**	0,003	**0,020**	0,002
-3	**0,240**	0,022	**0,231**	0,008	**0,270**	0,009	**0,201**	0,006	**0,165**	0,012	**0,160**	0,005	**0,100**	0,004	<LoD		**0,050**	0,002	**0,019**	0,002	**0,019**	0,002
-2	**0,181**	0,012	**0,216**	0,007	**0,267**	0,008	**0,182**	0,007	**0,168**	0,003	**0,148**	0,006	**0,097**	0,005	<LoD		**0,050**	0,002	**0,022**	0,002	**0,019**	0,002
-1	**0,169**	0,004	**0,221**	0,005	**0,271**	0,010	**0,203**	0,006	**0,158**	0,006	**0,146**	0,009	**0,102**	0,003	<LoD		**0,046**	0,006	**0,023**	0,004	**0,019**	0,002
0	**0,201**	0,013	**0,199**	0,011	**0,253**	0,013	**0,190**	0,006	**0,155**	0,005	**0,146**	0,007	**0,092**	0,002	<LoD		**0,047**	0,004	**0,019**	0,002	**0,020**	0,002
1	**0,192**	0,006	**0,180**	0,015	**0,191**	0,005	**0,193**	0,005	**0,163**	0,014	**0,136**	0,004	**0,074**	0,002	<LoD		**0,057**	0,003	**0,024**	0,002	**0,016**	0,002
2	**0,094**	0,006	**0,083**	0,005	**0,162**	0,006	**0,162**	0,011	**0,176**	0,005	**0,154**	0,002	**0,097**	0,019	<LoD		**0,075**	0,005	**0,040**	0,004	**0,025**	0,002
3	**0,117**	0,005	**0,115**	0,006	**0,138**	0,006	**0,142**	0,006	**0,144**	0,008	**0,141**	0,005	**0,102**	0,005	<LoD		**0,096**	0,002	**0,057**	0,005	**0,042**	0,004
4	**0,152**	0,007	**0,170**	0,006	**0,130**	0,006	**0,140**	0,006	**0,140**	0,007	**0,147**	0,007	**0,116**	0,005	**0,082**	0,009	**0,111**	0,006	**0,085**	0,009	**0,039**	0,005
5	**0,150**	0,006	**0,189**	0,011	**0,133**	0,009	**0,135**	0,005	**0,143**	0,009	**0,147**	0,007	**0,132**	0,006	**0,117**	0,013	**0,116**	0,002	**0,133**	0,007	**0,074**	0,006
6	**0,158**	0,008	**0,198**	0,013	**0,123**	0,007	**0,132**	0,005	**0,145**	0,005	**0,146**	0,007	**0,143**	0,004	**0,135**	0,005	**0,242**	0,008	**0,168**	0,003	**0,116**	0,004
7	**0,124**	0,009	**0,187**	0,011	**0,118**	0,007	**0,132**	0,007	**0,154**	0,011	**0,146**	0,008	**0,153**	0,002	**0,143**	0,011	**0,224**	0,004	**0,201**	0,013	**0,132**	0,005
8	**0,118**	0,007	**0,175**	0,011	**0,106**	0,007	**0,121**	0,007	**0,154**	0,010	**0,154**	0,006	**0,171**	0,007	**0,144**	0,007	**0,199**	0,005	**0,186**	0,009	**0,134**	0,011
9	**0,112**	0,007	**0,163**	0,009	**0,104**	0,008	**0,120**	0,005	**0,153**	0,003	**0,155**	0,006	**0,185**	0,008	**0,140**	0,003	**0,152**	0,009	**0,180**	0,005	**0,144**	0,008
10	**0,121**	0,010	**0,156**	0,005	**0,108**	0,003	**0,126**	0,005	**0,153**	0,007	**0,166**	0,004	**0,194**	0,011	**0,140**	0,008	**0,141**	0,004	**0,200**	0,012	**0,132**	0,010
11	**0,104**	0,005	**0,159**	0,006	**0,109**	0,005	**0,133**	0,010	**0,156**	0,004	**0,185**	0,012	**0,204**	0,008	**0,156**	0,002	**0,131**	0,004	**0,279**	0,009	**0,127**	0,008
12	**0,102**	0,005	**0,160**	0,005	**0,122**	0,003	**0,132**	0,005	**0,156**	0,012	**0,192**	0,005	**0,205**	0,015	**0,183**	0,003	**0,126**	0,004	**0,270**	0,024	**0,109**	0,003
13	**0,122**	0,008	**0,150**	0,005	**0,123**	0,005	**0,124**	0,007	**0,158**	0,008	**0,202**	0,006	**0,199**	0,002	**0,192**	0,008	**0,124**	0,003	**0,214**	0,016	**0,098**	0,007
14	**0,127**	0,006	**0,146**	0,007	**0,126**	0,008	**0,123**	0,007	**0,166**	0,010	**0,195**	0,006	**0,198**	0,007	**0,232**	0,003	**0,188**	0,014	**0,230**	0,003	**0,121**	0,006
15	**0,126**	0,002	**0,151**	0,011	**0,135**	0,014	**0,127**	0,007	**0,166**	0,009	**0,203**	0,006	**0,195**	0,005	**0,203**	0,006	**0,154**	0,006	**0,337**	0,021	**0,131**	0,005
16	**0,135**	0,005	**0,145**	0,003	**0,111**	0,002	**0,134**	0,006	**0,176**	0,007	**0,204**	0,013	**0,206**	0,005	**0,281**	0,007	**0,171**	0,013	**0,236**	0,007	**0,138**	0,010
LoD	0,004		0,020		0,020		0,008		0,008		0,008		0,005		0,052		0,005		0,002		0,006	
LoQ	0,009		0,057		0,057		0,021		0,021		0,021		0,014		0,153		0,013		0,003		0,017	

Table A1. 18: Nickel concentration across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth \ day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**12,27**	0,17	**8,01**	0,24	**3,97**	0,12	**7,64**	0,10	**8,94**	0,21	**9,94**	0,09	**10,44**	0,30	**20,81**	0,08	**24,80**	0,20	**28,11**	0,31	**36,16**	0,33
-4	**14,08**	0,55	**11,28**	0,48	**5,00**	0,09	**7,38**	0,09	**9,66**	0,10	**10,54**	0,07	**11,43**	0,33	**20,61**	0,18	**24,87**	0,23	**26,44**	0,36	**36,13**	1,02
-3	**12,81**	1,04	**11,30**	0,28	**5,13**	0,11	**7,67**	0,03	**10,19**	0,95	**10,74**	0,06	**11,49**	0,22	**20,66**	0,09	**24,85**	0,52	**26,57**	0,05	**37,28**	0,62
-2	**10,63**	0,54	**11,12**	0,38	**5,23**	0,14	**7,58**	0,05	**9,89**	0,09	**10,61**	0,08	**11,35**	0,26	**20,61**	0,10	**24,29**	0,16	**25,87**	0,14	**37,75**	0,46
-1	**9,94**	0,15	**11,46**	0,28	**5,49**	0,18	**8,53**	0,08	**10,02**	0,18	**10,89**	0,08	**11,56**	0,24	**20,70**	0,18	**24,34**	0,16	**27,13**	0,25	**40,27**	1,15
0	**11,56**	0,68	**11,67**	0,79	**6,01**	0,09	**8,62**	0,09	**10,58**	0,87	**10,93**	0,05	**11,27**	0,29	**20,63**	0,17	**23,91**	0,17	**27,06**	0,22	**39,61**	0,47
1	**10,86**	0,23	**11,63**	0,72	**6,92**	0,20	**9,12**	0,11	**10,67**	0,12	**13,67**	0,21	**11,72**	0,33	**19,89**	0,19	**21,58**	0,16	**21,21**	0,12	**22,57**	0,50
2	**7,45**	0,33	**7,13**	0,36	**3,89**	0,08	**10,07**	0,09	**6,19**	0,01	**9,46**	0,07	**6,03**	0,08	**8,29**	0,02	**7,85**	0,07	**7,87**	0,16	**4,01**	0,05
3	**3,52**	0,20	**3,70**	0,05	**2,27**	0,03	**6,03**	0,10	**3,36**	0,04	**5,29**	0,04	**2,90**	0,07	**1,65**	0,01	**1,81**	0,03	**1,44**	0,04	**0,52**	0,03
4	**2,24**	0,11	**2,75**	0,07	**1,36**	0,02	**3,70**	0,06	**2,16**	0,05	**3,51**	0,01	**1,75**	0,05	**0,91**	0,01	**0,77**	0,01	**0,90**	0,05	**0,82**	0,03
5	**1,27**	0,04	**2,07**	0,06	**0,98**	0,07	**2,64**	0,02	**1,67**	0,03	**2,64**	0,03	**1,16**	0,02	**0,73**	0,01	**0,56**	0,01	**0,74**	0,03	**0,56**	0,02
6	**0,70**	0,04	**1,68**	0,05	**0,76**	0,02	**2,16**	0,04	**1,37**	0,02	**2,26**	0,02	**1,12**	0,03	**0,55**	0,01	**0,62**	0,02	**0,71**	0,02	**0,45**	0,02
7	**0,49**	0,04	**1,45**	0,04	**1,00**	0,02	**1,87**	0,02	**1,26**	0,10	**1,77**	0,03	**0,83**	0,02	**0,76**	0,01	**0,54**	0,01	**0,98**	0,02	**0,44**	0,01
8	**0,44**	0,02	**1,17**	0,05	**0,99**	0,05	**1,32**	0,09	**1,57**	0,02	**1,60**	0,03	**0,74**	0,03	**6,69**	0,03	**0,48**	0,01	**0,62**	0,03	**0,41**	0,01
9	**0,43**	0,01	**1,09**	0,04	**0,91**	0,03	**1,13**	0,03	**1,00**	0,03	**1,44**	0,10	**0,73**	0,02	**0,56**	0,01	**0,46**	0,01	**0,54**	0,01	**0,44**	0,01
10	**0,45**	0,03	**0,93**	0,03	**0,98**	0,03	**1,08**	0,01	**0,99**	0,01	**1,27**	0,03	**0,63**	0,02	**0,86**	0,02	**0,46**	0,01	**0,55**	0,01	**0,35**	0,02
11	**0,36**	0,01	**0,87**	0,02	**0,77**	0,02	**1,08**	0,04	**0,94**	0,02	**1,21**	0,02	**0,57**	0,02	**0,55**	0,01	**0,42**	0,00	**1,45**	0,02	**0,34**	0,02
12	**0,32**	0,01	**0,77**	0,02	**0,62**	0,01	**0,92**	0,02	**0,87**	0,03	**1,10**	0,01	**0,55**	0,05	**0,44**	0,01	**0,40**	0,01	**0,56**	0,01	**0,31**	0,01
13	**0,34**	0,01	**0,72**	0,04	**0,49**	0,01	**0,79**	0,02	**0,78**	0,02	**1,08**	0,03	**0,49**	0,02	**0,39**	0,00	**0,39**	0,01	**0,40**	0,01	**0,32**	0,01
14	**0,31**	0,01	**0,70**	0,01	**0,44**	0,01	**0,75**	0,02	**0,82**	0,02	**1,08**	0,03	**0,44**	0,01	**0,44**	0,01	**0,54**	0,03	**0,48**	0,01	**0,35**	0,01
15	**0,67**	0,01	**0,67**	0,04	**0,49**	0,02	**0,74**	0,01	**0,80**	0,01	**0,97**	0,02	**0,43**	0,03	**0,36**	0,01	**0,39**	0,01	**0,56**	0,01	**0,33**	0,01
16	**0,30**	0,01	**0,60**	0,02	**0,68**	0,01	**0,74**	0,02	**0,81**	0,03	**0,99**	0,02	**0,43**	0,02	**0,51**	0,01	**0,44**	0,04	**0,52**	0,02	**0,27**	0,00
LoD	0,00		0,02		0,02		0,13		0,13		0,13		0,03		0,09		0,02		0,00		0,01	
LoQ	0,01		0,06		0,06		0,28		0,28		0,28		0,06		0,19		0,04		0,00		0,02	

Table A1. 19: Silver concentration across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth \ day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**0,075**	0,004	**0,058**	0,001	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**1,065**	0,024
-4	**0,086**	0,007	**0,053**	0,004	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,140**	0,010	**0,766**	0,006
-3	**0,098**	0,031	**0,036**	0,001	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,164**	0,014	**0,584**	0,006
-2	**0,079**	0,010	**0,022**	0,001	0,012	0,002	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,168**	0,014	**0,496**	0,008
-1	**0,085**	0,012	**0,022**	0,003	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,159**	0,005	**0,115**	0,008	**0,485**	0,011
0	**0,079**	0,004	0,013	0,001	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,187**	0,005	**0,196**	0,009	**0,362**	0,004
1	**0,076**	0,002	0,013	0,001	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,203**	0,007	**1,505**	0,020	**0,418**	0,009
2	**0,048**	0,021	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,879**	0,008	**1,477**	0,006	**0,112**	0,004
3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,346**	0,006	<LoD		<LoD	
4	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,071**	0,005	<LoD		<LoD	
5	<LoD		<LoD		0,007	0,001	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
6	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
7	0,009	0,004	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
8	0,011	0,003	0,011	0,002	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
9	<LoD		0,015	0,002	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
10	0,010	0,002	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
11	0,010	0,001	0,007	0,001	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
12	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
13	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
14	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
15	<LoD		0,008	0,001	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
16	<LoD		**0,020**	0,001	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
LoD	0,009		0,006		0,006		0,041		0,041		0,041		0,048		0,062		0,033		0,025		0,012	
LoQ	0,023		0,017		0,017		0,123		0,123		0,123		0,102		0,160		0,077		0,046		0,028	

Table A1. 20: Cadmium concentration across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth \ day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**0,038**		<LoD		<LoD		**0,010**	0,009	**0,202**	0,009	0,003	0,001	**0,029**	0,003	**0,479**	0,011	**0,418**	0,019	**0,373**	0,014	**0,432**	0,006
-4	**0,084**		<LoD		<LoD		<LoD		**0,043**	0,003	**0,012**	0,002	**0,025**	0,002	**0,487**	0,042	**0,512**	0,020	**0,392**	0,018	**0,469**	0,031
-3	**0,103**		<LoD		<LoD		<LoD		**0,037**	0,007	0,006	0,001	**0,027**	0,002	**0,468**	0,017	**0,529**	0,010	**0,463**	0,028	**0,487**	0,021
-2	**0,091**	0,009	**0,043**	0,003	<LoD		<LoD		**0,026**	0,002	**0,016**	0,003	**0,026**	0,002	**0,461**	0,011	**0,536**	0,023	**0,479**	0,028	**0,491**	0,009
-1	**0,090**	0,002	**0,055**	0,004	<LoD		<LoD		**0,017**	0,004	**0,033**	0,001	**0,030**	0,004	**0,467**	0,014	**0,587**	0,052	**0,556**	0,026	**0,552**	0,025
0	**0,094**	0,004	**0,056**	0,006	<LoD		**0,011**	0,008	**0,041**	0,008	**0,098**	0,004	**0,033**	0,002	**0,466**	0,014	**0,567**	0,021	**0,611**	0,063	**0,583**	0,010
1	**0,109**	0,004	**0,072**	0,003	<LoD		**0,014**	0,003	**0,040**	0,003	**0,030**	0,003	**0,039**	0,004	**0,891**	0,021	**0,728**	0,027	**0,572**	0,027	**0,312**	0,011
2	**0,130**		0,034		<LoD		**0,017**	0,010	**0,274**	0,010	<LoD	0,000	<LoD		**0,402**	0,017	**0,325**	0,020	**0,092**	0,009	<LoD	
3	**0,035**		<LoD		<LoD		<LoD		**0,040**	0,003	<LoD		<LoD		<LoD		**0,021**	0,005	**0,011**	0,003	<LoD	
4	0,007		<LoD		<LoD		<LoD		**0,014**	0,003	0,009	0,001	<LoD		<LoD		**0,005**	0,002	<LoD		<LoD	
5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,016**	0,003
6	<LoD		<LoD		<LoD		<LoD		**0,010**	0,003	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
7	<LoD		<LoD		<LoD		<LoD		**0,015**	0,002	0,005	0,001	<LoD		<LoD		<LoD		<LoD		<LoD	
8	<LoD		<LoD		<LoD		<LoD		<LoD		**0,035**	0,001	<LoD		<LoD		<LoD		<LoD		<LoD	
9	<LoD		<LoD		<LoD		<LoD		**0,054**	0,002	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
10	<LoD		<LoD		<LoD		<LoD		**0,011**	0,002	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
11	<LoD		<LoD		<LoD		<LoD		**0,019**	0,003	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
12	<LoD		<LoD		<LoD		<LoD		**0,017**	0,005	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
13	<LoD		<LoD		<LoD		<LoD		0,003	0,002	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
14	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,004**	0,002	<LoD		<LoD	
15	<LoD		<LoD		<LoD		<LoD		**0,037**	0,004	<LoD		<LoD		<LoD		<LoD		**0,006**	0,003	<LoD	
16	<LoD		<LoD		<LoD		<LoD		**0,030**	0,003	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
LoD	0,006		0,013		0,013		0,003		0,003		0,003		0,005		0,011		0,001		0,001		0,002	
LoQ	0,017		0,037		0,037		0,007		0,007		0,007		0,013		0,028		0,003		0,003		0,006	

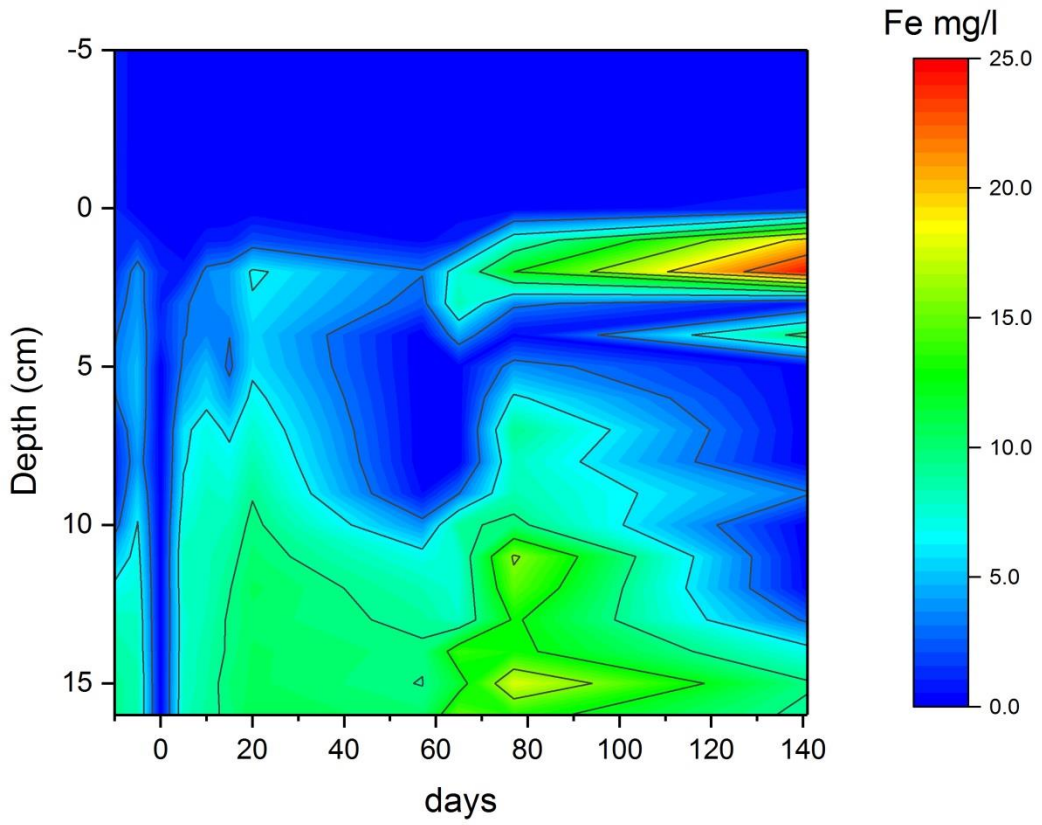


Figure A1. 5: Heatplot Iron concentration across the SWI (<16 µm) (values < LoD set to 0).

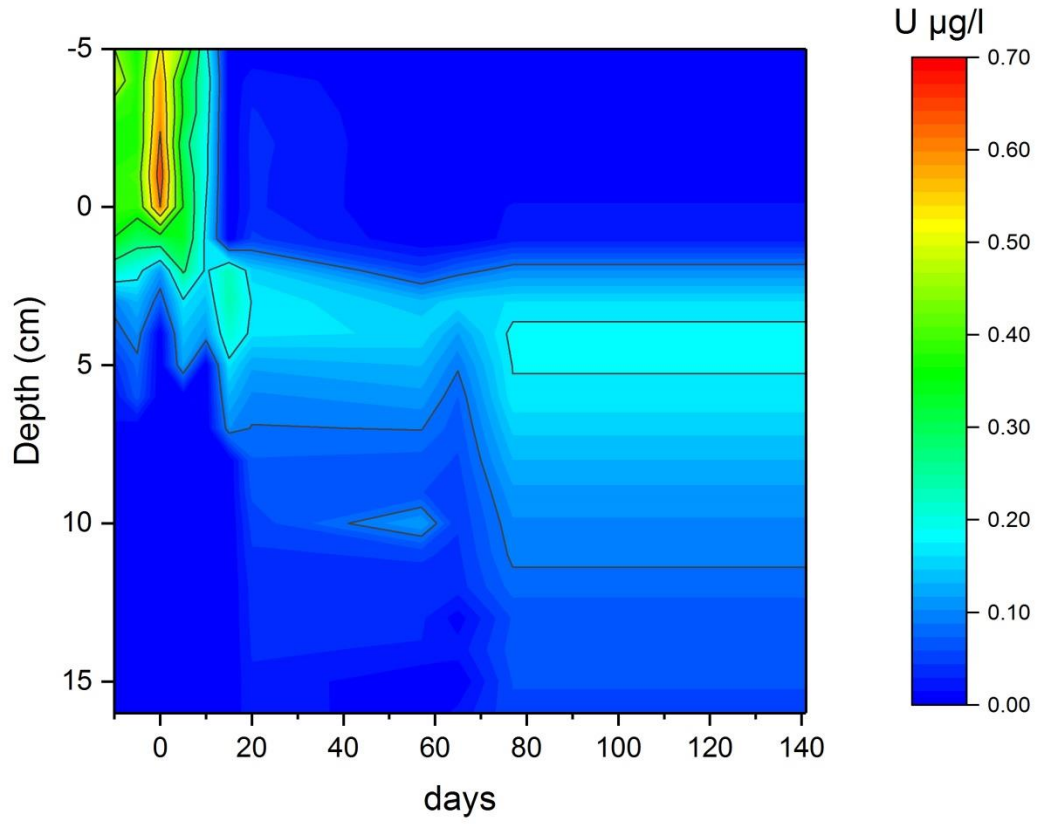


Figure A1. 6: Heatplot Uranium concentration across the SWI (<16 µm) (values <LoD set to 0).

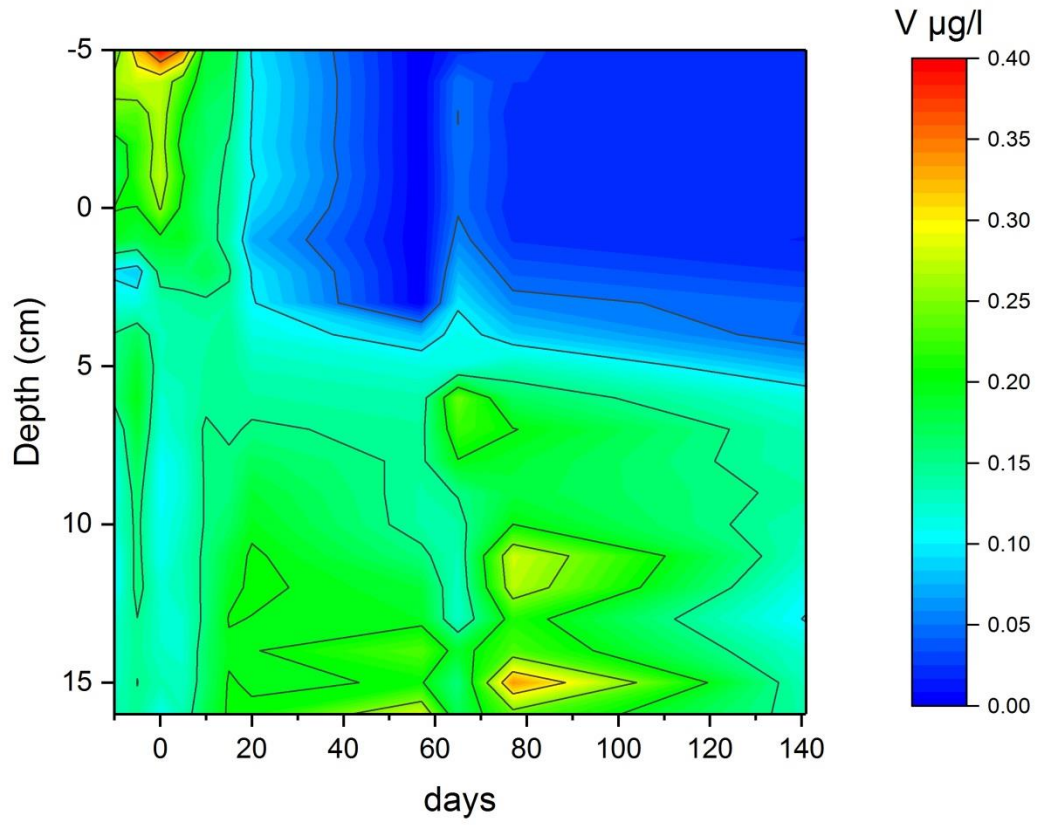


Figure A1. 7: Heatplot Vanadium concentration across the SWI (<16 µm) (values < LoD set to 0).

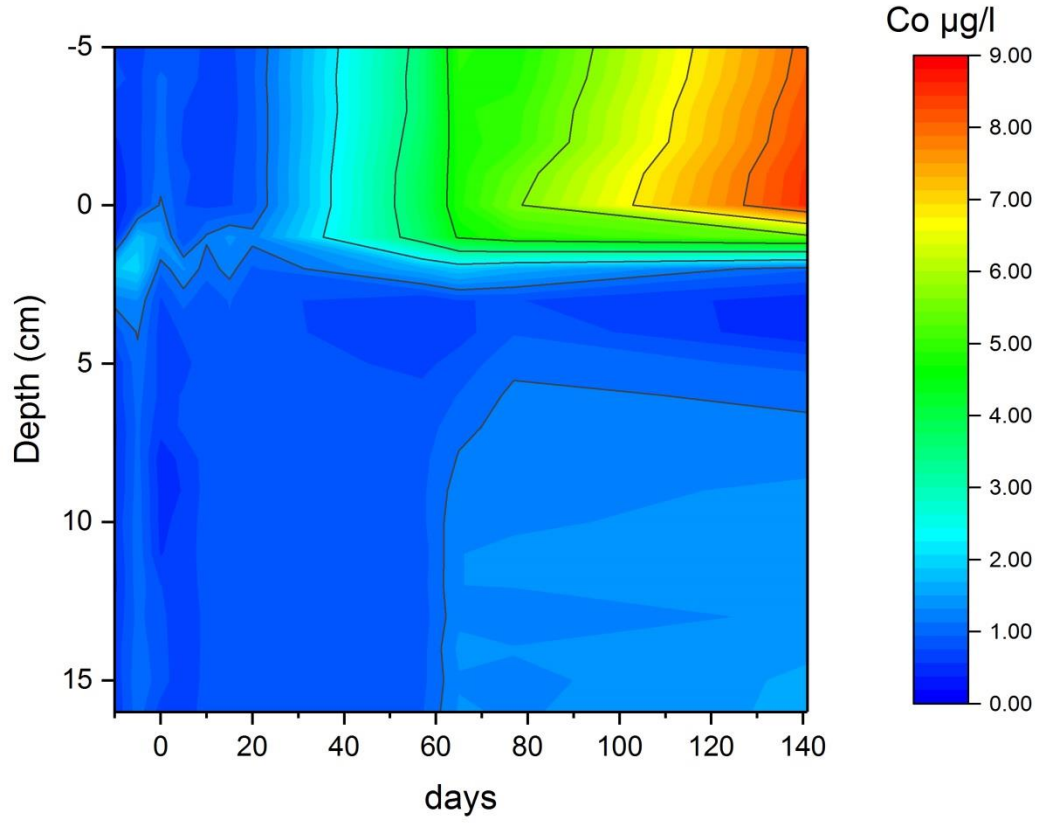


Figure A1. 8: Heatplot Cobalt concentration across the SWI (<16 µm) (values < LoD set to 0).

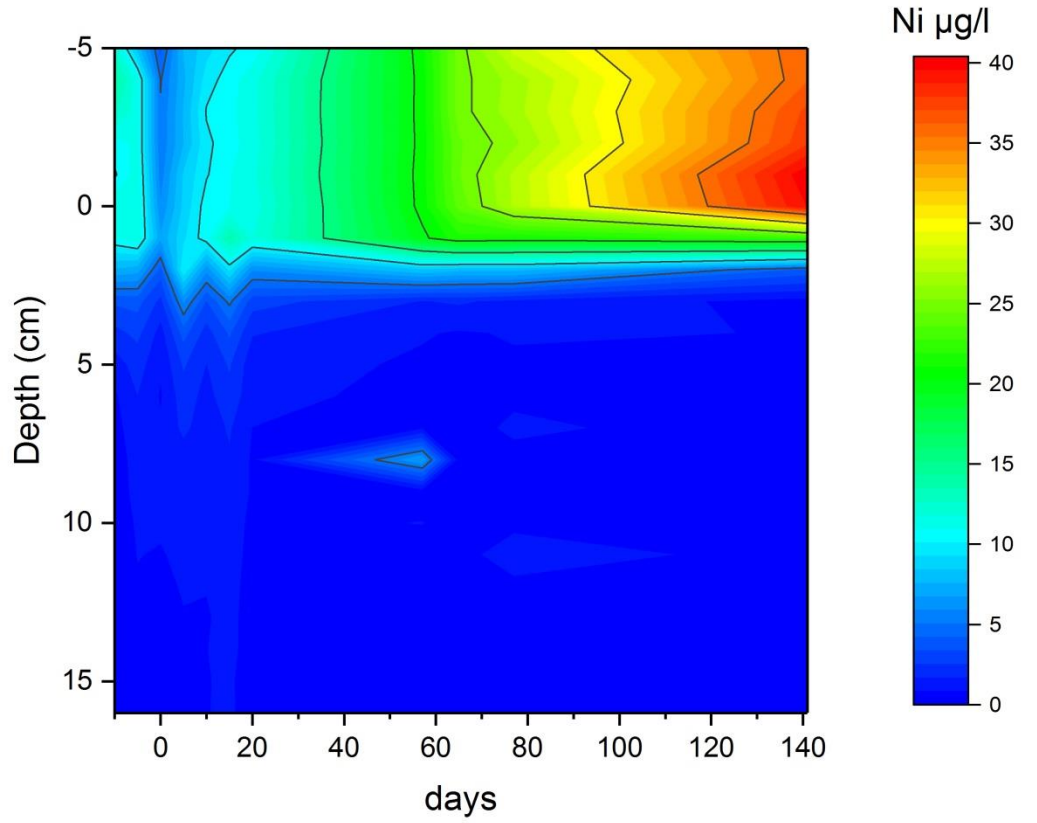


Figure A1. 9: Heatplot Nickel concentration across the SWI (<16 µm) (values < LoD set to 0).

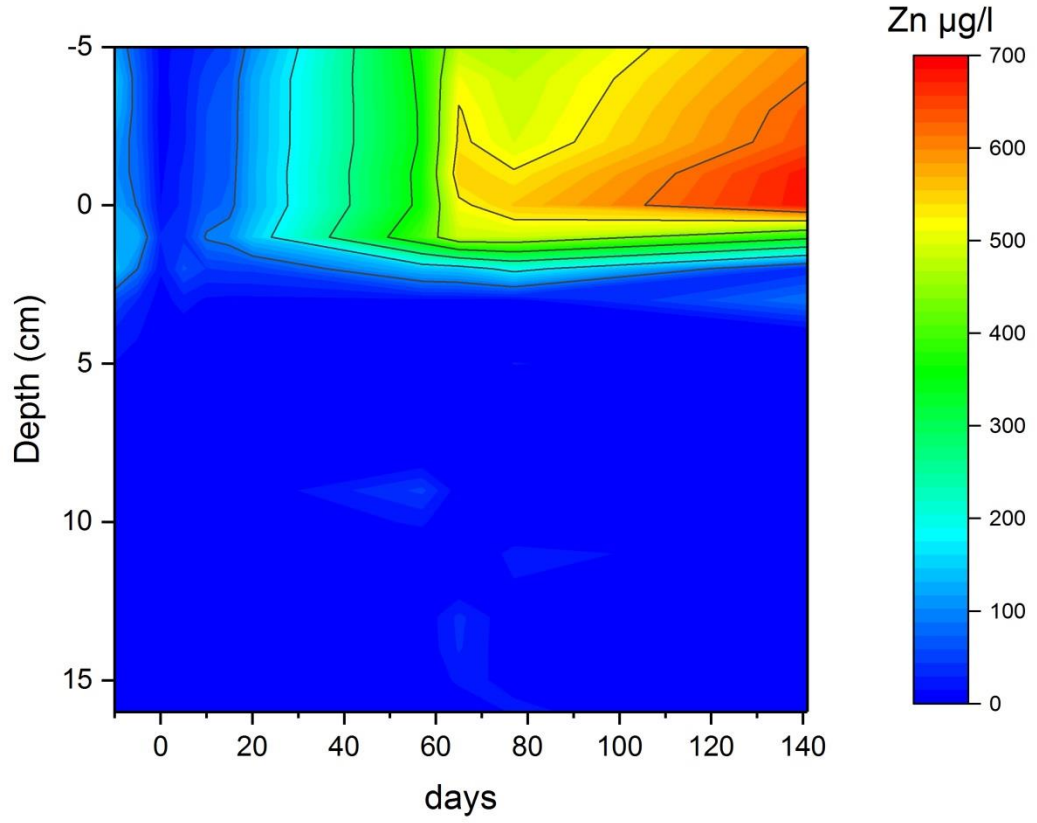


Figure A1. 10: Heatplot Zink concentration across the SWI (<16 µm) (values < LoD set to 0).

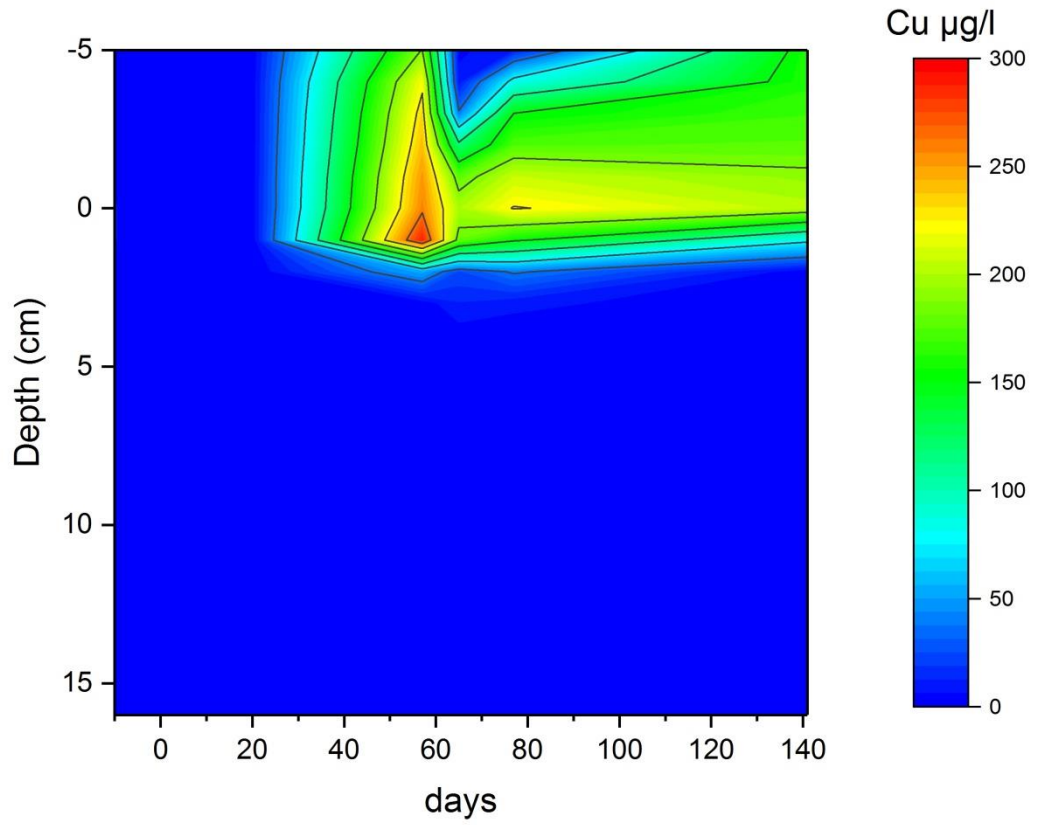


Figure A1. 11: Heatplot Copper concentration across the SWI (<16 µm) (values < LoD set to 0).

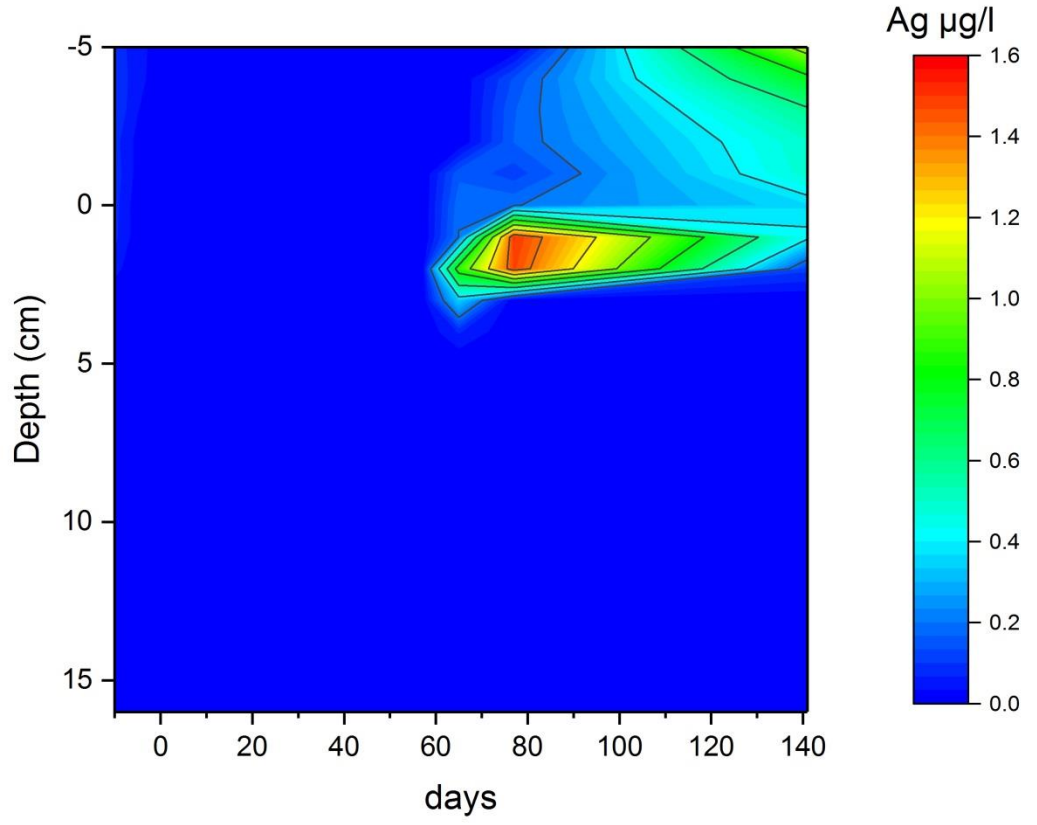


Figure A1. 12: Heatplot Silver concentration across the SWI (<16 µm) (values < LoD set to 0).

AI.VIII Spearman based correlations

Table A1. 21: Calculated Spearman Correlations

correlation factor	profiles 1-11	profile 1-4	profiles 8-11
>0.9		Cd/Zn, Co/Zn, Cd/Co, Ni/Zn,	
>0.8		Cu/Zn, Cu/Cd, Ni/Cd, Mn/Co, Cu/Co, Ni/Co, Mo/Sb	Cd/Zn, Ni/Zn, Cu/Cd, Ni/Cd, Ni/Cu
>0.7	Cd/Zn, Cu/Zn, Ni/Zn, Ni/Cd, Cu/Ni	Mn/Zn, NI/Cu, U/Sb	Mn/Zn, Cu/Zn, Co/Cd, Mn/Cd, Mn/Co, Cu/Mn, U/As, V/As
>0.6	Mn/Co, Cu/Cd Sb/Zn, Sb/Cu, Sb/Mo	Cu/Mn, Mo/U	Co/Zn, Ag/Cd, Ag/Mn, Ag/Ni, Sb/Mn
>0.5	Mo/U, Sb/Ni	Ag/Zn, Ag/Co, Ag/Mn, Ni/Mn, V/U	Ag/Zn, Ag/Co, Ag/Cu, Cu/Co, Ni/Co, V/Fe
<-0.5	Cd/As, Fe/Zn, Cu/As, Cu/Fe, Mo/Mn, Ni/Fe, Sb/Fe,	As/Zn, Mo/Mn, V/Co, V/Cu	Cu/As, Ni/As, U/Zn, V/Co, V/Ag
<-0.6		V/Zn, V/Cd, V/Mn	As/Zn, As/Co, As/Mn, U/Cd
<-0.7			As/Cd, U/Co, V/Zn, V/Cd, V/Mn, V/Cu, V/Ni

AI.IX Concentrations of As(III/V) and Sb(III/V)species in pore water samples

Table A1. 22: Arsenic (III) concentration across the SWI (<16 µm) and LoDs. Values <LoD were removed from the data set. All values in µg/L.

depth / day	-10	-5	0	5	10	15	20	57	65	77	141
-5	0,20	0,50	1,49	0,37	0,29	0,25	0,41	0,29	0,42	0,22	0,30
-4	0,24	0,44	1,26	0,32	0,29	0,24	0,30	0,29	0,42	0,21	0,37
-3	0,34	0,43	1,24	0,33	0,33	0,28	0,37	0,32	0,33	0,19	0,39
-2	0,32	0,47	0,78	0,42	0,19	0,31	0,39	0,33	0,25	0,11	0,38
-1	0,24	0,47	0,39	0,25	0,21	0,26	0,34	0,27	0,17	0,12	0,35
0	0,35	0,49	0,80	0,29	0,10	0,22	0,40	0,29	0,19	0,09	0,40
1	0,36	0,71	1,30	0,87	0,64	1,26	0,86	0,26	0,12	0,16	0,75
2	0,53	0,85	1,33	1,30	1,14	0,63	1,56	0,36	0,33	0,56	0,48
3	0,74	1,02	1,23	1,44	0,99	1,53	1,42	0,99	0,90	1,09	0,38
4	0,78	1,07	1,33	1,64	1,06	1,49	1,10	1,24	0,94	1,43	0,56
5	0,78	1,10	0,91	1,23	0,87	1,36	0,93	1,26	1,02	0,97	0,73
6	0,43	1,12	0,80	0,92	0,87	1,21	0,99	1,39	0,90	1,38	0,73
7	0,40	1,02	0,79	1,14	0,73	0,97	0,89	1,13	1,06	1,27	0,73
8	0,37	0,98	1,21	0,96	0,73	0,65	0,74	0,61	0,95	0,92	0,73
9	0,35	0,73	1,28	1,21	0,81	1,01	0,71	0,93	0,78	1,00	0,57
10	0,35	0,78	1,11	0,88	0,75	0,86	0,55	0,99	0,70	0,90	0,47
11	0,35	0,79	1,06	0,90	0,77	0,68	0,39	0,98	0,81	0,92	0,40
12	0,26	0,78	0,83	0,73	0,64	0,81	0,41	0,99	0,96	0,99	0,47
13	0,29	0,75	0,75	0,82	0,74	0,72	0,32	1,10	0,35	0,98	0,43
14	0,20	0,73	0,77	0,90	0,70	0,68	0,36	1,34	0,66	0,89	0,39
15	0,25	0,73	0,70	1,10	0,51	0,68	0,33	1,14	0,63	0,85	0,33
16	0,21	0,64	0,85	0,94	0,61	0,72	0,30	1,42	0,62	1,01	0,34
LoD	0,09	0,09	0,09	0,09	0,09	0,09	0,09	0,09	0,09	0,09	0,09

Table A1. 23: Arsenic (V) concentration across the SWI (<16 µm) and LoDs. Values <LoD were removed from the data set. All values in µg/L.

depth / day	-10	-5	0	5	10	15	20	57	65	77	141
-5	0,06	0,18	0,04	0,38	0,24	0,05	0,10	<LoD	<LoD	0,19	<LoD
-4	0,29	0,21	0,12	0,61	0,24	0,16	0,11	<LoD	<LoD	0,19	<LoD
-3	0,17	0,09	0,07	0,54	0,20	0,10	0,22	<LoD	<LoD	0,21	<LoD
-2	0,12	0,12	0,32	0,43	0,23	0,18	0,18	<LoD	<LoD	0,17	<LoD
-1	0,22	0,13	0,75	0,55	0,40	0,16	0,09	<LoD	<LoD	0,13	<LoD
0	0,14	0,07	0,09	0,52	0,25	0,14	0,11	<LoD	<LoD	0,10	<LoD
1	0,13	0,08	0,32	0,27	0,42	0,79	0,12	<LoD	<LoD	0,13	<LoD
2	0,10	0,21	0,98	1,20	1,05	0,16	0,91	<LoD	<LoD	0,16	<LoD
3	0,27	0,32	1,00	0,94	0,93	0,90	0,68	0,08	0,17	0,14	<LoD
4	0,27	0,27	0,56	0,57	0,47	0,47	0,46	0,08	0,19	0,12	<LoD
5	0,22	0,29	0,72	0,69	0,62	0,53	0,49	0,13	0,23	0,08	<LoD
6	0,18	0,16	0,68	0,70	0,70	0,42	0,41	0,23	0,15	0,12	0,19
7	0,06	0,19	0,77	0,52	0,60	0,47	0,40	0,36	0,15	0,09	0,22
8	0,06	0,16	0,79	0,67	0,51	0,35	0,34	0,80	0,13	0,07	0,19
9	0,07	0,12	0,70	0,41	0,50	0,55	0,33	0,39	0,17	0,07	0,17
10	0,05	0,11	0,91	0,59	0,54	0,39	0,44	0,50	0,18	0,05	0,12
11	0,05	0,09	0,70	0,45	0,46	0,32	0,41	0,42	0,30	0,08	0,07
12	<LoD	0,12	0,65	0,74	0,42	0,57	0,30	0,45	0,28	0,12	0,07
13	0,07	0,09	0,55	0,30	0,63	0,58	0,41	0,27	0,21	0,10	0,09
14	0,10	0,09	0,48	0,41	0,59	0,29	0,29	0,26	0,29	0,08	0,10
15	0,09	0,06	0,52	0,24	0,39	0,28	0,25	0,17	0,30	0,10	0,09
16	0,07	0,05	0,59	0,35	0,39	0,42	0,26	0,29	0,26	0,11	<LoD
LoD	0,04	0,04	0,04	0,04	0,04	0,04	0,04	0,04	0,04	0,04	0,04

Table A1. 24: Antimony concentration across the SWI (<16 µm) and LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

depth \ day	-10	SD	-5	SD	0	SD	5	SD	10	SD	15	SD	20	SD	57	SD	65	SD	77	SD	141	SD
-5	**0,607**	0,028	**0,782**	0,020	**1,287**	0,054	**0,870**	0,014	**0,686**	0,038	**0,897**	0,014	**0,547**	0,013	0,128	0,004	**0,282**	0,019	**0,352**	0,027	**0,169**	0,010
-4	**0,649**	0,007	**0,784**	0,018	**1,335**	0,048	**0,818**	0,027	**0,713**	0,024	**0,783**	0,031	**0,553**	0,025	<LoD		**0,286**	0,019	**0,311**	0,027	**0,131**	0,010
-3	**0,607**	0,059	**0,794**	0,016	**1,389**	0,065	**0,745**	0,028	**0,668**	0,020	**0,756**	0,046	**0,543**	0,018	<LoD		**0,268**	0,018	**0,277**	0,041	**0,125**	0,012
-2	**0,517**	0,026	**0,768**	0,023	**1,247**	0,028	**0,701**	0,024	**0,677**	0,021	**0,748**	0,027	**0,547**	0,019	<LoD		**0,247**	0,007	**0,259**	0,019	**0,120**	0,006
-1	**0,502**	0,010	**0,800**	0,027	**1,236**	0,027	**0,734**	0,029	**0,642**	0,019	**0,741**	0,052	**0,539**	0,012	<LoD		**0,225**	0,018	**0,255**	0,027	**0,129**	0,011
0	**0,560**	0,025	**0,789**	0,048	**1,130**	0,037	**0,737**	0,033	**0,641**	0,014	**0,733**	0,029	**0,516**	0,017	<LoD		**0,203**	0,007	**0,190**	0,011	**0,120**	0,005
1	**0,501**	0,025	**0,615**	0,046	**0,637**	0,016	**0,702**	0,018	**0,466**	0,023	**0,574**	0,026	**0,422**	0,010	<LoD		**0,213**	0,006	**0,328**	0,022	**0,162**	0,008
2	0,272	0,017	**0,228**	0,009	**0,158**	0,010	**0,531**	0,024	**0,152**	0,015	**0,238**	0,019	**0,149**	0,006	<LoD		**0,227**	0,009	**0,297**	0,028	**0,214**	0,015
3	<LoD		**0,083**	0,003	**0,100**	0,025	0,120	0,008	<LoD		**0,155**	0,011	**0,061**	0,004	<LoD		**0,190**	0,014	**0,232**	0,014	**0,209**	0,007
4	<LoD		**0,071**	0,002	**0,101**	0,010	<LoD		<LoD		0,128	0,008	**0,037**	0,003	<LoD		**0,112**	0,005	**0,176**	0,011	**0,229**	0,008
5	<LoD		**0,061**	0,002	**0,077**	0,012	<LoD		<LoD		<LoD		**0,180**	0,006	<LoD		<LoD		**0,174**	0,015	**0,207**	0,014
6	<LoD		**0,077**	0,001	**0,068**	0,004	<LoD		<LoD		<LoD		**0,039**	0,003	<LoD		<LoD		0,150	0,017	**0,164**	0,013
7	<LoD		**0,069**	0,002	**0,198**	0,011	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		0,147	0,012	**0,164**	0,006
8	<LoD		**0,067**	0,001	**0,123**	0,007	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		0,154	0,008	**0,153**	0,009
9	<LoD		**0,058**	0,016	**0,074**	0,005	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		0,141	0,011	**0,139**	0,006
10	<LoD		**0,063**	0,007	**0,096**	0,008	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		0,146	0,015	**0,128**	0,008
11	<LoD		**0,061**	0,000	**0,081**	0,007	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		**0,167**	0,025	**0,134**	0,010
12	<LoD		**0,056**	0,006	**0,078**	0,008	<LoD		<LoD		<LoD		<LoD		0,153	0,009	<LoD		**0,183**	0,011	**0,123**	0,007
13	<LoD		**0,077**	0,002	**0,059**	0,003	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		0,151	0,021	**0,128**	0,010
14	<LoD		**0,057**	0,009	**0,059**	0,006	<LoD		<LoD		<LoD		<LoD		<LoD		0,104	0,010	0,141	0,010	**0,116**	0,006
15	<LoD		**0,066**	0,007	**0,065**	0,015	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		0,141	0,019	**0,130**	0,014
16	<LoD		**0,054**	0,010	**0,132**	0,006	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD		0,140	0,011	**0,126**	0,012
LoD	0,112		0,010		0,010		0,050		0,050		0,050		0,015		0,128		0,032		0,057		0,013	
LoQ	0,273		0,024		0,024		0,145		0,145		0,145		0,035		0,329		0,076		0,165		0,035	

Table A1. 25: Antimony (V) concentration across the SWI (<16 µm) and LoDs. Values <LoD were removed from the data set. All values in µg/L.

depth / day	-10	-5	0	5	10	15	20	57	65	77	141
-5	0,61	0,60	0,97	0,61	0,57	0,35	0,59	0,15	0,27	0,32	0,10
-4	0,76	0,60	0,98	0,64	0,53	0,48	0,61	0,17	0,24	0,31	0,12
-3	0,65	0,66	1,01	0,64	0,51	0,45	0,60	0,12	0,24	0,24	0,10
-2	0,51	0,54	0,89	0,64	0,44	0,41	0,69	0,11	0,15	0,24	0,09
-1	0,49	0,55	0,80	0,64	0,46	0,45	0,44	0,13	0,19	0,20	0,06
0	0,47	0,54	0,86	0,61	0,43	0,47	0,48	0,12	0,17	0,23	0,09
1	0,44	0,45	0,46	0,45	0,29	0,12	0,42	0,20	0,12	0,22	0,09
2	0,30	0,16	0,09	0,16	<LoD	0,39	0,15	0,21	0,19	0,17	0,23
3	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	0,15	0,14	0,20	0,15
4	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	0,08	<LoD	0,14	0,10
5	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	0,06	0,06	0,13	0,14
6	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	0,04	0,06	<LoD	0,10
7	<LoD	<LoD	0,14	<LoD	<LoD	<LoD	<LoD	0,06	0,06	0,05	0,11
8	<LoD	<LoD	0,05	<LoD	<LoD	<LoD	<LoD	0,07	0,05	<LoD	0,07
9	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	0,05	0,07	<LoD	0,09
10	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	0,08	<LoD	<LoD	0,08
11	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	0,08	0,05	<LoD	<LoD
12	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	0,05	0,21	<LoD	<LoD
13	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	0,07	<LoD	<LoD	<LoD
14	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	0,07	0,06	<LoD	<LoD
15	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	<LoD	0,08	0,08	0,13	<LoD
16	<LoD	<LoD	0,08	<LoD	<LoD	<LoD	<LoD	0,07	<LoD	0,10	<LoD
LoD	0,05	0,05	0,05	0,05	0,05	0,05	0,05	0,05	0,05	0,17	0,05

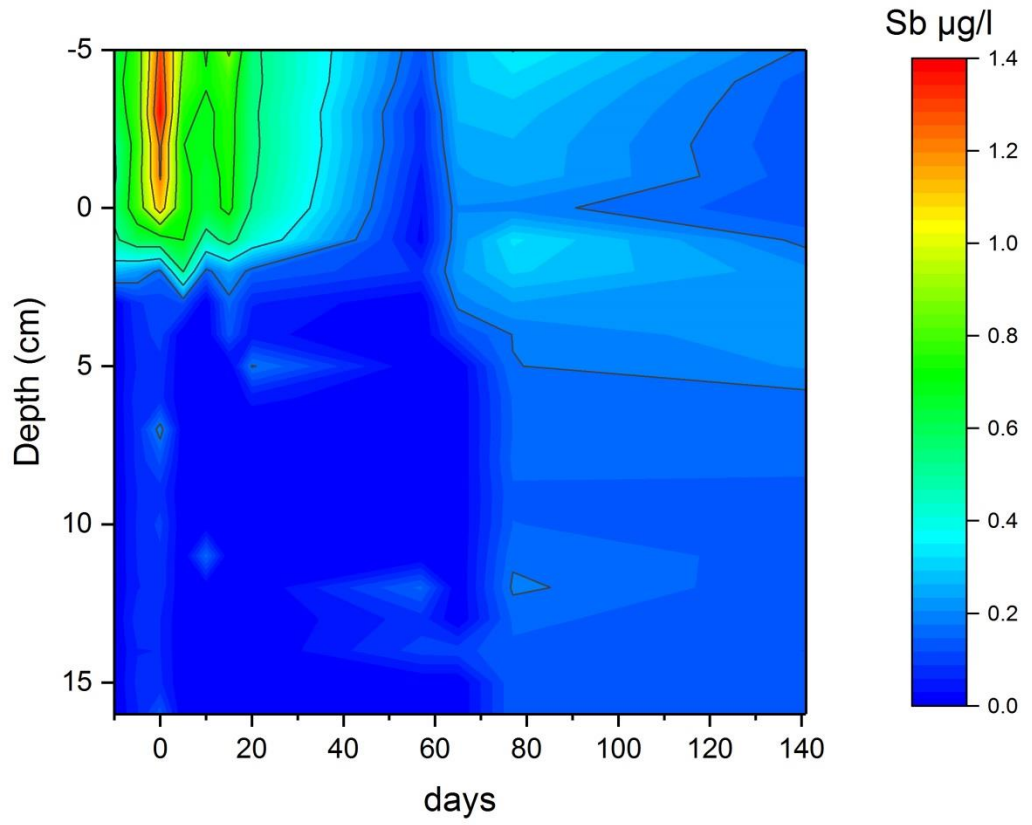


Figure A1. 13: Heatplot Antimony concentration across the SWI (<16 µm) (values < LoD set to 0).

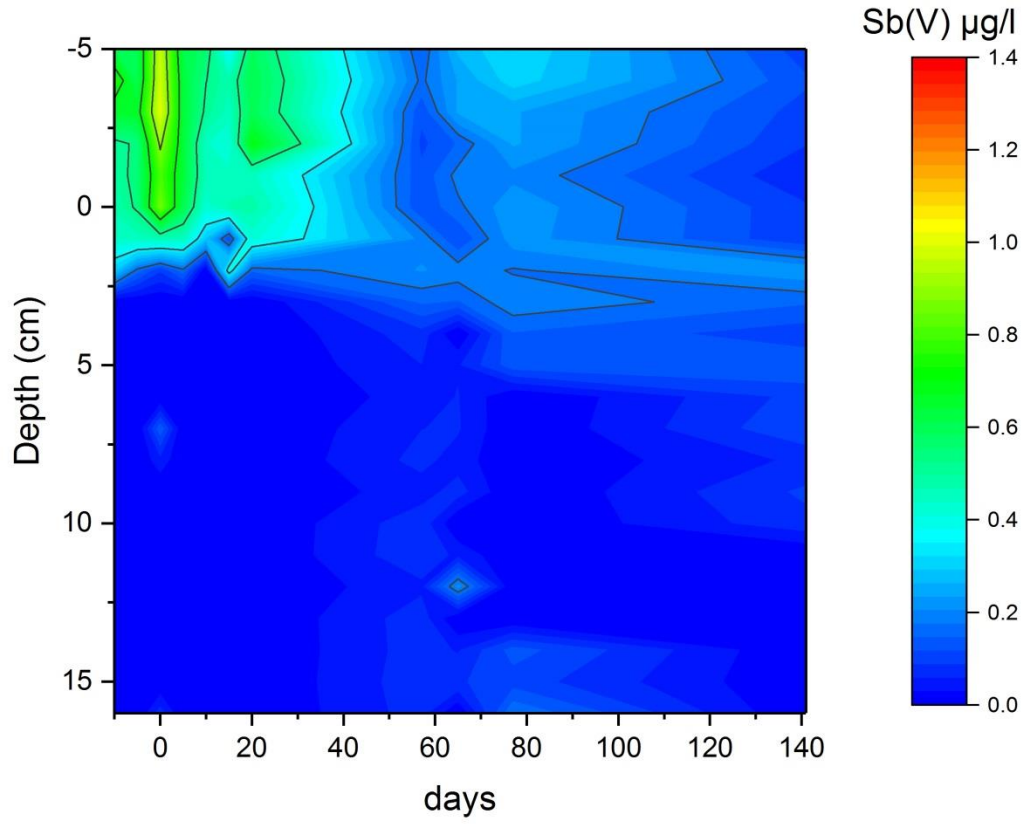


Figure A1. 14: Heatplot Antimony (V) concentration across the SWI (<16 µm) (values < LoD set to 0).

AI.X Size fractionation: Calculated colloidal fraction

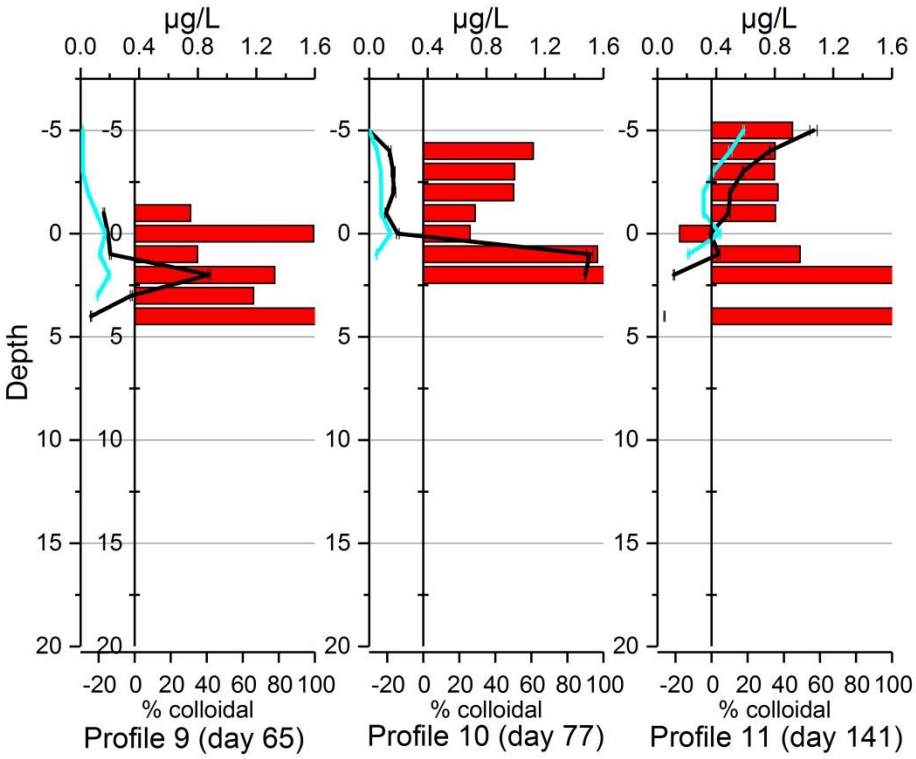


Fig. Figure A1. 15: Profiles of total (<16 µm) and dissolved (<0.45 µm) silver concentration and calculated colloidal fraction in % across the SWI.

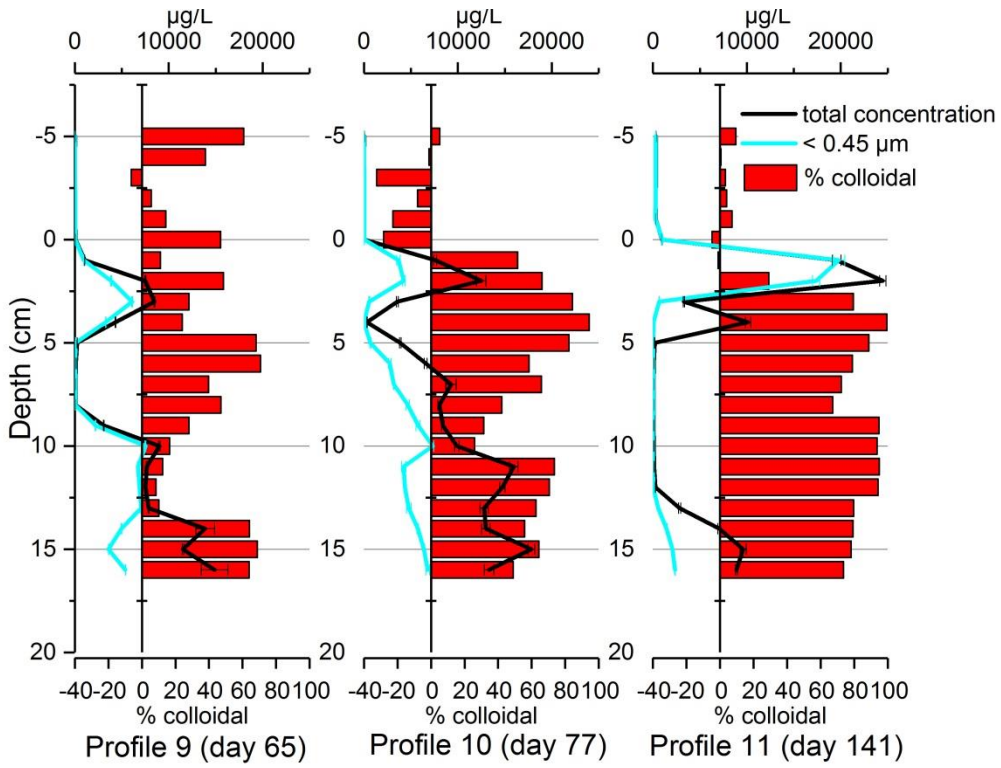


Figure A1. 16: Profiles of total (<16 µm) and dissolved (<0.45 µm) iron concentration and calculated colloidal fraction in % across the SWI.

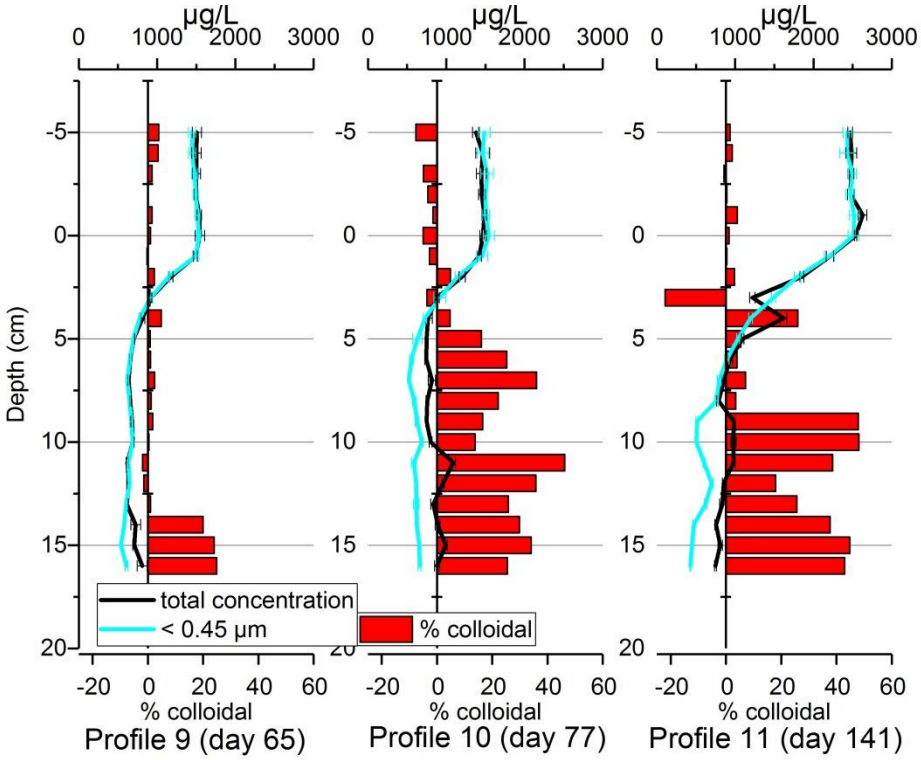


Figure A1. 17: Profiles of total (<16 µm) and dissolved (<0.45 µm) manganese concentration and calculated colloidal fraction in % across the SWI.

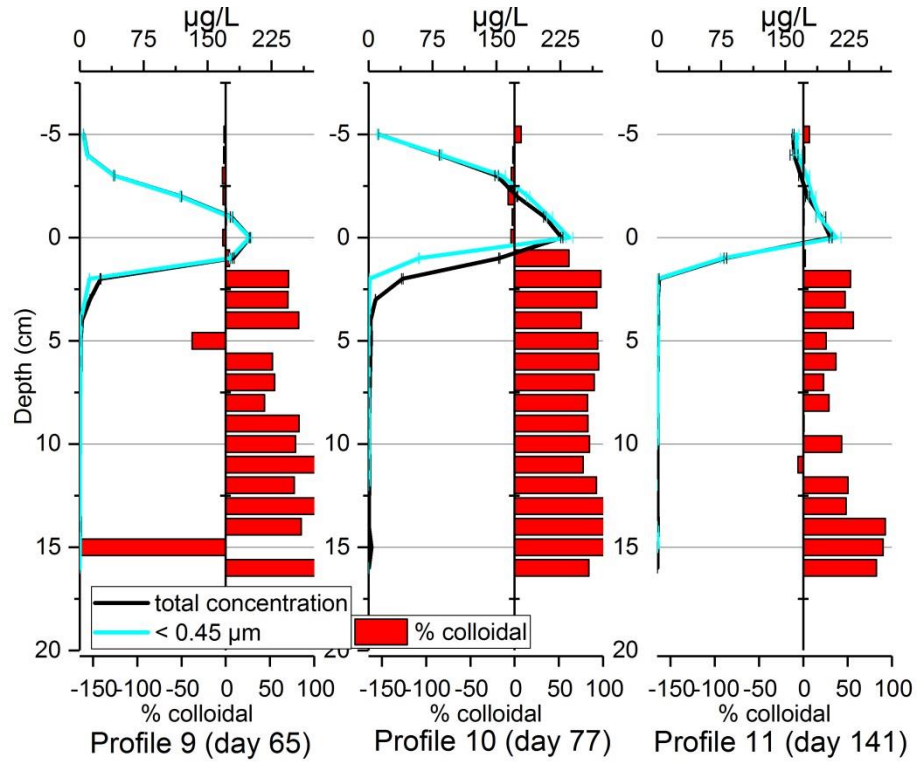


Figure A1. 18: Profiles of total (<16 µm) and dissolved (<0.45 µm) copper concentration and calculated colloidal fraction in % across the SWI.

Appendix II

Supporting Information Chapter 3:

Impact of mechanical disturbance and acidification on the metal(loid) and C, P, S mobility at the sediment water interface examined using a fractionation meso profiling ICP-QQQ-MS approach

Henning Schroeder, Anne-Lena Fabricius, Dennis Ecker, Thomas A. Ternes and Lars Duester

AII.I Sediment characteristics

AII.I.I Metal(loid)s content of the sediment at the end of the experiment

Subsequently to the experiment, a sediment core was sampled from each Experiment in the laboratory, frozen and cut with a ceramic knife into 1 cm slices. The sediment samples were freeze dried (Christ Gefriertrocknungsanlagen GmbH, Germany), milled (planetary mill pulverisette, Fritsch, Germany) and digested by application of a microwave assisted procedure. Therefore, 1 g of the sediment was mixed with 10 mL of reverse *aqua regia* (2,5 mL 30% HCl + 7,5 mL 65% HNO_3) and digested in a five-step power-controlled program (refer to table S2) using a Multiwave PRO (Anton Paar, Austria). After digestion, samples were diluted to 100 mL and analysed by means of ICP-OES (Optima 8300, Perkin Elmer,).

Table A2. 1: Micro wave program.

Step	Program	Power	Time
		W	mm:ss
1	Power ramp	600	11:00
2	Power ramp	1500	3:00
3	Power hold	1500	13:00
4	Power ramp	860	9:30
5	Power hold	750	13:30

Table A2. 2: Metal(loid)s content of the sediment of Experiment A at the end of the experiment. All values in mg/kg.

Depth (cm)	Al	SD	As	SD	Ca	SD	Cd	SD
0-1 cm	33,145	153.96	28.39	0.37	9,052	38.10	5.94	0.04
1-2 cm	34,564	333.28	27.88	0.87	7,659	63.88	5.85	0.16
2-3 cm	29,697	176.11	22.73	2.22	8,446	33.29	5.16	0.07
3-4 cm	24,691	145.34	19.43	0.78	9,960	55.65	4.37	0.10
4-5 cm	21,717	179.38	15.72	0.91	11,123	88.38	3.58	0.06
5-6 cm	23,853	137.49	15.59	0.69	11,097	57.75	3.66	0.07
6-7 cm	22,057	61.40	16.64	0.94	11,264	38.46	3.71	0.15
7-8 cm	23,346	244.90	19.75	0.18	10,912	87.61	4.04	0.05
8-9 cm	23,874	144.74	19.25	0.63	10,663	41.41	4.15	0.10
9-10 cm	28,255	265.02	23.06	0.27	10,689	88.81	4.34	0.21
10-11 cm	27,413	547.46	24.07	1.24	10,445	167.54	4.19	0.20
11-12 cm	27,754	128.08	23.57	1.86	10,453	52.79	4.46	0.08
12-13 cm	29,776	308.40	23.26	1.68	10,749	78.92	4.18	0.03
13-14 cm	27,168	384.98	24.31	1.35	10,555	153.64	4.28	0.18
14-15 cm	26,956	116.63	23.72	1.59	10,721	21.31	4.51	0.04
15-16 cm	27,741	86.26	22.31	0.44	10,735	11.14	4.23	0.16

Depth (cm)	Cr	SD	Cu	SD	Fe	SD	Li	SD
0-1 cm	146.69	1.29	2,870.79	36.79	79,188	214.68	29.95	0.34
1-2 cm	154.82	1.62	2,832.87	40.64	84,847	477.66	30.37	0.08
2-3 cm	136.01	0.41	2,618.31	3.73	78,668	232.39	26.65	0.34
3-4 cm	114.33	0.55	2,321.30	15.09	79,811	429.27	21.93	0.29
4-5 cm	114.30	0.82	2,279.52	22.77	71,357	508.45	18.44	0.22
5-6 cm	114.77	0.96	2,253.92	23.01	71,943	179.42	19.45	0.21
6-7 cm	103.40	1.11	2,328.25	21.57	73,405	394.58	19.30	0.13
7-8 cm	111.40	1.00	2,335.49	19.41	76,808	398.62	20.90	0.42
8-9 cm	111.84	0.10	2,381.55	10.69	76,506	97.88	21.14	0.12
9-10 cm	112.55	0.35	2,322.62	10.26	86,013	434.49	23.20	0.25
10-11 cm	110.04	0.58	2,224.47	14.92	84,461	1,060.11	22.79	0.54
11-12 cm	112.08	0.77	2,369.63	17.79	86,052	350.88	22.91	0.07
12-13 cm	131.45	0.26	2,379.95	16.45	85,582	364.40	23.77	0.30
13-14 cm	112.70	0.30	2,340.87	19.98	85,815	884.25	22.87	0.32
14-15 cm	110.96	1.76	2,376.94	39.78	86,303	115.03	23.00	0.23
15-16 cm	114.35	1.15	2,370.86	30.19	84,570	92.77	22.90	0.17

Depth (cm)	Mg	SD	Mn	SD	Ni	SD	P	SD
0-1 cm	5,061	17.71	651.09	5.86	132.64	0.37	2.23	0.04
1-2 cm	4,957	22.74	669.83	6.22	128.44	0.33	2.69	0.04
2-3 cm	4,710	56.70	728.54	8.36	120.99	0.23	2.75	0.01
3-4 cm	4,296	65.09	766.07	11.61	111.29	0.28	2.65	0.02
4-5 cm	4,399	9.01	844.62	1.95	106.68	0.16	2.37	0.02
5-6 cm	4,542	4.69	828.87	0.59	107.43	0.16	2.40	0.02
6-7 cm	4,386	5.38	834.52	2.18	104.73	0.32	2.61	0.03
7-8 cm	4,473	9.61	809.28	2.86	111.53	0.16	2.58	0.03
8-9 cm	4,483	9.09	797.87	1.20	108.44	0.16	2.54	0.01
9-10 cm	4,752	12.58	832.12	2.93	108.72	0.16	2.66	0.01
10-11 cm	4,584	8.57	798.60	1.54	106.75	0.20	2.66	0.02
11-12 cm	4,706	11.65	805.69	2.68	109.88	0.22	2.74	0.02
12-13 cm	4,829	14.33	798.60	2.19	109.19	0.06	2.68	0.01
13-14 cm	4,622	11.41	802.27	2.17	110.23	0.13	2.66	0.03
14-15 cm	4,560	4.05	808.72	0.80	109.11	0.10	2.69	0.04
15-16 cm	4,647	13.31	799.96	2.58	109.50	0.29	2.65	0.03

Depth (cm)	Pb	SD	Zn	SD
0-1 cm	513.58	1.34	3,181	21.34
1-2 cm	507.63	0.50	3,000	37.87
2-3 cm	475.07	0.75	2,738	34.12
3-4 cm	421.09	0.93	2,348	37.99
4-5 cm	368.13	0.65	1,994	3.85
5-6 cm	382.11	0.79	2,102	2.69
6-7 cm	378.57	0.32	2,077	1.62
7-8 cm	416.27	1.17	2,241	3.83
8-9 cm	419.66	0.80	2,267	1.95
9-10 cm	401.63	0.47	2,247	0.88
10-11 cm	400.48	0.86	2,218	7.34
11-12 cm	436.86	1.34	2,276	5.57
12-13 cm	407.43	0.18	2,252	8.27
13-14 cm	417.08	0.17	2,290	6.87
14-15 cm	428.81	1.85	2,267	2.99
15-16 cm	414.42	0.77	2,249	9.82

Table A2. 3: Metal(loid)s content of the sediment of Experiment B at the end of the experiment. All values in mg/kg.

Depth (cm)	Al	SD	As	SD	Ca	SD	Cd	SD
0-1 cm	31,412	382.87	26.73	1.31	10,671	95.93	5.09	0.02
1-2 cm	32,071	336.32	27.28	2.25	11,629	84.09	5.34	0.07
2-3 cm	30,397	266.50	24.58	1.02	9,315	81.40	4.92	0.05
3-4 cm	33,692	309.19	26.09	0.56	9,672	76.90	4.99	0.17
4-5 cm	32,111	481.02	25.82	0.84	9,649	119.11	5.20	0.08
5-6 cm	31,691	247.53	29.31	2.20	9,529	66.40	5.35	0.10
6-7 cm	32,254	258.21	28.00	0.88	9,670	68.93	5.43	0.08
7-8 cm	37,061	114.00	28.72	0.47	9,941	15.88	5.56	0.02
8-9 cm	26,539	377.19	21.88	1.36	12,100	144.09	3.97	0.06
9-10 cm	21,630	117.66	15.60	0.51	12,935	71.29	3.07	0.18
10-11 cm	23,900	355.17	18.28	0.98	11,663	120.45	3.32	0.08
11-12 cm	28,041	212.12	22.27	1.31	10,957	69.95	4.12	0.09
12-13 cm	29,013	315.77	23.34	0.66	10,801	102.30	4.13	0.15
13-14 cm	29,310	78.50	22.71	1.27	11,058	23.19	4.17	0.19
14-15 cm	28,870	377.06	22.09	0.20	10,844	110.60	4.27	0.02
15-16 cm	30,348	387.73	22.64	1.49	11,306	99.33	4.31	0.16

Depth (cm)	Cr	SD	Cu	SD	Fe	SD	Li	SD
0-1 cm	121.95	1.32	2,322	28.42	87,125	660.44	27.97	0.38
1-2 cm	128.35	0.78	2,346	10.93	99,093	619.61	27.69	0.26
2-3 cm	119.41	0.88	2,259	28.12	85,924	647.33	27.36	0.64
3-4 cm	128.94	0.79	2,267	9.05	86,240	441.62	28.91	0.26
4-5 cm	123.57	0.45	2,332	4.40	87,308	980.81	28.90	0.58
5-6 cm	123.92	1.02	2,385	17.01	89,660	430.14	29.12	0.23
6-7 cm	126.46	1.44	2,451	32.92	90,067	479.06	29.43	0.15
7-8 cm	142.99	0.17	2,443	14.02	92,043	298.65	31.18	0.55
8-9 cm	114.43	0.64	2,166	13.37	83,218	632.62	21.34	0.41
9-10 cm	91.23	0.36	1,919	5.19	74,865	311.72	17.29	0.16
10-11 cm	95.17	0.40	2,291	15.01	76,939	585.63	19.37	0.27
11-12 cm	114.88	0.80	2,131	18.52	81,976	504.76	23.06	0.33
12-13 cm	115.46	0.70	2,264	21.01	82,797	619.51	23.95	0.15
13-14 cm	116.29	0.58	2,221	14.00	83,784	179.30	24.74	0.16
14-15 cm	116.55	0.24	2,119	15.03	81,435	671.60	23.54	0.14
15-16 cm	129.31	1.12	2,245	19.40	84,731	669.11	24.71	0.26

Depth (cm)	Mg	SD	Mn	SD	Ni	SD	P	SD
0-1 cm	4,988	49.87	727.17	9.99	112.05	0.18	2.75	0.03
1-2 cm	5,337	8.60	747.34	1.54	118.09	0.12	2.83	0.03
2-3 cm	4,760	88.07	747.59	27.15	111.37	0.18	2.66	0.01
3-4 cm	5,035	39.88	751.93	9.35	111.85	0.16	2.65	0.02
4-5 cm	4,909	55.17	753.53	10.43	111.91	0.19	2.60	0.03
5-6 cm	4,875	48.81	744.09	9.84	114.68	0.55	2.58	0.02
6-7 cm	4,875	4.69	730.93	2.70	114.98	0.32	2.41	0.03
7-8 cm	5,093	93.43	749.02	21.52	115.84	0.63	2.44	0.02
8-9 cm	4,453	11.91	786.53	2.79	109.20	0.09	2.36	0.01
9-10 cm	4,406	11.55	877.99	3.36	97.35	0.08	2.25	0.02
10-11 cm	4,501	4.84	860.35	2.56	99.22	0.06	2.41	0.01
11-12 cm	4,700	7.92	809.75	1.74	106.83	0.19	2.46	0.02
12-13 cm	4,613	53.79	776.68	13.19	105.71	0.07	2.49	0.02
13-14 cm	4,625	23.07	849.15	6.23	107.62	0.18	2.52	0.03
14-15 cm	4,664	17.61	799.04	2.81	106.06	0.25	2.60	0.02
15-16 cm	4,835	26.62	795.85	6.04	109.46	0.24	2.52	0.02

Depth (cm)	Pb	SD	Zn	SD
0-1 cm	458.00	0.42	2,590	19.26
1-2 cm	484.51	1.23	2,692	6.99
2-3 cm	456.16	1.13	2,516	56.11
3-4 cm	460.42	0.89	2,558	15.79
4-5 cm	459.63	1.25	2,656	52.89
5-6 cm	470.71	1.84	2,744	36.04
6-7 cm	472.08	1.44	2,743	15.18
7-8 cm	472.88	2.35	2,780	28.19
8-9 cm	381.39	0.57	2,139	0.69
9-10 cm	325.47	0.20	1,680	6.09
10-11 cm	348.68	1.71	1,861	6.26
11-12 cm	389.58	0.83	2,151	7.44
12-13 cm	384.81	1.74	2,165	43.03
13-14 cm	417.51	0.83	2,237	11.37
14-15 cm	397.61	0.37	2,214	17.20
15-16 cm	406.63	0.89	2,271	9.92

AII.I.II Carbon, Nitrogen and Sulfur content of the sediment at the end of the experiment

To determine the total content of carbon, nitrogen and sulphur, 100 mg of the freeze-dried and milled sediment samples were analysed by means of a total content analyser (Vario Macro, Elementar, Germany). For the analyses sulphur measurements, 120 mg of tungsten oxide (WO_3) were added to support the combustion process. Calibration was performed using sulphanilamide and verified by measurements of acetanilide. Two certified reference materials were included in the measurements (Leco 308, Leco 309). Results are presented in Table S3.

Table A2. 4: Total CNS content of the sediment at the end of the experiment.

	Depth [cm]	C [%]	TOC [%]	N [%]	S [%]	C/N	C/S
Experiment A	0-1	9.42	9.31	0.7	6.78	13.53	1.39
	2-Jan	9.78	9.76	0.71	6.69	13.82	1.46
	3-Feb	9.58	9.54	0.71	6.43	13.6	1.49
	4-Mar	9.64	9.53	0.68	6.4	14.17	1.51
	5-Apr	9.51	9.43	0.74	6.57	6.73	1.46
	6-May	9.57	9.69	0.72	7.04	13.21	1.36
	7-Jun	9.97	9.82	0.73	7.13	13.58	1.4
	8-Jul	12.5	12.03	0.86	6.84	14.5	1.87
	9-Aug	16.03	16.04	0.95	5.62	16.89	2.88
	10-Sep	15.84	15.84	0.91	5.07	17.45	3.13
	11-Oct	13.8	13.38	0.86	5.43	16.04	2.55
	12-Nov	13.32	12.73	0.87	5.88	15.36	2.26
	13-Dec	12.48	12.37	0.81	6.27	15.41	1.99
	13-14	12.48	12.45	0.84	6.41	14.93	1.95
	14-15	12.97	12.96	0.85	6.01	15.31	2.16
	15-16	13.26	13.26	0.83	6.2	15.96	2.14
Experiment B	0-1	9.81	9.79	0.79	7.61	12.36	1.29
	2-Jan	9.77	9.37	0.79	7.35	12.43	1.33
	3-Feb	10.77	10.48	0.8	6.49	13.42	1.66
	4-Mar	12.79	12.41	0.85	6.44	14.98	1.99
	5-Apr	12.52	12.06	0.82	5.82	15.36	2.15
	6-May	12.61	12.36	0.85	5.96	14.88	2.12
	7-Jun	12.58	11.92	0.8	5.97	15.67	2.11
	8-Jul	11.86	11.13	0.8	6.15	14.82	1.93
	9-Aug	12.1	11.67	0.82	6.2	14.85	1.95
	10-Sep	11.95	11.69	0.8	6.49	14.97	1.84
	11-Oct	12.29	11.93	0.8	6.41	15.35	1.92
	12-Nov	12.12	11.76	0.81	6.56	14.98	1.85
	13-Dec	12.11	11.73	0.83	6.22	14.6	1.95
	13-14	12.08	11.2	0.98	6.22	12.66	1.95
	14-15	12.07	11.81	0.8	6.37	15.09	1.9
	15-16	12.08	11.85	0.81	6.55	14.99	1.85

AII.I.III Grain size distribution of the sediment at the end of the experiment

The grain size distributions were determined by laser diffraction particle size analyser (Beckman Coulter LS200, Beckman Coulter , Inc., USA).

Very similar results were obtained for both experiments. Due to their faster settling velocities coarse grain sizes were enriched in the deeper sediment layers subsequent to the mechanical disturbance. Results are shown in Table S6 and S7.

Table A2. 5: Grain size distribution of the sediment of Experiment A at the end of the experiment. All values in volume %.

depth (cm) / size class	0-1	1-2	2-3	3-4	4-5	5-6	6-7
0.63-2 mm	0.000	0.000	2.774	9.390	8.124	15.837	5.497
0.2-0.63 mm	0.498	0.087	10.680	21.210	21.620	27.300	22.890
0.063-0.2 mm	14.150	17.660	20.320	23.100	23.460	24.000	22.800
0.02-0.063 mm	33.880	39.180	34.060	21.290	20.830	18.110	20.820
0.0063-0.02 mm	29.000	26.910	19.860	13.870	13.960	8.770	15.190
0.002-0.0063 mm	14.250	11.110	8.000	6.890	7.330	3.790	7.770
<0.002 mm	7.009	5.064	4.303	4.205	4.658	2.204	5.034
depth (cm) / size class	7-8	8-9	9-10	10-11	11-12	12-13	13-14
0.63-2 mm	15.781	14.721	13.408	14.381	13.688	11.997	16.676
0.2-0.63 mm	23.790	22.970	21.840	23.590	23.380	21.250	22.270
0.063-0.2 mm	21.760	21.460	26.320	23.250	22.820	26.640	20.690
0.02-0.063 mm	18.630	19.610	21.740	20.090	20.640	24.060	19.390
0.0063-0.02 mm	11.360	12.180	10.200	10.890	11.490	10.290	12.050
0.002-0.0063 mm	5.470	5.730	4.250	4.970	5.090	3.820	5.670
<0.002 mm	3.210	3.332	2.240	2.802	2.870	1.940	3.286

Table A2. 6: Grain size distribution of the sediment of Experiment B at the end of the experiment. All values in volume %.

depth (cm) / size class	0-1	1-2	2-3	3-4	4-5	5-6	6-7
0.63-2 mm	0.000	0.241	0.000	0.000	0.092	0.000	0.677
0.2-0.63 mm	0.028	3.217	1.532	0.606	2.206	0.412	3.660
0.063-0.2 mm	35.740	36.790	16.370	25.080	38.770	23.490	26.910
0.02-0.063 mm	36.480	38.710	36.570	37.780	37.900	40.920	39.550
0.0063-0.02 mm	15.470	14.270	28.120	22.110	14.180	21.760	18.830
0.002-0.0063 mm	6.150	4.540	11.630	9.370	4.560	8.710	6.770
<0.002 mm	3.323	2.239	5.794	5.070	2.297	4.738	3.612
depth (cm) / size class	7-8	8-9	9-10	10-11	11-12	12-13	13-14
0.63-2 mm	7.769	6.739	7.919	12.324	14.990	11.713	18.066
0.2-0.63 mm	27.990	27.720	31.660	30.100	25.250	23.350	26.890
0.063-0.2 mm	32.540	29.220	31.480	27.320	25.860	27.480	18.770
0.02-0.063 mm	19.270	16.640	15.140	16.330	19.020	21.690	18.020
0.0063-0.02 mm	8.020	10.530	7.320	7.780	8.630	9.400	10.310
0.002-0.0063 mm	2.960	5.490	3.930	3.800	3.910	3.970	4.930
<0.002 mm	1.474	3.661	2.512	2.352	2.354	2.355	3.042

AII.II Sediment parameters

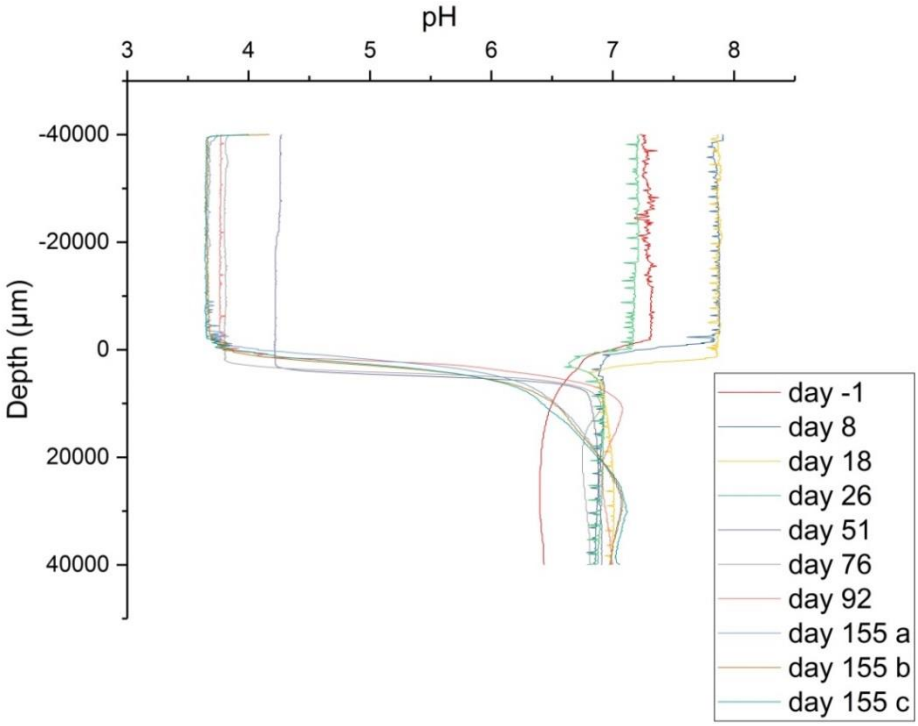
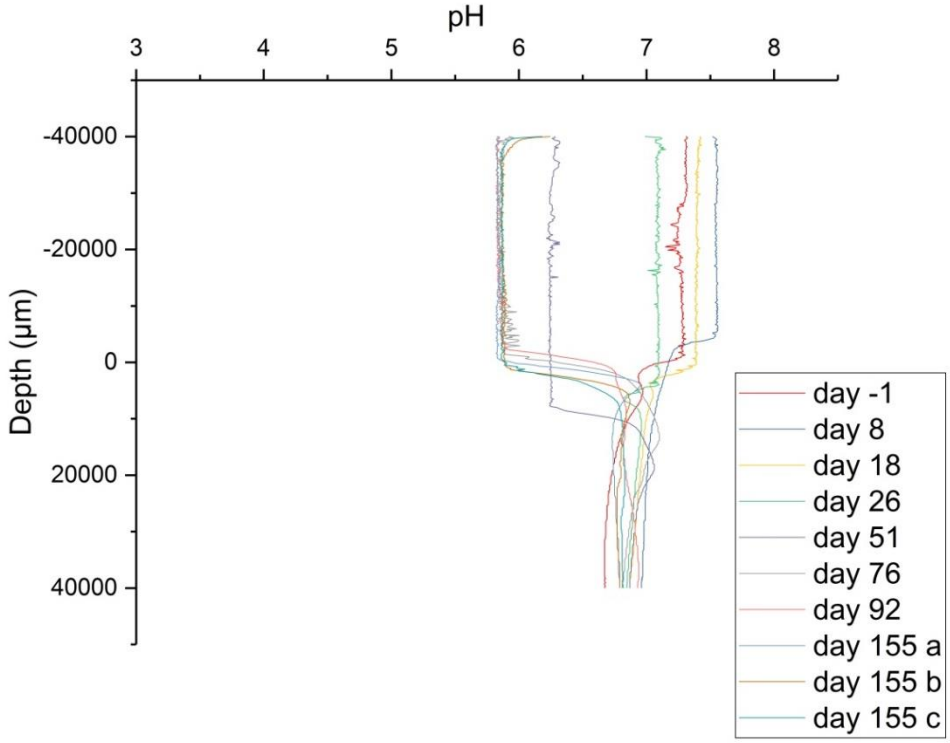


Figure A2. 1: pH profiles in between the respective *messy* profiles of Experiment A.

Figure A2. 2: pH profiles in between the respective *messy* profiles of Experiment B.



AII.III Element concentrations in sediment pore water samples

AII.III.I ICP-MS Analyses of sediment pore water samples

The information about the measurements of the metal(loid) concentrations in the pore water samples in the different size fractions are given in Table A3. 8-A3. 68. Elements were measured by application of a collision cell (He) with a He gas flow of 5 ml/min, or application of a collision cell (O_2) with 30% O_2 content. Limits of detection (LoD, blank + 3 sigma) and limits of quantification (LoQ, blank + 10 sigma) are given together with the results.

Table A2. 7: Information about ICP-QQQMS analyses of sediment pore water samples

Isotope	Gas	Mode	CRM	TMRain**	TM25.4**	1640a**	SPS-SW 1**	SPS-SW 2**		tartaric acid
^{12}C	O_2	MS/MS	certified value							200.000
^{31}P	O_2	MS/MS					100.000	500.000		
^{32}S	O_2	MS/MS					2000.000	10000.000		
^{55}Mn	He	SingleQuad		6.700	25.100	40.390	10.000	50.000		
^{56}Fe	He	SingleQuad		24.700	31.000	36.800	20.000	100.000		
^{60}Ni	He	SingleQuad		0.908	16.200	25.320	10.000	50.000		
^{63}Cu	O_2	MS/MS		7.030	26.700	85.750	20.000	100.000		
^{51}V	O_2	MS/MS		0.683	27.400	15.050	10.000	50.000		
^{52}Cr	O_2	MS/MS		0.866	24.000	40.540	2.000	10.000		
^{59}Co	O_2	MS/MS		0.246	27.500	20.240	2.000	10.000		
^{75}As	O_2	MS/MS		1.140	27.100	8.075	10.000	50.000		
^{114}Cd	O_2	MS/MS		0.524	23.500	3.992	0.520	2.500		
^{121}Sb	O_2	MS/MS		0.353	23.800	5.105				
^{205}Tl	O_2	MS/MS		0.377	30.500	1.619	0.500	2.500		
^{208}Pb	He	SingleQuad		0.346	27.000	12.101	5.000	25.000		
**Certified Reference Material for Trace Elements, Environment Canada										

AII.III.II Methodological blank value correction

All measured concentrations were corrected by means of 3-5 methodological blank values to take into account the possibility of sample contaminations occurring in the glove boxes. To determine the methodological blank values 15 ml centrifuge tubes (VWR catalyst Laboratory Services, USA) were filled with ultrapure water (USF ELGA Purelab Plus system, ELGA LabWater, Germany) and left in the glove box for the approximately same amount of time as the samples during each pore water profile sampled. For some blank samples the values determined this way exceeded the concentrations of certain analytes found in all samples of the corresponding profiles. Hence, in these cases the blank values did obviously not reflect a possible contamination of the samples and measured concentrations of the samples were corrected by means of the blank values of all other profiles. The values used for correction are given with the results.

AII.III.III Measured concentrations in sediment pore water samples

Table A2. 8: Carbon concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in mg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**45**	4.08	**57**	2.82	**69**	2.25	**60**	1.90	**175**	5.42	**91**	5.26
-4.5	**66**	2.94	**68**	4.43	**70**	4.51	**80**	2.51	**191**	11.00	**89**	4.19
-3.5	**68**	0.42	**79**	10.13	**67**	5.87	**94**	4.30	**173**	8.41	**59**	6.54
-2.5	**68**	4.98	**58**	2.49	**71**	4.57	**81**	2.24	**83**	2.93	**88**	2.62
-1.5	**59**	5.99	**83**	4.90	**70**	11.17	**72**	4.01	**52**	2.71	**59**	4.76
-0.5	**72**	14.57	**71**	3.96	**85**	2.89	**73**	4.39	**174**	8.92	**67**	1.98
0.5	**64**	3.13	**89**	10.06	**98**	9.34	**90**	3.68	**33**	1.35	**58**	5.81
1.5	**72**	6.09	**64**	8.97	**97**	6.33	**65**	1.18	**71**	2.30	**65**	4.55
2.5	**100**	13.77	**70**	6.36	**162**	2.92	**78**	1.87	**118**	3.28	**108**	8.14
3.5	**83**	9.72	**79**	3.74	**125**	7.53	**109**	4.18	**118**	6.56	**160**	10.83
4.5	**120**	23.44	**88**	1.57	**149**	15.79	**116**	4.80	**158**	5.64	**295**	18.61
5.5	**165**	15.17	**122**	16.37	**184**	23.65	**101**	1.82	**131**	4.05	**226**	10.14
6.5	**181**	9.38	**117**	17.73	**186**	18.89	**91**	3.09	**141**	3.77	**176**	9.12
7.5	**182**	11.22	**152**	19.74	**198**	7.71	**115**	3.23	**182**	9.55	**186**	9.17
8.5	**559**	37.06	**121**	6.63	**444**	38.48	**93**	3.35	**136**	5.48	**162**	8.93
9.5	**193**	17.22	**139**	3.16	**625**	71.42	**85**	4.62	**173**	10.88	**142**	3.66
10.5	**413**	34.32	**218**	3.26	**632**	25.42	**67**	4.02	**114**	6.04	**201**	12.46
11.5	**360**	34.73	**191**	12.92	**821**	23.20	**81**	1.47	**57**	1.15	**145**	12.35
12.5	**469**	44.04	**211**	12.61	**753**	48.68	**81**	3.09	**128**	5.83	**137**	5.19
13.5	**368**	8.32	**185**	10.28	**782**	84.62	**61**	3.43	**102**	2.08	**68**	5.70
14.5	**424**	95.59	**530**	80.37	**710**	50.99	**65**	2.69	**61**	5.25	**76**	3.41
15.5	**200**	21.42	**177**	20.69	**859**	70.55	**74**	1.06	**88**	4.42	**45**	1.45
blank 1	<LoD		14.42	0.35	<LoD		3.00	0.32	11.23	1.40	10.73	0.40
blank 2	<LoD		9.92	0.70	<LoD		3.09	0.23	8.68	0.70	11.46	0.91
blank 3	<LoD		8.88	0.68	<LoD		4.27	0.15	8.53	0.85	11.11	0.57
blank 4	<LoD		<LoD		<LoD		4.28	0.19	7.28	0.39	12.34	0.52
blank 5	<LoD		<LoD		<LoD		4.07	0.28	7.69	0.72	9.76	0.25
correction value	0.00		6.65		0.00		3.74		8.68		11.08	
LoD	7.96		7.96		7.96		2.65		2.65		9.20	
LoQ	16.63		16.63		16.63		7.04		7.04		25.11	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**31**	0.83	4	0.36	<LoD		<LoD		<LoD	0.26	**24**	0.61
-4.5	**33**	0.87	4	0.16	<LoD		<LoD		<LoD	0.27	**24**	1.16
-3.5	**27**	0.96	3	0.30	<LoD		<LoD		<LoD	0.61	**21**	0.79
-2.5	**21**	0.61	4	0.24	7	0.82	<LoD		9	0.92	**23**	1.43
-1.5	**19**	0.43	3	0.20	<LoD		<LoD		<LoD	0.60	20	0.84
-0.5	**20**	0.52	2	0.25	<LoD		<LoD		<LoD	0.84	19	0.37
0.5	**15**	0.52	3	0.20	**29**	1.31	**47**	0.83	<LoD	0.35	22	1.55
1.5	**25**	0.36	30	0.89	**142**	4.04	**167**	6.30	**127**	4.70	**44**	1.82
2.5	**61**	1.16	62	1.91	**267**	7.75	**321**	3.55	**184**	5.10	**65**	2.94
3.5	**148**	3.66	113	2.81	**323**	5.08	**357**	2.52	**337**	13.45	**90**	1.86
4.5	**137**	3.74	115	3.21	**524**	49.25	**439**	11.27	**448**	8.90	**49**	0.59
5.5	**168**	3.79	176	4.87	**657**	44.84	**519**	14.39	**491**	8.07	**93**	1.70
6.5	**194**	5.00	132	3.58	no sample *	no sample *	**731**	22.30	**682**	25.24	**102**	4.08
7.5	**238**	4.70	153	3.73	no sample *	no sample *	**611**	17.24	**593**	11.50	**158**	3.89
8.5	**163**	5.13	166	3.93	no sample *	no sample *	**1003**	13.19	**664**	25.95	**160**	2.70
9.5	**104**	1.72	188	3.90	**236**	6.00	**999**	27.96	**653**	14.18	**169**	5.37
10.5	**91**	4.03	162	2.90	**664**	13.80	**872**	21.62	**718**	21.89	**122**	4.10
11.5	**140**	3.70	202	4.31	**707**	27.96	**985**	32.42	**569**	14.24	**147**	7.64
12.5	**93**	2.15	217	5.04	**697**	10.17	**809**	28.25	**793**	21.43	**142**	4.59
13.5	**110**	0.60	232	5.74	**701**	15.71	**719**	33.18	**776**	25.16	**77**	1.68
14.5	**111**	3.85	216	5.07	**568**	16.87	**771**	15.43	**788**	26.27	no sample **	no sample **
15.5	**80**	2.03	256	8.06	**663**	22.72	**836**	18.48	**842**	17.22	**213**	5.20
blank 1	6.84	0.16	6.15	0.18	12.46	1.68	10.22	0.56	<LoD		<LoD	
blank 2	6.56	0.17	5.80	0.20	13.72	1.29	13.01	0.49	<LoD		<LoD	
blank 3	7.98	0.31	6.00	0.07	14.25	1.47	12.85	0.69	<LoD		<LoD	
blank 4	6.89	0.27	5.95	0.19	16.02	1.39	12.93	0.25	<LoD		<LoD	
blank 5	7.76	0.06	5.73	0.29	15.04	0.67	14.36	1.16	<LoD		<LoD	
correction value	7.20		5.93		14.30		12.67		0.00		0.00	
LoD	4.20		4.20		6.81		4.49		4.49		9.32	
LoQ	11.32		11.32		18.73		9.23		9.23		22.86	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 9: Carbon concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in mg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**143**	1.08	**163**	3.39	**86**	2.90	**180**	7.72	**89**	3.26	**35**	1.81
-4.5	**96**	0.81	**150**	5.23	**150**	3.64	**136**	4.89	**161**	7.63	**36**	1.74
-3.5	**134**	1.47	**125**	3.35	**140**	6.42	**102**	2.29	**205**	8.79	**10**	0.45
-2.5	**166**	2.21	**145**	3.30	**150**	5.77	**114**	2.56	**164**	3.51	**10**	0.64
-1.5	**168**	3.13	**117**	3.31	**157**	2.96	**119**	3.24	**165**	3.36	**26**	1.13
-0.5	**154**	2.56	**201**	7.78	**119**	2.81	**65**	2.66	**102**	2.80	**10**	0.38
0.5	**257**	5.27	**91**	1.44	**193**	1.95	**358**	14.09	**107**	2.30	<LoD	
1.5	**227**	11.51	**128**	3.78	**252**	9.41	**73**	1.07	**84**	3.45	<LoD	
2.5	**293**	4.69	**220**	11.46	**174**	4.52	**55**	3.01	**206**	10.87	**17**	0.35
3.5	**273**	9.01	**255**	7.90	**200**	4.19	**55**	3.95	**163**	4.90	**49**	1.48
4.5	**242**	9.00	**291**	8.96	**329**	3.53	**67**	6.11	**234**	6.51	**60**	1.49
5.5	**314**	2.43	**395**	10.54	**336**	10.00	**95**	6.90	**251**	20.11	**38**	1.69
6.5	**341**	9.90	**361**	10.44	**408**	4.02	no sample ***	no sample ***	**247**	5.94	**59**	1.11
7.5	**403**	9.62	**485**	25.79	**547**	17.85	no sample ***	no sample ***	**244**	8.27	**51**	0.75
8.5	**400**	19.61	**447**	8.04	**482**	16.16	no sample ***	no sample ***	**287**	7.85	**69**	2.35
9.5	**596**	23.29	**490**	14.78	**383**	8.83	no sample ***	no sample ***	**255**	6.06	**121**	3.97
10.5	**638**	21.56	**400**	9.27	**441**	16.69	**247**	8.17	**182**	5.76	**95**	1.72
11.5	**636**	42.42	**448**	13.50	**395**	6.33	**129**	7.09	**185**	6.34	**83**	1.42
12.5	**515**	21.02	**482**	15.16	**525**	14.49	**110**	3.44	**100**	4.35	**106**	2.65
13.5	**600**	21.47	**543**	32.67	**678**	16.44	**125**	1.87	**170**	2.24	**113**	3.00
14.5	**540**	4.80	**362**	11.14	**731**	16.10	**261**	8.54	**201**	5.80	**113**	0.75
15.5	**729**	38.54	**531**	21.76	**534**	18.48	no sample ***	no sample ***	**234**	10.81	**116**	2.92
blank 1	<LoD		14.07	1.78	<LoD		<LoD		<LoD		4.64	0.12
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		5.40	0.12
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		4.86	0.23
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		4.97	0.15
blank 5	<LoD		<LoD		<LoD		<LoD				5.17	0.20
correction value	0.00		2.81		0.00		0.00		0.00		5.01	
LoD	11.87		11.87		11.87		9.52		9.52		2.16	
LoQ	31.23		31.23		31.23		21.36		21.36		5.06	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**52**	0.96	<LoD		<LoD	1.75	<LoD		**68**	6.24	14	1.26
-4.5	**32**	0.46	<LoD		<LoD	1.71	<LoD		**32**	2.27	14	1.60
-3.5	**30**	0.35	<LoD		<LoD	1.72	<LoD		**19**	0.34	13	0.97
-2.5	**31**	0.36	<LoD		<LoD	1.10	<LoD		**14**	0.86	13	2.22
-1.5	**30**	0.19	<LoD		<LoD	1.28	<LoD		**11**	0.94	13	0.74
-0.5	**21**	0.52	<LoD		<LoD	2.16	<LoD		**10**	0.77	13	0.75
0.5	**18**	0.21	<LoD		**32**	2.10	**54**	3.14	**12**	1.71	18	0.68
1.5	**30**	1.04	**37**	2.18	**154**	12.22	**237**	7.35	**148**	3.57	22	0.67
2.5	**89**	2.71	**136**	6.92	**275**	13.45	**353**	25.03	**190**	4.33	**41**	1.28
3.5	**134**	2.27	**128**	6.25	**457**	5.92	**424**	10.90	**303**	10.32	**79**	2.68
4.5	**247**	9.68	**148**	5.86	**510**	26.69	**513**	14.68	**435**	16.44	**69**	2.58
5.5	**247**	6.18	**223**	7.18	**411**	33.46	**761**	20.30	**470**	2.94	no sample **	no sample **
6.5	**232**	11.50	**304**	14.62	no sample *	no sample *	**632**	30.94	**581**	14.46	**78**	2.06
7.5	**208**	8.12	**309**	18.26	no sample *	no sample *	**774**	8.10	**704**	14.81	**85**	1.55
8.5	**274**	11.25	**354**	24.92	no sample *	no sample *	**784**	27.75	**751**	23.51	**93**	3.63
9.5	**239**	6.19	**213**	6.54	**282**	11.09	**810**	16.26	**613**	6.65	**82**	4.67
10.5	**270**	8.42	**246**	8.76	**477**	32.67	**802**	14.56	**184**	6.86	**34**	1.56
11.5	**268**	5.50	**257**	12.94	**523**	15.55	**816**	32.28	**753**	14.09	no sample **	no sample **
12.5	**263**	10.05	**274**	10.09	**610**	28.35	**839**	64.91	**400**	13.42	no sample **	no sample **
13.5	**283**	11.01	**248**	10.48	**504**	14.72	**917**	28.76	**419**	6.61	no sample **	no sample **
14.5	**352**	9.97	**247**	10.78	**753**	51.45	**1,202**	29.27	**487**	16.75	no sample **	no sample **
15.5	**310**	10.74	**297**	6.66	**472**	17.70	**1,038**	58.73	**474**	15.33	no sample **	no sample **
blank 1	11.35	0.83	<LoD		14.87	1.51	26.63	0.85	12.98	0.93	<LoD	
blank 2	10.33	0.53	<LoD		12.66	2.15	18.38	2.91	10.17	1.09	<LoD	
blank 3	8.83	0.51	<LoD		13.02	1.81	17.98	1.85	<LoD		<LoD	
blank 4	9.19	0.56	<LoD		<LoD		18.40	5.45			<LoD	
blank 5	9.09	0.35	<LoD		9.44	2.22	14.44	1.45			<LoD	
correction value	9.76		0.00		10.00		19.17		7.71		0.00	
LoD	2.16		9.20		9.29		6.81		4.49		9.32	
LoQ	5.06		25.11		22.81		18.73		9.23		22.86	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 10: Carbon concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in mg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**86**	7.90	**31**	2.20	**57**	8.29	**79**	5.50	**99**	3.04	**108**	2.74
-4.5	**63**	5.93	**36**	1.67	**62**	3.63	**110**	6.44	**45**	1.50	**149**	3.67
-3.5	**49**	2.56	**30**	1.87	**63**	3.89	**66**	4.18	**85**	4.03	**121**	3.19
-2.5	**36**	2.30	**35**	3.96	**60**	3.91	**124**	1.28	**47**	1.37	**123**	2.03
-1.5	**57**	9.12	**30**	4.66	**64**	2.96	**51**	2.19	**104**	1.73	**128**	2.32
-0.5	**59**	5.75	**53**	7.05	**93**	3.46	**100**	4.79	**75**	3.85	**152**	3.06
0.5	**56**	4.00	**77**	0.82	**187**	40.04	**87**	3.62	**134**	9.53	**92**	2.22
1.5	**74**	0.77	**123**	6.69	**192**	10.93	**69**	3.50	**66**	1.58	**128**	3.92
2.5	**85**	2.67	**103**	8.08	**109**	9.00	**58**	3.96	**158**	4.76	**158**	5.81
3.5	**92**	6.30	**103**	4.81	**166**	4.89	**69**	3.66	**94**	1.05	**239**	5.29
4.5	**160**	16.12	**146**	8.71	**343**	13.03	**75**	3.39	**160**	7.20	**251**	7.11
5.5	**209**	10.12	**132**	13.65	**216**	11.67	**68**	3.99	**184**	1.42	**305**	10.06
6.5	**188**	14.33	**194**	36.76	**443**	47.88	**59**	1.52	**437**	16.24	**350**	26.53
7.5	**249**	81.95	**186**	9.71	**530**	30.10	**72**	2.32	**229**	9.72	**286**	2.16
8.5	**299**	90.82	**615**	35.71	**381**	32.46	**54**	2.90	**178**	7.05	**293**	9.57
9.5	**608**	68.76	**136**	20.43	**536**	33.31	**63**	2.99	**211**	6.89	**347**	5.77
10.5	**387**	51.89	**485**	15.90	**606**	50.04	**67**	2.28	**226**	8.80	**365**	16.72
11.5	**610**	62.24	**365**	20.40	**495**	15.25	**64**	2.89	**291**	9.37	**329**	19.82
12.5	**435**	49.31	**486**	47.68	**595**	20.68	**68**	1.98	**184**	1.62	**358**	14.97
13.5	**425**	46.85	**508**	30.11	**618**	36.93	**75**	2.75	**234**	6.57	**349**	12.15
14.5	**304**	93.03	**776**	44.34	**600**	32.10	**60**	1.70	**430**	25.13	**354**	3.09
15.5	**573**	58.30	**451**	10.59	**705**	60.03	**80**	2.35	**263**	7.39	**465**	17.12
blank 1	12.15	1.78	18.70	2.85	14.46	0.69	5.69	0.64	4.95	0.34	16.72	1.99
blank 2	11.51	0.47	10.99	2.37	11.49	1.80	4.89	0.31	4.78	0.39	19.03	2.62
blank 3	11.06	0.75	9.01	1.53	11.27	1.66	5.41	0.54	4.08	0.41	20.64	2.16
blank 4	9.75	2.15	<LoD		9.78	0.88	5.70	0.52	4.07	0.52	22.75	4.56
blank 5	19.48	3.12	<LoD		9.82	2.03	5.52	0.25	3.76	0.28	17.39	1.47
correction value	12.79		7.74		11.36		5.44		4.33		19.31	
LoD	7.96		7.96		7.96		2.65		2.65		9.29	
LoQ	16.63		16.63		16.63		7.04		7.04		22.81	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**55**	1.39	<LoD		<LoD		**26**	1.33	**23**	2.93	10	1.27
-4.5	**43**	1.20	4	0.13	<LoD		**54**	1.81	**14**	2.06	13	2.65
-3.5	**36**	0.82	5	0.51	**39**	3.01	**35**	1.75	**18**	1.10	<LoD	
-2.5	**25**	0.41	5	0.26	14	3.60	**32**	2.78	**17**	1.03	10	1.64
-1.5	**20**	0.56	6	0.40	**20**	1.63	**27**	2.42	**12**	1.54	10	0.99
-0.5	**18**	0.45	10	0.41	<LoD		**47**	1.52	6	0.39	11	1.20
0.5	**24**	0.57	**71**	1.94	**15**	1.53	**193**	5.90	6	1.14	**38**	1.72
1.5	**30**	1.10	**139**	2.47	**119**	7.36	**107**	1.26	**23**	1.56	**45**	1.81
2.5	**52**	2.08	**76**	3.07	**96**	6.27	**115**	2.48	**269**	13.38	**219**	8.38
3.5	**57**	1.83	**115**	2.72	**274**	7.42	**107**	3.55	**18**	1.69	**190**	6.17
4.5	**70**	2.66	**117**	3.76	**393**	20.51	**135**	3.80	8	1.60	**162**	7.20
5.5	**93**	3.36	**166**	5.21	**338**	20.55	**114**	3.45	8	0.75	**149**	3.05
6.5	**70**	2.74	**127**	3.78	**519**	12.73	**170**	6.20	**78**	2.34	**93**	4.35
7.5	**77**	2.08	**160**	3.78	**418**	13.22	**154**	5.03	**78**	5.07	**146**	4.01
8.5	**37**	1.62	**153**	3.99	**449**	16.29	**204**	14.74	**21**	1.48	**116**	0.51
9.5	**37**	1.93	**166**	4.15	**581**	26.01	**124**	1.49	**18**	1.05	**90**	2.42
10.5	no sample**	no sample**	**145**	3.00	**634**	24.96	**196**	5.99	**11**	1.37	**88**	3.25
11.5	**25**	1.06	**154**	4.24	**343**	7.18	**193**	5.33	7	1.32	**121**	1.89
12.5	no sample**	no sample**	**160**	3.61	**827**	37.75	**492**	14.70	**10**	0.81	**76**	2.79
13.5	**34**	0.62	**123**	2.34	**700**	54.06	**255**	8.16	**12**	1.93	**13**	0.46
14.5	no sample**	no sample**	**185**	3.87	**321**	22.13	**261**	17.82	8	1.56	**10**	0.51
15.5	**37**	2.17	**154**	1.57	no sample**	no sample**	**200**	3.69	9	0.60	**71**	4.30
blank 1	12.10	0.38	8.91	0.50	68.14	2.84	30.82	3.05	21.18	2.17	13.39	0.32
blank 2	10.27	0.37	8.48	0.39	34.71	1.41	27.11	2.42	15.98	1.26	13.41	0.38
blank 3	5.40	0.28	7.71	0.33	26.27	1.60	23.55	2.00	14.20	1.45	12.13	0.46
blank 4	4.78	0.27	7.87	0.39	21.12	1.33	23.00	1.13	11.19	0.82	13.15	0.77
blank 5	4.79	0.18	7.46	0.22	18.55	1.44	21.36	2.06	10.54	0.70	14.03	1.86
correction value	7.47		8.08		33.76		25.17		15.90		13.22	
LoD	4.20		4.20		6.81		4.49		4.49		9.32	
LoQ	11.32		11.32		18.73		9.23		9.23		22.86	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 11: Carbon concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in mg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**157**	4.85	**45**	1.41	**87**	2.41	**139**	2.66	**198**	7.57	**101**	3.11
-4.5	**289**	9.90	**74**	2.76	**126**	3.53	**115**	4.17	**150**	3.53	**71**	0.83
-3.5	**155**	2.88	**107**	5.13	**85**	3.39	**179**	2.69	**244**	3.41	**92**	3.47
-2.5	**146**	2.92	**116**	3.65	**101**	3.28	**82**	3.88	**275**	6.24	**99**	2.41
-1.5	**125**	3.88	**106**	2.49	**95**	2.64	**146**	5.12	**264**	8.40	**83**	2.15
-0.5	**149**	5.59	**119**	1.97	**183**	4.38	**70**	0.66	**226**	7.54	**69**	1.33
0.5	**184**	4.01	**194**	5.06	**157**	5.30	**68**	4.36	**278**	11.59	**84**	2.75
1.5	**199**	7.71	**303**	5.43	**207**	3.57	**41**	1.89	**132**	6.33	**147**	3.56
2.5	**217**	6.20	**270**	8.38	**244**	9.20	no sample ***	no sample ***	**190**	5.14	**176**	6.03
3.5	**204**	2.98	**305**	11.40	**260**	9.26	no sample ***	no sample ***	**276**	14.71	**258**	11.34
4.5	**270**	8.27	**401**	7.00	**333**	7.11	**100**	2.95	**340**	11.49	**246**	7.11
5.5	**296**	6.41	**419**	17.57	**366**	12.46	**97**	2.45	**384**	5.70	**315**	7.37
6.5	**530**	23.73	**606**	10.68	**582**	27.84	**96**	4.40	**216**	11.14	**327**	10.32
7.5	**530**	21.20	**591**	24.53	**480**	8.76	**142**	5.40	**208**	5.47	**357**	14.01
8.5	**531**	19.82	**490**	26.20	**479**	7.62	**150**	7.81	**342**	14.02	**408**	11.82
9.5	**484**	14.84	**484**	19.18	**813**	39.38	**122**	2.97	**304**	16.39	**430**	10.86
10.5	**730**	44.44	**486**	20.35	**964**	58.19	**69**	3.17	**287**	12.24	**291**	4.42
11.5	**646**	27.51	**536**	28.15	**924**	50.01	**172**	6.77	**220**	14.66	**358**	18.97
12.5	**574**	24.87	**474**	15.38	**916**	51.22	no sample ***	no sample ***	**194**	2.67	**332**	5.53
13.5	**451**	19.36	**582**	28.38	**885**	38.48	**193**	3.76	**276**	6.08	**405**	16.05
14.5	**645**	38.59	**642**	35.34	**957**	59.26	no sample ***	no sample ***	**265**	15.17	**231**	7.28
15.5	**364**	17.49	**712**	28.98	**987**	58.32	no sample ***	no sample ***	**187**	8.95	**272**	11.39
blank 1	15.68	2.12	15.68	2.12	17.64	2.67	9.65	0.68	11.40	0.96	7.93	0.54
blank 2	12.89	1.66	12.89	1.66	17.14	1.86	10.63	0.70	11.05	0.94	6.03	0.22
blank 3	<LoD		<LoD		13.43	1.34	9.55	0.49	10.82	0.87	7.07	0.24
blank 4	<LoD		<LoD		<LoD		<LoD		9.58	0.40	5.97	0.27
blank 5	<LoD		<LoD		<LoD						5.97	0.11
correction value	5.71		5.71		9.64		5.97		8.57		6.59	
LoD	11.87		11.87		11.87		9.52		9.52		2.16	
LoQ	31.23		31.23		31.23		21.36		21.36		5.06	

Day	27.00		43.00		69.00		85.00		110.00		148.00	
Profile	7.00		8.00		9.00		10.00		11.00		12.00	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**29**	1.43	10	0.50	**73**	4.15	**26**	1.50	**19**	1.95	12	0.56
-4.5	**49**	1.54	12	0.23	**45**	6.47	7	1.21	**15**	1.19	14	1.04
-3.5	**34**	0.84	12	0.35	**58**	5.07	19	1.36	**20**	2.78	13	0.69
-2.5	**26**	0.59	12	0.35	**51**	3.74	**19**	1.50	8	1.58	13	0.96
-1.5	20	0.41	11	0.24	**52**	3.69	17	1.37	6	0.78	12	1.46
-0.5	13	0.32	16	0.46	**26**	2.40	**27**	1.22	5	0.36	13	0.82
0.5	11	0.40	**59**	1.45	**116**	6.92	**116**	7.48	6	1.36	**25**	0.65
1.5	13	0.68	**82**	2.71	**245**	9.34	**173**	6.86	**13**	1.23	**71**	2.59
2.5	14	0.70	**122**	4.00	**347**	21.95	**258**	19.20	**10**	1.01	**101**	5.04
3.5	18	0.56	**155**	4.03	**378**	26.50	**86**	7.09	**75**	1.46	**144**	8.35
4.5	16	0.28	**169**	4.28	**73**	6.00	**82**	2.61	**69**	3.54	**83**	4.13
5.5	16	0.46	**166**	4.52	**293**	11.72	**102**	6.01	**40**	1.88	**99**	4.12
6.5	16	0.60	**185**	5.17	**448**	18.21	**98**	3.59	no sample**	no sample**	**102**	4.19
7.5	17	0.41	**191**	2.41	**389**	18.45	**79**	2.68	no sample**	no sample**	**55**	1.79
8.5	23	0.75	**198**	5.25	**661**	26.47	**94**	2.98	no sample**	no sample**	**66**	1.12
9.5	**47**	0.54	**177**	4.45	**289**	13.87	**111**	5.32	no sample**	no sample**	**62**	1.73
10.5	**31**	0.66	**163**	2.70	**396**	16.99	**59**	2.12	no sample**	no sample**	**79**	2.83
11.5	**34**	0.58	**219**	6.16	**329**	25.55	**60**	3.72	no sample**	no sample**	**56**	0.86
12.5	**64**	1.24	**172**	2.73	**386**	9.37	<LoD		no sample**	no sample**	no sample**	no sample**
13.5	24	0.55	**134**	3.00	**711**	46.34	no sample ***	no sample ***	no sample**	no sample**	**26**	0.34
14.5	**45**	1.01	**143**	2.55	**752**	13.19	no sample ***	no sample ***	no sample**	no sample**	**87**	3.39
15.5	21	0.70	**175**	6.29	**757**	30.02	no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	<LoD		9.49	0.78	20.32	3.43	26.63	0.85	15.14	8.83	9.33	0.40
blank 2	<LoD		<LoD		14.44	1.74	18.38	2.91	12.97	11.61	<LoD	
blank 3	<LoD		<LoD		14.47	1.67	17.98	1.85	13.02	14.22	9.79	0.57
blank 4	<LoD		<LoD		11.25	1.22	18.40	5.45	10.21	13.84	<LoD	
blank 5	<LoD		<LoD		11.79	1.72	14.44	1.45	7.75	16.38	<LoD	
correction value	0.00		1.90		14.46		19.17		11.95		3.83	
LoD	9.20		9.20		9.29		6.81		4.49		9.32	
LoQ	25.11		25.11		22.81		18.73		9.23		22.86	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 12: Sulfur concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in mg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**61.81**	0.59	**84.02**	2.23	**82.57**	2.51	**22.38**	1.90	**83.91**	2.10	**57.18**	4.03
-4.5	**75.60**	3.17	**88.97**	3.25	**79.55**	1.73	**31.97**	2.21	**84.87**	6.56	**50.93**	5.06
-3.5	**69.79**	0.59	**92.51**	5.18	**81.89**	2.39	**36.68**	2.00	**91.30**	3.17	**54.55**	6.52
-2.5	**64.60**	1.25	**68.75**	3.25	**76.42**	0.56	**31.96**	0.89	**48.64**	2.33	**52.68**	5.21
-1.5	**63.98**	2.35	**90.28**	2.11	**86.30**	4.34	**29.20**	3.24	**47.07**	1.72	**57.19**	6.05
-0.5	**71.47**	1.29	**71.47**	7.60	**78.07**	5.92	**35.18**	2.27	**83.37**	6.04	**40.37**	1.62
0.5	**60.41**	2.87	**70.70**	2.92	**46.96**	2.28	**41.77**	2.91	**60.36**	2.85	**61.71**	5.03
1.5	**49.94**	0.33	**41.87**	1.65	**35.15**	1.48	**33.19**	1.95	**47.71**	2.94	**36.71**	2.37
2.5	**44.89**	1.93	**24.83**	0.62	**28.41**	2.61	**30.55**	2.89	**35.30**	1.08	**33.67**	2.86
3.5	**43.25**	3.43	**22.46**	1.41	**23.00**	1.03	**23.65**	1.68	**18.26**	1.63	**16.31**	1.00
4.5	**31.76**	0.84	**15.47**	1.06	**13.74**	1.57	**17.97**	0.85	**14.24**	1.53	**17.95**	1.02
5.5	**19.29**	0.24	**11.28**	0.60	**11.68**	1.81	**18.07**	2.53	**7.52**	1.44	**12.92**	0.36
6.5	**11.40**	1.51	**9.01**	0.75	**5.29**	2.08	**12.21**	1.57	3.79	1.25	**8.61**	0.31
7.5	**9.69**	1.12	**4.76**	0.02	**3.26**	0.75	**11.81**	1.03	3.13	1.15	**6.21**	0.24
8.5	**8.50**	0.96	2.31	0.64	1.44	0.23	**9.42**	0.99	<LoD		**2.86**	0.10
9.5	**2.65**	0.59	0.99	0.78	1.18	0.61	**8.76**	1.11	<LoD		**1.60**	0.07
10.5	1.81	0.56	<LoD		<LoD		7.00	1.14	<LoD		**1.54**	0.11
11.5	1.31	1.26	<LoD		1.00	0.62	5.28	1.17	<LoD		<LoD	
12.5	<LoD		<LoD		1.41	0.59	<LoD		<LoD		<LoD	
13.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
14.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
15.5	1.07	1.08	<LoD		<LoD		<LoD		<LoD		<LoD	
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		0.03	0.00
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		0.03	0.00
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		0.03	0.00
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		0.05	0.00
blank 5	<LoD		<LoD		<LoD		<LoD		<LoD		0.03	0.00
correction value	0.00		0.00		0.00		0.00		0.00		0.04	
LoD	0.99		0.99		0.99		2.89		2.89		0.02	
LoQ	2.57		2.57		2.57		7.47		7.47		0.06	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**118.97**	5.54	**133.77**	1.79	**191.40**	4.66	**271.25**	23.67	**243.91**	14.90	**235.98**	7.99
-4.5	**110.05**	3.00	**135.27**	5.51	**190.01**	6.96	**285.99**	11.57	**250.66**	11.96	**235.01**	10.08
-3.5	**99.28**	1.55	**130.92**	0.87	**198.31**	2.74	**293.64**	22.38	**240.83**	9.02	**238.90**	4.72
-2.5	**90.81**	2.18	**131.03**	1.45	**230.49**	3.42	**187.02**	8.31	**293.78**	17.34	**227.17**	4.19
-1.5	**90.16**	2.45	**130.65**	2.67	**176.05**	5.78	**282.50**	10.82	**264.95**	9.55	**221.80**	3.35
-0.5	**92.05**	2.48	**129.12**	1.73	**180.68**	2.89	**302.28**	14.80	**266.31**	5.39	**229.09**	10.14
0.5	**91.71**	1.57	**130.59**	2.97	**188.92**	4.64	**303.76**	11.35	**224.24**	10.17	**229.01**	5.19
1.5	**72.86**	0.69	**107.66**	1.34	**149.91**	3.28	**217.31**	9.68	**212.32**	11.79	**215.28**	9.04
2.5	**44.87**	1.13	**67.21**	1.88	**102.16**	3.35	**146.50**	4.60	**159.05**	2.90	**160.28**	5.99
3.5	**24.73**	0.42	**44.10**	1.01	**67.79**	0.98	**99.77**	4.97	**112.37**	7.48	**117.88**	3.16
4.5	**12.71**	0.25	**22.13**	0.68	**35.69**	1.43	**72.03**	2.77	**63.62**	2.82	**85.28**	1.70
5.5	**7.46**	0.14	**11.14**	0.09	**18.58**	0.61	**33.89**	1.76	**41.53**	2.22	**58.92**	2.66
6.5	**3.94**	0.20	**5.68**	0.12	no sample *	no sample *	**31.47**	2.21	**28.54**	0.75	**40.71**	0.62
7.5	**2.03**	0.02	**2.35**	0.10	no sample *	no sample *	**15.02**	0.22	**14.72**	0.84	**26.86**	0.65
8.5	**1.18**	0.05	**1.89**	0.07	no sample *	no sample *	**8.68**	0.41	**7.68**	0.32	**16.53**	0.34
9.5	<LoD		<LoD		**6.25**	0.20	**5.04**	0.29	**9.03**	0.54	**11.43**	0.12
10.5	<LoD		<LoD		**4.95**	0.09	**2.42**	0.17	**3.86**	0.14	**7.46**	0.32
11.5	<LoD		<LoD		**1.91**	0.02	**1.31**	0.06	**2.76**	0.18	**5.23**	0.17
12.5	<LoD		<LoD		**1.26**	0.03	**1.01**	0.06	**1.59**	0.05	**3.41**	0.10
13.5	<LoD		<LoD		**1.13**	0.04	**1.05**	0.04	**1.09**	0.04	**2.95**	0.08
14.5	<LoD		<LoD		<NWG	0.04	<LoD		**1.08**	0.02	no sample **	no sample **
15.5	<LoD		<LoD		**1.04**	0.02	**1.01**	0.05	**1.15**	0.04	**2.44**	0.12
blank 1	0.09	0.00	0.06	0.00	<LoD		0.03	0.00	0.05	0.00	<LoD	
blank 2	0.09	0.00	0.07	0.00	0.09	0.00	0.03	0.00	0.07	0.01	<LoD	
blank 3	0.09	0.00	0.07	0.00	0.07	0.00	0.03	0.00	<LoD		<LoD	
blank 4	0.09	0.00	0.08	0.00	0.07	0.00	0.03	0.00	<LoD		<LoD	
blank 5	0.10	0.00	0.06	0.00	0.08	0.00	<LoD		<LoD		<LoD	
correction value	0.09		0.07		0.06		0.03		0.02		0.00	
LoD	0.03		0.03		0.06		0.03		0.03		0.14	
LoQ	0.08		0.08		0.17		0.08		0.08		0.33	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 13: Sulfur concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in mg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**69.29**	3.95	**86.33**	3.06	**69.40**	3.54	**13.43**	2.58	**35.42**	1.37	**46.22**	3.30
-4.5	**61.12**	2.36	**77.69**	3.04	**87.53**	5.16	**11.13**	1.10	**61.13**	2.92	**51.33**	3.04
-3.5	**71.78**	1.64	**70.56**	1.99	**81.18**	1.57	**11.25**	0.89	**56.59**	2.58	**47.23**	3.13
-2.5	**79.92**	3.94	**75.67**	6.08	**79.36**	4.98	**12.33**	1.70	**59.11**	2.87	**47.78**	4.26
-1.5	**79.54**	3.35	**75.18**	3.10	**87.87**	2.75	**12.28**	1.30	**44.30**	2.03	**50.31**	3.50
-0.5	**73.10**	2.70	**77.68**	0.72	**67.54**	3.28	**13.13**	1.70	**38.42**	3.49	**48.39**	3.23
0.5	**86.64**	4.27	**49.42**	2.74	**48.11**	1.08	**15.63**	2.21	**42.92**	3.57	<LoD	0.62
1.5	**64.41**	2.46	**39.69**	2.74	**34.91**	2.65	**15.83**	1.52	**29.73**	1.90	**6.54**	1.51
2.5	**52.14**	1.03	**26.55**	1.27	**14.04**	2.37	**15.30**	2.16	**14.89**	2.03	**16.09**	2.56
3.5	**41.38**	2.48	**17.86**	2.15	**13.43**	1.22	**7.79**	1.19	2.54	1.44	<LoD	
4.5	**17.48**	2.13	**13.47**	1.20	**10.23**	1.66	5.21	1.57	<LoD		<LoD	
5.5	**10.76**	1.53	**9.14**	1.24	2.57	0.69	4.99	1.05	<LoD		<LoD	
6.5	**4.84**	0.92	**6.85**	0.37	<LoD		no sample ***	no sample ***	<LoD		<LoD	
7.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
8.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
9.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
10.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
11.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
12.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
13.5	<LoD	21.47	<LoD		<LoD		<LoD		<LoD		<LoD	
14.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
15.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
blank 1	11.78	0.13	6.05	0.33	8.67	0.27	10.63	0.55	10.63	0.55	10.06	0.85
blank 2	6.84	0.24	6.56	0.21	8.67	0.43	10.14	0.59	10.14	0.59	9.45	0.76
blank 3	7.40	0.31	6.87	0.39	8.03	0.35	12.94	0.65	12.94	0.65	13.97	1.03
blank 4	10.52	0.24	6.80	0.15	9.40	0.20	9.59	0.51	9.59	0.51	29.53	2.64
blank 5	7.99	0.24	5.94	0.26	7.16	0.20	14.25	0.36	14.25	0.36	34.53	2.93
correction value	8.907		6.442		8.385		11.511		11.511		19.507	
LoD	1.205		1.205		1.205		1.898		1.898		1.710	
LoQ	2.868		2.868		2.868		5.021		5.021		4.050	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**148.68**	6.50	**65.24**	2.31	**200.29**	9.88	**276.46**	6.08	**295.12**	7.08	**215.50**	3.40
-4.5	**114.69**	4.42	**64.41**	0.63	**185.38**	18.88	**264.65**	7.77	**271.55**	22.64	**224.07**	8.00
-3.5	**112.96**	3.84	**64.15**	1.63	**164.95**	4.97	**236.72**	5.12	**320.00**	10.91	**232.74**	9.32
-2.5	**120.13**	3.95	**65.32**	1.34	**151.31**	7.35	**246.95**	9.10	**316.75**	13.81	**238.93**	17.16
-1.5	**116.82**	3.29	**64.47**	0.89	**145.46**	8.29	**256.48**	8.66	**238.78**	11.41	**230.83**	10.28
-0.5	**96.06**	2.95	**63.70**	1.57	**145.16**	3.51	**259.79**	8.95	**233.35**	10.43	**233.91**	11.34
0.5	**92.88**	1.91	**65.64**	1.64	**150.97**	9.38	**292.78**	7.70	**274.18**	7.19	**241.95**	13.67
1.5	**62.60**	4.95	**54.90**	3.24	**104.42**	10.20	**221.27**	11.55	**237.55**	10.90	**207.87**	9.72
2.5	**36.86**	3.06	**29.15**	0.50	**71.76**	5.62	**116.06**	3.16	**168.67**	3.81	**164.52**	9.09
3.5	**12.62**	0.64	**15.85**	0.46	**42.61**	3.38	**91.74**	2.42	**105.83**	5.56	**124.31**	6.25
4.5	**5.69**	1.23	**4.78**	0.35	**16.26**	2.40	**51.02**	2.37	**67.99**	2.90	**90.47**	4.58
5.5	<LoD		<LoD		**4.54**	1.29	**23.11**	0.77	**44.48**	2.21	no sample **	no sample **
6.5	<LoD		<LoD		no sample *	no sample *	**34.97**	1.95	**28.81**	1.56	**39.40**	0.23
7.5	<LoD		<LoD		no sample *	no sample *	**4.67**	0.49	**13.46**	1.41	**26.79**	1.55
8.5	<LoD		<LoD		no sample *	no sample *	<LoD		**6.19**	0.63	**14.52**	0.88
9.5	<LoD		<LoD		<LoD		<LoD		**6.85**	0.30	**9.59**	0.35
10.5	<LoD		<LoD		<LoD		<LoD		<LoD		**5.19**	0.29
11.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
12.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
13.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
14.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
15.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
blank 1	7.57	0.57	7.07	0.13	6.71	0.56	8.78	0.82	3.44	0.26	3.06	0.05
blank 2	10.81	1.03	7.34	0.47	5.94	0.30	8.83	0.25	4.12	0.21	1.43	0.11
blank 3	16.46	1.18	8.05	0.49	7.98	0.42	8.45	0.65	4.16	0.29	2.74	0.18
blank 4	18.17	1.18	7.00	0.41	15.55	0.94	6.85	0.58	2.71	0.20	1.53	0.22
blank 5	12.30	0.94	6.87	0.29	11.68	0.76	10.30	0.55			2.47	0.22
correction value	13.06		7.27		9.57		8.64		2.88		2.25	
LoD	1.71		1.20		0.16		0.29		0.15		0.41	
LoQ	4.05		3.07		0.37		0.79		0.39		1.07	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 14: Sulfur concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in mg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**68.72**	0.70	**85.66**	2.99	**93.84**	2.91	**24.78**	2.24	**56.20**	3.03	**57.02**	1.33
-4.5	**64.17**	6.90	**78.73**	8.95	**106.79**	4.23	**30.30**	1.73	**54.52**	3.26	**61.47**	2.78
-3.5	**61.37**	2.35	**73.36**	1.47	**103.23**	3.08	**19.93**	0.56	**78.25**	2.08	**57.28**	1.02
-2.5	**63.63**	1.02	**84.32**	1.48	**106.03**	2.11	**34.04**	2.47	**55.94**	2.65	**62.95**	2.87
-1.5	**73.96**	3.25	**78.68**	1.23	**118.05**	4.45	**24.93**	1.64	**114.29**	4.48	**61.02**	1.74
-0.5	**75.93**	2.39	**71.08**	4.59	**74.54**	1.29	**31.35**	1.64	**84.27**	3.94	**70.31**	2.39
0.5	**68.17**	3.45	**46.45**	0.92	**53.85**	1.00	**27.03**	2.49	**70.19**	2.29	**48.33**	1.78
1.5	**73.41**	1.69	**26.25**	0.05	**37.81**	1.23	**25.64**	1.31	**28.83**	1.46	**33.68**	0.82
2.5	**68.52**	1.03	**16.38**	1.00	**26.85**	2.08	**21.88**	0.93	**22.10**	0.84	**20.62**	0.85
3.5	**39.15**	3.66	**9.73**	1.54	**20.36**	2.84	**17.52**	2.37	**9.17**	0.94	**13.61**	0.38
4.5	**34.31**	0.71	**7.48**	0.06	**17.94**	0.23	**14.81**	1.25	5.20	1.18	<LoD	
5.5	**23.04**	1.97	**5.96**	1.07	**9.66**	0.53	**14.26**	0.78	5.90	1.33	**13.00**	0.53
6.5	**15.85**	1.98	2.13	0.65	**4.58**	0.73	**13.65**	0.29	5.02	0.49	<LoD	
7.5	**14.61**	1.50	<LoD		**3.32**	0.74	**11.46**	1.40	3.10	1.04	**10.10**	0.26
8.5	**3.92**	0.87	<LoD		1.27	0.60	**10.07**	1.23	<LoD		<LoD	
9.5	**3.79**	0.35	<LoD		1.17	0.93	**8.46**	0.79	<LoD		**6.79**	0.23
10.5	1.29	1.10	<LoD		<LoD		6.88	0.44	<LoD		**4.22**	0.17
11.5	<LoD		<LoD		<LoD		4.33	0.46	<LoD		**2.32**	0.12
12.5	<LoD		<LoD		1.05	0.65	3.53	0.93	<LoD		**1.18**	0.04
13.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
14.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
15.5	1.11	0.11	<LoD		<LoD		<LoD		<LoD		<LoD	
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		0.05	0.00
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		0.05	0.00
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		0.04	0.00
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		0.08	0.01
blank 5	1.03	0.86	<LoD		<LoD		<LoD		<LoD		0.03	0.00
correction value	0.21		0.00		0.00		0.00		0.00		0.05	
LoD	0.99		0.99		0.99		2.89		2.89		0.03	
LoQ	2.57		2.57		2.57		7.47		7.47		0.07	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**111.64**	3.45	**143.48**	3.82	**177.87**	4.59	**167.76**	4.11	**157.26**	7.89	**110.82**	4.41
-4.5	**94.83**	2.11	**141.26**	1.49	**159.72**	5.12	**221.87**	11.68	**146.18**	7.33	**110.76**	4.54
-3.5	**91.75**	2.39	**142.00**	4.68	**156.90**	4.01	**201.43**	7.54	**184.51**	9.44	**104.93**	3.61
-2.5	**82.86**	3.48	**139.41**	4.27	**152.21**	4.69	**211.12**	15.57	**169.16**	5.21	**107.21**	4.39
-1.5	**81.53**	1.71	**143.52**	13.12	**130.06**	4.92	**187.19**	4.70	**166.80**	4.79	**111.09**	3.72
-0.5	**82.47**	2.49	**141.25**	2.03	**133.98**	2.60	**184.89**	12.54	**141.64**	1.59	**114.01**	4.68
0.5	**83.32**	2.33	**121.31**	2.58	**119.88**	1.11	**147.85**	8.33	**146.81**	4.49	**101.57**	3.18
1.5	**59.09**	1.58	**86.63**	2.34	**109.56**	1.48	**95.19**	6.60	**133.92**	4.10	**68.33**	2.92
2.5	**34.40**	0.61	**54.10**	1.41	**81.64**	1.09	**52.46**	2.64	**124.21**	7.45	**44.03**	1.56
3.5	**20.46**	0.39	**36.86**	3.43	**51.81**	1.30	**36.79**	2.10	**70.08**	4.05	**23.63**	1.07
4.5	**11.15**	0.39	**20.83**	0.65	**41.05**	1.20	**20.01**	0.77	**50.77**	2.47	**14.25**	0.59
5.5	**5.49**	0.15	**9.86**	0.22	**25.90**	0.83	**13.56**	0.75	**33.78**	1.03	**9.71**	0.44
6.5	**3.13**	0.15	**6.68**	0.12	**10.23**	0.21	**8.81**	0.68	**22.57**	1.26	**6.18**	0.39
7.5	**1.62**	0.07	**4.72**	0.06	**15.45**	0.68	**8.00**	0.25	**12.28**	0.96	**2.20**	0.10
8.5	**1.19**	0.03	**2.70**	0.04	**18.32**	0.37	**7.16**	0.31	**8.29**	0.20	**1.56**	0.04
9.5	<LoD		**3.10**	0.09	**6.45**	0.09	**6.86**	0.27	**5.88**	0.16	**1.37**	0.06
10.5	no sample**	no sample**	**1.28**	0.08	**3.31**	0.07	**6.67**	0.35	**5.12**	0.17	**1.35**	0.09
11.5	<LoD		**1.00**	0.01	**2.39**	0.06	**6.66**	0.30	**4.61**	0.22	**1.42**	0.05
12.5	no sample**	no sample**	<LoD		**2.34**	0.05	**7.29**	0.20	**4.31**	0.20	**1.34**	0.07
13.5	<LoD		<LoD		**2.13**	0.04	**7.41**	0.16	**5.94**	0.05	<LoD	
14.5	no sample**	no sample**	<LoD		**1.51**	0.03	**7.16**	0.55	**6.71**	0.25	<LoD	
15.5	<LoD		<LoD		no sample**	no sample**	**7.60**	0.60	**4.20**	0.12	**1.50**	0.07
blank 1	0.14	0.00	0.06	0.00	0.10	0.00	0.08	0.01	0.06	0.00	0.22	0.01
blank 2	0.12	0.01	0.07	0.00	0.09	0.00	0.06	0.00	0.04	0.00	0.18	0.01
blank 3	0.06	0.00	0.08	0.00	0.09	0.00	0.07	0.01	0.03	0.00	0.17	0.01
blank 4	0.06	0.00	0.06	0.00	0.08	0.00	0.05	0.00	0.21	0.01	0.18	0.00
blank 5	0.06	0.00	0.10	0.00	0.07	0.00	0.05	0.00	0.04	0.00	0.21	0.01
correction value	0.09		0.07		0.09		0.06		0.05		0.19	
LoD	0.03		0.03		0.06		0.03		0.03		0.14	
LoQ	0.08		0.08		0.17		0.08		0.08		0.33	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 15: Sulfur concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in mg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**75.57**	1.24	**79.81**	2.04	**87.99**	2.16	**21.07**	1.96	**50.36**	3.05	**79.50**	5.14
-4.5	**95.32**	2.99	**93.83**	3.22	**112.20**	3.25	**19.56**	1.99	**44.78**	2.10	**57.36**	1.37
-3.5	**86.05**	5.49	**100.36**	3.18	**97.62**	1.37	**24.23**	0.97	**63.07**	4.11	**81.62**	2.29
-2.5	**87.00**	6.13	**108.05**	2.83	**97.31**	2.91	**20.87**	1.09	**71.62**	2.35	**98.80**	3.50
-1.5	**85.95**	2.80	**96.16**	4.38	**90.13**	4.74	**21.71**	2.33	**74.15**	2.01	**87.46**	3.03
-0.5	**88.20**	3.32	**72.61**	3.10	**70.76**	2.35	**20.99**	2.60	**65.59**	2.05	**77.83**	2.84
0.5	**93.24**	4.25	**55.37**	1.16	**39.69**	3.28	**22.45**	0.86	**70.97**	2.67	**79.70**	3.35
1.5	**94.23**	2.74	**31.46**	1.49	**34.24**	1.85	**24.57**	1.39	**25.68**	3.33	**58.96**	1.73
2.5	**65.21**	3.69	**18.10**	1.31	**25.51**	0.56	no sample ***	no sample ***	**15.37**	2.09	**40.71**	0.80
3.5	**47.04**	2.08	**11.51**	1.05	**19.54**	0.58	no sample ***	no sample ***	**8.67**	1.25	**21.90**	0.94
4.5	**29.40**	2.87	**9.53**	0.79	**16.18**	0.95	**17.13**	1.45	**5.76**	1.15	**18.73**	0.83
5.5	**24.30**	2.29	**5.90**	0.69	**7.10**	1.31	**14.37**	1.26	**4.73**	0.96	**14.38**	1.09
6.5	**20.35**	0.73	**3.42**	0.74	**4.71**	0.75	**13.02**	1.62	**3.23**	0.71	**4.42**	0.61
7.5	**13.00**	0.69	1.38	0.57	2.96	0.64	**10.76**	1.17	1.53	1.29	<LoD	
8.5	**4.36**	0.98	<LoD		<LoD		**10.18**	1.11	<LoD		<LoD	
9.5	2.30	1.01	<LoD		<LoD		**8.17**	2.09	1.69	1.52	<LoD	
10.5	1.93	0.35	<LoD		<LoD		**5.95**	1.07	<LoD		<LoD	
11.5	<LoD		<LoD		<LoD		3.15	1.28	<LoD		<LoD	
12.5	<LoD		<LoD		1.94	0.93	no sample ***	no sample ***	<LoD		<LoD	
13.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
14.5	<LoD		1.42	0.71	<LoD		no sample ***	no sample ***	<LoD		<LoD	
15.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		41.41	0.70
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD						<LoD	
correction value	0.00		0.00		0.00		0.00		0.00		8.28	
LoD	1.27		1.27		1.27		1.26		1.26		0.02	
LoQ	3.24		3.24		3.24		3.23		3.23		0.04	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**41.55**	2.23	**78.76**	2.26	**103.81**	2.11	**152.10**	2.79	**155.51**	11.27	**106.33**	4.82
-4.5	**50.64**	1.43	**77.48**	2.14	**108.71**	8.78	**125.70**	3.02	**161.09**	10.15	**107.43**	4.16
-3.5	**48.71**	1.40	**77.49**	1.76	**103.07**	4.23	**141.89**	5.26	**191.31**	9.83	**107.96**	2.70
-2.5	**42.80**	1.57	**75.86**	1.94	**100.99**	6.16	**152.76**	6.75	**145.90**	7.02	**108.02**	2.07
-1.5	**42.13**	0.96	**76.50**	1.05	**95.34**	3.81	**161.18**	3.85	**131.41**	4.76	**108.00**	2.27
-0.5	**42.51**	1.64	**77.04**	0.89	**87.03**	3.59	**153.98**	4.03	**129.22**	5.29	**111.66**	4.95
0.5	**43.54**	1.18	**70.10**	1.53	**106.69**	5.27	**110.58**	2.99	**141.22**	5.33	**104.41**	3.05
1.5	**30.67**	1.39	**48.93**	1.80	**71.40**	3.21	**82.83**	2.77	**128.89**	4.46	**72.72**	1.74
2.5	**18.19**	0.38	**31.59**	1.11	**59.34**	5.09	**55.64**	2.18	**115.00**	7.24	**45.48**	2.18
3.5	**10.95**	0.11	**20.11**	0.40	**32.15**	1.25	**37.75**	1.10	**83.00**	2.53	**24.80**	0.57
4.5	**5.81**	0.09	**11.89**	0.31	**20.61**	1.06	**21.40**	1.04	**59.74**	2.32	**14.64**	0.51
5.5	**3.10**	0.12	**5.76**	0.13	**15.63**	0.69	**14.57**	0.18	**39.68**	1.41	**10.16**	0.46
6.5	**1.69**	0.07	**3.94**	0.09	**10.52**	0.33	**10.07**	0.57	no sample**	no sample**	**5.58**	0.44
7.5	<LoD		**2.74**	0.10	**11.03**	0.67	**9.17**	0.39	no sample**	no sample**	**2.29**	0.10
8.5	<LoD		**1.60**	0.02	**9.31**	0.47	**7.83**	0.39	no sample**	no sample**	**1.65**	0.07
9.5	<LoD		**1.90**	0.04	**3.48**	0.09	**7.49**	0.36	no sample**	no sample**	**1.50**	0.05
10.5	<LoD		<LoD		**1.88**	0.06	**7.23**	0.51	no sample**	no sample**	**1.46**	0.07
11.5	<LoD		<LoD		**1.41**	0.15	**7.52**	0.23	no sample**	no sample**	**1.33**	0.03
12.5	<LoD		<LoD		<LoD		<LoD		no sample**	no sample**	no sample**	no sample**
13.5	<LoD		<LoD		**1.34**	0.10	no sample ***	no sample ***	no sample**	no sample**	**1.40**	0.07
14.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	no sample**	no sample**	**1.41**	0.06
15.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	0.03	0.00	<LoD		<LoD		<LoD		0.09	3.72	<LoD	
blank 2	<LoD		<LoD		0.04	0.00	<LoD		0.04	4.35	<LoD	
blank 3	0.06	0.00	<LoD		<LoD		<LoD		0.05	4.02	<LoD	
blank 4	0.06	0.00	<LoD		<LoD		<LoD		0.04	5.66	<LoD	
blank 5	0.05	0.00	<LoD		<LoD		<LoD		0.04	9.38	<LoD	
correction value	0.04		0.00		0.01		0.00		0.06		0.00	
LoD	0.02		0.02		0.03		0.06		0.03		0.14	
LoQ	0.06		0.06		0.07		0.17		0.08		0.33	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 16: Phosphorous concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**9**	7.45	**383**	16.26	**83**	39.48	**33**	2.91	**52**	2.50	<LoD	
-4.5	**59**	9.80	**220**	17.88	**38**	15.67	**34**	2.64	**37**	4.49	<LoD	
-3.5	**73**	20.71	**192**	13.30	**19**	12.51	**1,260**	76.36	**33**	3.06	<LoD	
-2.5	**16**	18.46	**118**	40.79	<LoD		**463**	27.98	1	1.37	<LoD	
-1.5	**25**	16.79	**81**	28.65	<LoD		**22**	3.08	0	1.45	7	4.72
-0.5	**33**	18.22	**71**	14.78	**65**	25.22	**209**	16.32	**23**	2.24	<LoD	
0.5	**77**	39.32	**40**	23.12	**112**	37.22	**56**	3.92	**29**	2.59	**102**	12.70
1.5	**136**	26.92	**7**	5.04	**148**	13.99	**11**	1.23	**284**	10.40	**472**	30.65
2.5	**116**	28.99	**62**	11.42	**387**	56.40	**186**	8.25	**864**	41.39	**1,125**	74.56
3.5	**63**	14.55	**164**	53.05	**517**	26.51	**167**	9.81	**776**	46.13	**1,085**	47.67
4.5	**266**	55.77	**236**	27.16	**751**	81.87	**29**	4.19	**707**	44.30	**1,860**	96.56
5.5	**661**	29.43	**493**	57.54	**570**	121.00	**12**	1.46	**535**	23.32	**1,591**	104.71
6.5	**292**	30.15	**472**	18.15	**306**	46.16	**9**	1.04	**524**	7.60	**1,879**	82.46
7.5	**119**	45.17	**131**	30.79	**109**	22.07	**29**	2.20	**606**	44.03	**805**	26.32
8.5	**245**	32.20	**67**	2.86	**70**	42.69	**75**	4.32	**484**	28.45	**907**	34.42
9.5	**353**	43.09	**182**	33.30	**41**	14.01	**5**	1.08	**513**	31.79	**864**	36.24
10.5	**463**	32.56	**676**	83.94	**27**	10.35	**15**	1.83	**108**	7.42	**1,401**	91.36
11.5	**393**	50.07	**734**	56.96	**36**	22.54	**16**	1.62	**136**	5.71	**834**	45.07
12.5	**888**	169.23	**854**	20.69	**267**	32.48	**11**	1.28	**181**	6.90	**773**	9.42
13.5	**334**	39.24	**690**	16.86	**872**	67.18	**8**	2.06	**173**	3.34	**927**	34.42
14.5	**602**	72.08	**1,583**	193.72	**995**	189.79	**9**	1.27	**173**	3.30	**690**	42.63
15.5	**902**	39.43	**1,122**	39.55	**1,514**	169.00	**13**	1.46	**207**	8.05	**722**	33.12
blank 1	17.48	12.13	19.69	6.62	22.18	5.24	25.50	1.48	28.19	1.00	64.95	4.08
blank 2	<LoD		19.92	5.98	22.83	7.66	21.93	0.78	18.69	0.55	37.74	0.73
blank 3	21.35	8.67	<LoD		17.98	2.06	34.97	1.96	35.96	1.33	47.99	1.91
blank 4	20.05	10.01	18.19	20.28	23.35	17.35	40.84	0.83	22.86	0.55	54.69	1.39
blank 5	12.40	1.53	16.62	8.65	11.88	6.81	43.86	1.63	42.63	1.72	46.89	2.54
correction value	14.26		14.88		19.64		33.42		29.67		50.45	
LoD	10.26		10.26		10.26		2.48		2.48		1.20	
LoQ	27.66		27.66		27.66		7.10		7.10		3.07	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**2**	2.60	**39**	1.72	<LoD		<LoD		**47**	3.54	**17**	1.29
-4.5	<LoD		**26**	1.84	<LoD		<LoD		**13**	0.45	**15**	1.11
-3.5	<LoD		**22**	1.11	<LoD		**33**	10.65	**11**	0.71	**19**	0.92
-2.5	<LoD		**19**	0.71	<LoD		<LoD		**18**	1.38	**20**	1.48
-1.5	<LoD		**18**	1.30	<LoD		**63**	8.76	**12**	0.58	**13**	0.88
-0.5	<LoD		**14**	1.17	<LoD		**34**	7.62	**14**	0.57	**17**	0.96
0.5	<LoD		**7**	0.87	<LoD		**19**	6.33	**6**	0.60	**12**	0.80
1.5	<LoD		**7**	0.77	<LoD		**57**	4.98	**9**	0.86	**24**	2.65
2.5	**170**	9.72	**12**	1.51	<LoD		<LoD		**12**	1.02	**25**	1.92
3.5	**713**	19.25	**71**	1.25	<LoD		0	7.96	**13**	1.28	**23**	0.46
4.5	**1,050**	30.45	**307**	13.08	**256**	21.06	**150**	15.15	**47**	2.94	**21**	1.63
5.5	**1,166**	29.19	**641**	6.13	**990**	65.72	**525**	31.60	**567**	22.21	**17**	1.73
6.5	**1,208**	67.34	**678**	23.86	no sample *	no sample *	**1,981**	88.95	**1,138**	32.59	**16**	1.07
7.5	**1,082**	18.82	**573**	23.56	no sample *	no sample *	**3,162**	107.90	**1,643**	38.54	**19**	1.32
8.5	**826**	14.30	**561**	24.66	no sample *	no sample *	**4,986**	104.15	**2,186**	41.58	**90**	3.53
9.5	**723**	34.57	**459**	5.95	**1,147**	34.10	**5,195**	300.00	**2,567**	107.92	**553**	23.72
10.5	**654**	27.36	**400**	14.15	**2,124**	117.01	**1,369**	111.52	**3,329**	90.51	**897**	46.47
11.5	**601**	17.70	**367**	12.95	**2,807**	48.60	**1,653**	87.89	**3,743**	206.81	**931**	33.52
12.5	**589**	18.00	**323**	15.84	**3,473**	117.37	**2,213**	126.91	**1,628**	28.46	**627**	21.53
13.5	**648**	23.57	**293**	10.12	**3,963**	156.44	**3,146**	70.77	**2,445**	72.14	**299**	8.66
14.5	**615**	32.13	**266**	9.08	**4,041**	45.26	**4,161**	301.31	**3,424**	74.14	no sample **	no sample **
15.5	**708**	24.98	**284**	10.26	**5,331**	208.10	**5,326**	298.15	**4,815**	225.19	**128**	5.30
blank 1	27.56	1.22	9.29	0.61	18.57	1.27	130.93	2.61	7.88	0.14	3.06	0.05
blank 2	32.28	3.03	9.15	0.29	28.69	1.23	158.27	2.71	6.95	0.68	1.43	0.11
blank 3	43.74	1.81	10.80	0.69	23.52	1.52	178.34	13.26	8.09	0.28	2.74	0.18
blank 4	44.43	2.78	8.14	0.55	60.82	2.66	188.81	8.17	7.22	0.43	1.53	0.22
blank 5	45.48	2.36	9.76	0.50	58.92	2.30	72.70	1.70	7.40	0.60	2.47	0.22
correction value	38.70		9.43		38.11		145.81		7.51		2.25	
LoD	0.26		0.26		0.29		0.15		0.15		0.41	
LoQ	0.63		0.63		0.79		0.39		0.39		1.07	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 17: Phosphorous concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**22**	0.94	**520**	18.40	**255**	7.91	**102**	6.92	**87**	3.51	**13**	2.28
-4.5	**27**	0.69	**217**	11.67	**75**	2.12	**38**	1.23	**121**	2.99	**11**	1.31
-3.5	**17**	0.71	**232**	6.74	**55**	4.37	**46**	2.40	**80**	3.09	**16**	3.35
-2.5	**23**	1.08	**142**	6.50	**51**	3.29	**38**	0.65	**56**	2.72	**20**	1.91
-1.5	**24**	0.90	**96**	3.59	**36**	1.39	**35**	1.16	**55**	1.76	**39**	4.59
-0.5	**18**	1.06	**111**	4.71	**89**	3.80	**42**	1.50	**31**	1.01	**16**	3.27
0.5	**109**	3.57	**150**	3.40	**290**	7.48	**30**	1.55	**55**	4.46	3	1.89
1.5	**706**	44.81	**229**	5.62	**509**	15.96	**31**	0.86	**358**	5.09	**54**	5.87
2.5	**910**	30.72	**437**	23.33	**580**	13.00	**36**	2.55	**1,217**	48.72	**429**	33.46
3.5	**661**	19.87	**717**	20.58	**875**	26.94	**296**	4.84	**1,078**	15.75	**639**	44.74
4.5	**631**	15.45	**445**	18.85	**987**	24.86	**384**	13.95	**758**	27.17	**810**	47.40
5.5	**1,146**	25.54	**767**	28.38	**680**	18.70	**144**	3.31	**688**	101.29	**967**	79.03
6.5	**742**	36.01	**679**	23.61	**422**	17.49	no sample ***	no sample ***	**611**	15.86	**1,169**	69.89
7.5	**380**	21.76	**550**	21.77	**196**	8.97	no sample ***	no sample ***	**536**	14.27	**1,518**	27.07
8.5	**622**	13.53	**373**	13.23	**104**	3.29	no sample ***	no sample ***	**527**	10.92	**1,154**	46.57
9.5	**1,696**	32.50	**633**	19.80	**98**	2.10	no sample ***	no sample ***	**499**	14.89	**1,449**	58.48
10.5	**2,808**	163.93	**976**	23.38	**196**	10.55	**28**	1.27	**539**	6.69	**1,866**	30.06
11.5	**3,754**	254.95	**2,122**	87.26	**259**	8.32	**40**	0.57	**538**	12.39	**2,228**	76.51
12.5	**4,156**	279.49	**3,091**	35.98	**1,496**	53.39	**42**	1.69	**816**	18.62	**2,340**	108.20
13.5	**5,062**	21.47	**3,875**	217.19	**3,017**	97.15	**40**	0.72	**653**	10.85	**2,562**	22.37
14.5	**5,213**	176.65	**4,799**	75.92	**3,326**	169.56	**52**	1.14	**638**	14.03	**2,626**	70.03
15.5	**5,126**	295.18	**5,144**	171.46	**3,068**	92.81	no sample ***	no sample ***	**586**	24.125	**3,192**	114.46
blank 1	11.78	0.13	6.05	0.33	8.67	0.27	10.63	0.55	9.92	0.26	10.06	0.85
blank 2	6.84	0.24	6.56	0.21	8.67	0.43	10.14	0.59	19.16	1.01	9.45	0.76
blank 3	7.40	0.31	6.87	0.39	8.03	0.35	12.94	0.65	9.78	0.36	13.97	1.03
blank 4	10.52	0.24	6.80	0.15	9.40	0.20	9.59	0.51	15.82	0.61	29.53	2.64
blank 5	7.99	0.24	5.94	0.26	7.16	0.20	14.25	0.36			34.53	2.93
correction value	8.91		6.44		8.39		11.51		10.94		19.51	
LoD	1.20		1.20		1.20		1.90		1.90		1.71	
LoQ	2.87		2.87		2.87		5.02		5.02		4.05	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**30**	2.46	**32**	1.56	**9**	0.86	**15**	1.00	**14**	0.22	**13**	0.26
-4.5	**22**	0.95	**18**	1.08	**6**	1.44	**10**	1.36	**13**	0.85	**11**	0.86
-3.5	**26**	1.81	**18**	1.02	**5**	1.14	**9**	1.46	**17**	0.64	**39**	3.11
-2.5	**16**	1.89	**13**	0.89	**3**	0.13	**13**	1.30	**16**	1.23	**37**	3.28
-1.5	**19**	0.99	**11**	1.10	**3**	0.75	**8**	0.72	**10**	0.78	**12**	0.72
-0.5	**12**	0.88	**10**	0.88	**2**	0.48	**9**	0.57	**9**	0.89	**11**	0.89
0.5	**5**	0.46	**4**	0.64	**5**	0.70	**19**	1.45	**10**	0.14	**12**	0.78
1.5	**10**	2.06	**7**	0.07	**10**	1.53	**18**	1.37	**13**	0.72	**22**	1.89
2.5	**312**	12.08	**13**	1.47	**34**	3.08	**6**	0.93	**21**	0.75	**27**	2.14
3.5	**919**	36.07	**75**	4.99	**40**	1.47	**10**	0.62	**24**	1.85	**27**	1.82
4.5	**1,708**	126.78	**308**	14.96	**483**	30.95	**117**	3.89	**117**	4.02	**36**	1.92
5.5	**1,681**	53.71	**611**	34.53	**1,726**	120.79	**3,223**	77.40	**1,403**	53.57	no sample **	no sample **
6.5	**1,915**	76.78	**668**	31.96	no sample *	no sample *	**1,852**	94.01	**3,113**	127.95	**19**	1.17
7.5	**1,605**	50.64	**591**	26.87	no sample *	no sample *	**3,565**	214.36	**4,044**	297.86	**22**	1.41
8.5	**3,964**	114.81	**574**	20.15	no sample *	no sample *	**4,335**	188.99	**4,595**	218.14	**111**	5.98
9.5	**4,515**	64.92	**460**	20.10	**4,977**	200.35	**5,071**	104.81	**4,492**	82.68	**606**	32.50
10.5	**3,029**	117.66	**411**	18.00	**4,851**	240.68	**7,101**	297.34	**4,626**	164.00	**932**	41.87
11.5	**3,404**	43.14	**371**	14.77	**4,818**	214.71	**7,786**	324.44	**5,240**	64.79	no sample **	no sample **
12.5	**2,657**	88.82	**333**	14.38	**5,102**	285.27	**6,769**	357.36	**6,255**	564.47	no sample **	no sample **
13.5	**3,308**	113.77	**301**	13.06	**5,269**	355.23	**7,321**	397.36	**6,283**	295.60	no sample **	no sample **
14.5	**3,030**	26.85	**277**	10.99	**5,570**	114.10	**7,511**	401.11	**5,576**	226.18	no sample **	no sample **
15.5	**3,549**	147.06	**292**	11.67	**4,497**	221.41	**6,534**	355.77	**5,621**	208.32	no sample **	no sample **
blank 1	7.57	0.57	7.07	0.13	6.71	0.56	8.78	0.82	3.44	0.26	3.06	0.05
blank 2	10.81	1.03	7.34	0.47	5.94	0.30	8.83	0.25	4.12	0.21	1.43	0.11
blank 3	16.46	1.18	8.05	0.49	7.98	0.42	8.45	0.65	4.16	0.29	2.74	0.18
blank 4	18.17	1.18	7.00	0.41	15.55	0.94	6.85	0.58	2.71	0.20	1.53	0.22
blank 5	12.30	0.94	6.87	0.29	11.68	0.76	10.30	0.55			2.47	0.22
correction value	13.06		7.27		9.57		8.64		2.88		2.25	
LoD	1.71		1.20		0.16		0.29		0.15		0.41	
LoQ	4.05		3.07		0.37		0.79		0.39		1.07	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 18: Phosphorous concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	<LoD		**384**	16.26	**78**	39.48	**37**	5.86	**60**	1.94	**33**	4.14
-4.5	**39**	9.80	**221**	17.88	**34**	15.67	**24**	5.04	**45**	3.70	**57**	4.39
-3.5	**53**	20.71	**193**	13.30	15	12.51	<LoD		**36**	1.53	**33**	3.67
-2.5	<LoD		**120**	40.79	<LoD		<LoD		<NWG	1.42	**58**	4.83
-1.5	<LoD		**83**	28.65	<LoD		<LoD		**50**	1.69	**74**	2.25
-0.5	14	18.22	**72**	14.78	**60**	25.22	**17**	1.94	**25**	2.16	**43**	2.05
0.5	**58**	39.32	**41**	23.12	**107**	37.22	<LoD		**1,012**	83.37	**173**	7.32
1.5	**117**	26.92	<LoD		**143**	13.99	<LoD		**1,239**	41.13	**836**	25.64
2.5	**97**	28.99	**63**	11.42	**383**	56.40	<LoD		**1,772**	57.53	**1,179**	68.30
3.5	**44**	14.55	**165**	53.05	**513**	26.51	**24**	2.77	**1,266**	11.25	**1,679**	70.68
4.5	**247**	55.77	**237**	27.16	**747**	81.87	**12**	1.41	**1,498**	82.75	**973**	14.53
5.5	**642**	29.43	**495**	57.54	**566**	121.00	<LoD		**1,638**	26.81	**2,311**	48.98
6.5	**273**	30.15	**473**	18.15	**302**	46.16	**32**	1.56	**2,290**	124.13	**1,293**	110.38
7.5	**100**	45.17	**132**	30.79	**104**	22.07	**32**	2.00	**1,840**	96.58	**2,357**	73.23
8.5	**226**	32.20	**68**	2.86	**66**	42.69	**46**	1.16	**1,835**	82.21	**1,039**	39.82
9.5	**334**	43.09	**183**	33.30	**37**	14.01	**40**	2.93	**2,744**	75.14	**3,261**	59.05
10.5	**444**	32.56	**677**	83.94	**22**	10.35	**61**	3.20	**1,226**	53.15	**1,343**	48.59
11.5	**373**	50.07	**735**	56.96	**31**	22.54	**110**	5.81	**1,600**	69.37	**1,724**	81.61
12.5	**869**	169.23	**855**	20.69	**263**	32.48	**211**	8.58	**1,067**	16.29	**1,525**	38.77
13.5	**315**	39.24	**692**	16.86	**867**	67.18	**314**	6.72	**1,291**	38.51	**1,368**	67.60
14.5	**583**	72.08	**1,585**	193.72	**991**	189.79	**354**	9.79	**1,611**	98.90	**1,273**	43.07
15.5	**882**	39.43	**1,123**	39.55	**1,510**	169.00	**451**	10.22	**1,266**	55.03	**1,340**	49.67
blank 1	28.05	15.50	12.21	3.62	28.48	4.45	31.88	0.64	25.49	0.70	79.74	1.71
blank 2	39.95	8.68	26.30	7.15	19.48	13.28	44.23	1.56	25.71	1.00	34.87	3.19
blank 3	28.94	17.23	14.47	19.33	31.03	12.81	44.39	1.89	22.69	1.20	41.67	3.76
blank 4	33.97	20.81	<LoD		22.58	5.42	44.96	0.87	19.28	1.36	38.97	3.25
blank 5	36.51	18.27	15.68	10.65	18.58	16.40	35.19	0.50	17.72	0.82	42.78	3.65
correction value	33.49		13.73		24.03		40.13		22.18		47.61	
LoD	10.26		10.26		10.26		2.48		2.48		0.16	
LoQ	27.66		27.66		27.66		7.10		7.10		0.37	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**26**	3.52	**120**	3.89	**25**	1.65	**170**	5.28	**41**	1.31	**42**	2.95
-4.5	**16**	2.51	<LoD		**17**	4.62	**223**	11.21	**27**	1.40	**13**	1.28
-3.5	**20**	2.45	<LoD		**32**	1.57	**251**	4.32	**32**	1.60	<LoD	
-2.5	**12**	2.66	<LoD		<LoD		**196**	12.58	**20**	1.80	**11**	0.86
-1.5	**14**	2.74	<LoD		<LoD		**234**	6.45	**19**	1.30	**11**	0.27
-0.5	**15**	2.52	<LoD		<LoD		**210**	13.54	**16**	1.06	**11**	1.41
0.5	**15**	2.43	<LoD		**38**	3.78	**331**	22.08	**16**	0.89	**34**	2.50
1.5	**16**	2.32	<LoD		**53**	3.30	**252**	20.23	**34**	1.48	**36**	2.01
2.5	**182**	6.30	**45**	2.54	**43**	3.01	**241**	9.43	**61**	4.26	**34**	1.56
3.5	**612**	22.85	**304**	10.67	**279**	3.84	**520**	23.40	**29**	2.19	**199**	5.83
4.5	**1,002**	45.58	**801**	29.76	**1,187**	59.04	**707**	27.74	**25**	1.99	**619**	20.31
5.5	**1,179**	32.54	**1,799**	67.68	**2,145**	129.42	**818**	31.20	**39**	1.21	**846**	44.98
6.5	**1,264**	84.46	**1,634**	58.41	**1,912**	42.40	**1,148**	26.60	**49**	2.60	**853**	48.39
7.5	**1,170**	44.99	**2,539**	88.40	**2,365**	75.55	**1,554**	21.95	**37**	2.65	**1,000**	43.44
8.5	**985**	35.18	**3,235**	34.56	**2,524**	81.93	**1,539**	77.94	**39**	1.92	**1,345**	44.55
9.5	**950**	28.18	**1,840**	60.11	**1,760**	39.45	**1,598**	80.01	**73**	2.68	**1,584**	56.84
10.5	no sample**	no sample**	**1,324**	82.84	**1,727**	50.19	**1,081**	54.50	**151**	4.62	**1,759**	97.56
11.5	**809**	7.84	**2,039**	52.79	**1,480**	44.97	**820**	39.69	**446**	20.05	**1,885**	53.44
12.5	no sample**	no sample**	**2,139**	29.79	**1,476**	51.63	**972**	13.09	**597**	31.55	**1,737**	76.01
13.5	**741**	27.82	**2,769**	103.11	**1,668**	58.52	**757**	25.87	**495**	16.79	**753**	13.21
14.5	no sample**	no sample**	**3,146**	134.27	**1,114**	57.53	**712**	32.41	**288**	20.32	**653**	12.05
15.5	**728**	30.57	**3,925**	84.73	no sample**	no sample**	**683**	25.27	**486**	12.35	**1,178**	34.83
blank 1	26.01	1.57	13.68	0.94	56.03	1.03	16.04	0.41	6.46	0.20	5.57	0.51
blank 2	26.76	1.77	13.79	0.99	42.93	2.59	15.96	0.49	7.42	0.44	5.34	0.23
blank 3	12.63	0.76	14.07	0.98	56.45	2.93	16.65	1.05	7.63	0.60	4.76	0.34
blank 4	10.39	0.71	14.15	1.18	49.54	1.58	16.10	0.54	6.78	0.54	6.45	0.45
blank 5	12.29	0.84	13.36	0.75	40.55	2.71	16.02	1.08	7.95	0.23	7.09	0.40
correction value	17.62		13.81		49.10		16.15		7.28		5.84	
LoD	0.26		0.26		0.29		0.15		0.15		0.41	
LoQ	0.63		0.63		0.79		0.39		0.39		1.07	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 19: Phosphorous concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**15**	1.12	**203**	5.91	**84**	4.24	**87**	3.30	**113**	7.45	**49**	4.08
-4.5	**28**	0.87	**158**	5.70	**43**	2.04	**48**	2.21	**68**	3.83	**34**	0.65
-3.5	**21**	2.43	**135**	7.75	**29**	1.53	**74**	5.01	**101**	3.37	**37**	4.03
-2.5	**10**	1.07	**122**	4.25	**35**	1.81	**82**	2.79	**101**	4.46	**59**	4.17
-1.5	**17**	0.81	**207**	5.43	**130**	4.12	**44**	1.49	**99**	6.97	**56**	3.92
-0.5	**9**	1.13	**1621**	37.32	**795**	31.05	**55**	1.61	**79**	1.98	**35**	3.07
0.5	**109**	3.68	**2096**	63.20	**1056**	43.37	**69**	2.13	**1510**	58.87	**221**	12.60
1.5	**171**	6.06	**2688**	96.95	**1297**	29.95	**135**	3.66	**2030**	22.61	**1039**	31.75
2.5	**270**	8.34	**1733**	54.69	**889**	29.26	no sample ***	no sample ***	**2203**	66.44	**1778**	40.73
3.5	**467**	7.58	**1298**	42.13	**741**	23.97	no sample ***	no sample ***	**2728**	28.12	**2692**	26.68
4.5	**1005**	45.26	**1143**	22.81	**629**	6.57	**184**	5.54	**4193**	157.41	**4064**	108.88
5.5	**2950**	77.33	**784**	27.12	**375**	15.81	**107**	2.46	**5109**	253.64	**4625**	181.46
6.5	**4632**	352.40	**821**	14.89	**332**	9.96	**152**	5.54	**5472**	83.13	**4878**	161.43
7.5	**5259**	397.53	**489**	16.91	**199**	5.51	**154**	2.18	**4507**	172.55	**5638**	102.52
8.5	**5451**	247.56	**414**	24.90	**148**	6.15	**639**	9.56	**5303**	118.29	**5211**	164.72
9.5	**5447**	295.64	**425**	21.28	**270**	10.62	**723**	21.86	**5217**	277.68	**6596**	306.29
10.5	**6641**	441.23	**474**	21.29	**398**	21.79	**941**	21.35	**5490**	228.13	**6198**	121.78
11.5	**6618**	304.95	**516**	16.14	**840**	32.12	**1246**	57.47	**5034**	494.42	**7492**	365.74
12.5	**4907**	361.92	**1119**	36.71	**1624**	74.92	no sample ***	no sample ***	**6074**	221.78	**6339**	211.25
13.5	**6812**	450.40	**2093**	72.53	**3085**	80.98	1093	28.16	**6512**	168.96	**7388**	266.41
14.5	**6264**	263.66	**2880**	103.85	**3094**	178.12	no sample ***	no sample ***	**6890**	264.27	**6037**	258.66
15.5	**5187**	269.50	**3408**	204.39	**4194**	337.64	no sample ***	no sample ***	**7076**	405.11	**6849**	177.67
blank 1	16.96	0.53	5.19	0.25	11.22	0.29	15.05	1.17	11.03	0.65	17.89	0.38
blank 2	19.10	0.83	5.67	0.38	18.62	0.53	17.11	0.59	14.09	0.11	12.91	1.24
blank 3	23.73	1.16	6.43	0.37	9.37	0.39	18.05	0.82	11.72	0.54	15.34	0.95
blank 4	12.76	0.83	5.98	0.23	6.14	0.30	14.57	0.77	14.45	0.49	16.86	1.11
blank 5	10.11	0.22	7.89	0.53	6.94	0.42					23.71	1.29
correction value	16.53		6.23		10.46		12.96		10.26		17.34	
LoD	1.20		1.20		1.20		1.90		1.90		1.71	
LoQ	2.87		2.87		2.87		5.02		5.02		4.05	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**13**	2.95	**1198**	37.45	**23**	1.07	**55**	3.21	**117**	7.11	**76**	2.91
-4.5	**17**	2.99	**33**	2.22	**9**	1.93	**19**	0.40	**42**	2.34	**22**	1.43
-3.5	**15**	2.82	**27**	1.59	**5**	0.87	**18**	2.18	**43**	2.00	**17**	1.37
-2.5	**5**	2.18	**16**	1.17	**3**	0.59	**20**	2.66	**26**	1.57	**16**	1.09
-1.5	**4**	1.93	**16**	0.43	**2**	1.07	**17**	0.66	**19**	0.46	**14**	1.10
-0.5	**4**	2.06	**16**	1.32	**7**	1.00	**18**	0.94	**18**	0.90	**18**	1.85
0.5	**22**	3.84	**28**	0.50	**215**	11.29	**79**	3.46	**21**	1.46	**65**	4.21
1.5	**28**	3.47	**28**	2.00	**192**	4.85	**193**	3.69	**46**	2.63	**59**	1.72
2.5	**314**	14.59	**563**	20.78	**302**	19.83	**138**	7.23	**286**	5.01	**86**	3.14
3.5	**856**	35.80	**2516**	98.12	**218**	11.10	**486**	27.36	**62**	2.37	**282**	8.96
4.5	**1193**	44.83	**3905**	144.21	**620**	41.56	**869**	33.68	**43**	1.03	**703**	21.15
5.5	**1499**	77.37	**5455**	126.33	**1304**	73.93	**1055**	44.06	**77**	2.58	**919**	26.15
6.5	**1892**	109.04	**5732**	187.47	**1543**	37.77	**1495**	69.99	no sample**	no sample**	**942**	46.93
7.5	**1749**	38.60	**5589**	114.07	**1524**	85.19	**1579**	24.49	no sample**	no sample**	**1088**	54.87
8.5	**2038**	48.47	**5288**	190.91	**1761**	92.34	**1406**	60.42	no sample**	no sample**	**1408**	59.57
9.5	**1565**	37.92	**8092**	112.91	**976**	36.36	**1434**	46.63	no sample**	no sample**	**1673**	51.79
10.5	**1789**	75.17	**7944**	123.41	**1080**	38.14	**1870**	85.24	no sample**	no sample**	**1826**	84.01
11.5	**2192**	54.19	**7562**	242.32	**925**	16.52	**1733**	129.81	no sample**	no sample**	**1918**	57.66
12.5	**2540**	65.06	**8235**	168.78	**889**	63.26	**85**	10.49	no sample**	no sample**	no sample**	no sample**
13.5	**2789**	62.34	**7248**	160.01	**1153**	89.61	no sample ***	no sample ***	no sample**	no sample**	**1582**	73.17
14.5	**2920**	78.66	**6701**	172.24	**1074**	58.19	no sample ***	no sample ***	no sample**	no sample**	**1341**	60.81
15.5	**3161**	131.47	**6213**	157.00	**927**	56.71	no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	18.86	1.02	3.54	0.09	16.76	0.88	8.66	0.52	2.56	4.86	2.70	0.24
blank 2	14.89	0.84	3.09	0.14	17.41	1.11	8.45	0.57	2.17	7.41	2.61	0.13
blank 3	25.84	1.42	3.85	0.24	16.92	0.84	9.06	0.34	1.96	8.96	2.20	0.19
blank 4	20.39	1.30	3.11	0.23	20.28	0.90	7.92	0.72	2.31	7.25	2.04	0.16
blank 5	24.37	1.57	3.05	0.11	15.14	0.71	6.75	0.63	2.68	8.98	2.19	0.33
correction value	20.87		3.33		17.30		8.17		2.47		2.35	
LoD	1.20		1.20		0.16		0.29		0.15		0.41	
LoQ	3.07		3.07		0.37		0.79		0.39		1.07	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 20: Arsenic concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.277**	0.034	**0.276**	0.010	**0.549**	0.027	**1.821**	0.175	**1.797**	0.024	**1.026**	0.096
-4.5	**0.364**	0.016	**0.291**	0.039	**0.552**	0.011	**2.336**	0.117	**1.769**	0.069	**0.931**	0.081
-3.5	**0.370**	0.023	**0.376**	0.037	**0.492**	0.037	**2.414**	0.091	**1.833**	0.094	**0.987**	0.119
-2.5	**0.323**	0.034	**0.266**	0.036	**0.547**	0.072	**1.924**	0.108	**0.885**	0.039	**1.012**	0.072
-1.5	**0.301**	0.041	**0.341**	0.006	**0.525**	0.079	**1.682**	0.054	**0.811**	0.009	**1.040**	0.084
-0.5	**0.362**	0.090	**0.474**	0.014	**0.848**	0.042	**1.666**	0.121	**1.455**	0.103	**0.715**	0.031
0.5	**0.543**	0.019	**0.734**	0.109	**0.829**	0.088	**1.893**	0.061	**0.755**	0.032	**1.490**	0.143
1.5	**0.651**	0.047	**0.517**	0.046	**0.868**	0.056	**1.448**	0.090	**1.873**	0.109	**1.111**	0.069
2.5	**0.586**	0.139	**0.601**	0.021	**0.962**	0.039	**2.195**	0.183	**2.192**	0.106	**1.473**	0.125
3.5	**0.569**	0.052	**0.713**	0.043	**0.732**	0.077	**1.755**	0.118	**1.472**	0.044	**1.091**	0.105
4.5	**0.720**	0.100	**0.661**	0.027	**0.772**	0.107	**1.301**	0.052	**1.565**	0.096	**1.517**	0.081
5.5	**0.901**	0.047	**0.743**	0.085	**0.627**	0.079	**1.122**	0.048	**1.249**	0.095	**1.113**	0.097
6.5	**0.630**	0.031	**0.640**	0.102	**0.644**	0.075	**1.009**	0.044	**1.126**	0.035	**1.015**	0.035
7.5	**0.678**	0.045	**0.649**	0.110	**0.522**	0.026	**1.111**	0.071	**1.317**	0.101	**0.824**	0.035
8.5	**0.888**	0.094	**0.510**	0.039	**0.568**	0.045	**1.047**	0.032	**1.040**	0.041	**0.785**	0.031
9.5	**0.487**	0.044	**0.529**	0.024	**0.644**	0.115	**0.973**	0.041	**1.111**	0.045	**0.669**	0.054
10.5	**0.623**	0.051	**0.523**	0.015	**0.533**	0.058	**0.851**	0.034	**1.032**	0.066	**1.089**	0.086
11.5	**0.523**	0.076	**0.414**	0.020	**0.567**	0.021	**0.933**	0.054	**1.027**	0.048	**0.705**	0.053
12.5	**0.689**	0.055	**0.468**	0.027	**0.451**	0.030	**0.904**	0.045	**0.974**	0.051	**0.639**	0.036
13.5	**0.465**	0.014	**0.482**	0.029	**0.527**	0.059	**0.848**	0.032	**0.968**	0.042	**0.690**	0.060
14.5	**0.547**	0.115	**0.849**	0.111	**0.583**	0.033	**0.884**	0.031	**0.906**	0.042	**0.529**	0.047
15.5	**0.510**	0.060	**0.536**	0.007	**0.648**	0.045	**0.854**	0.059	**0.924**	0.047	**0.597**	0.052
blank 1	0.003	0.002	0.003	0.001	0.005	0.002	<LoD		<LoD		<LoD	
blank 2	0.002	0.002	<LoD		0.003	0.001	<LoD		<LoD		<LoD	
blank 3	0.003	0.004	0.004	0.001	0.004	0.004	<LoD		<LoD		<LoD	
blank 4	0.005	0.003	0.003	0.001	0.004	0.002	<LoD		<LoD		<LoD	
blank 5	0.002	0.001	0.003	0.002	0.005	0.003	<LoD		<LoD		<LoD	
correction value	0.003		0.003		0.004		0.000		0.000		0.000	
LoD	0.002		0.002		0.002		0.026		0.026		0.146	
LoQ	0.006		0.006		0.006		0.073		0.073		0.380	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.683**	0.052	**0.953**	0.053	**1.095**	0.059	**1.267**	0.021	**1.183**	0.067	**1.989**	0.064
-4.5	**0.605**	0.040	**0.967**	0.065	**1.003**	0.050	**1.233**	0.027	**1.172**	0.077	**1.136**	0.081
-3.5	**0.524**	0.034	**0.894**	0.022	**1.127**	0.062	**1.243**	0.081	**1.009**	0.098	**0.830**	0.033
-2.5	**0.451**	0.045	**0.845**	0.016	**1.305**	0.088	**0.702**	0.052	**1.315**	0.074	**0.693**	0.051
-1.5	**0.428**	0.040	**0.754**	0.049	**0.875**	0.092	**1.094**	0.032	**1.024**	0.049	**0.620**	0.026
-0.5	**0.424**	0.042	**0.670**	0.032	**1.036**	0.104	**1.200**	0.072	**1.044**	0.013	**0.684**	0.031
0.5	**0.416**	0.039	**0.488**	0.043	**0.749**	0.081	**0.886**	0.052	**1.219**	0.078	**0.810**	0.016
1.5	**0.762**	0.021	**0.293**	0.035	**0.641**	0.054	**0.582**	0.050	**0.631**	0.034	**0.460**	0.040
2.5	**1.165**	0.065	**0.725**	0.054	**0.890**	0.064	**0.725**	0.042	**0.388**	0.046	**0.450**	0.018
3.5	**1.467**	0.060	**1.186**	0.044	**1.627**	0.049	**0.794**	0.033	**0.486**	0.018	**0.366**	0.039
4.5	**1.141**	0.061	**1.387**	0.075	**1.536**	0.080	**1.434**	0.093	**0.713**	0.040	**0.311**	0.025
5.5	**1.039**	0.049	**1.451**	0.038	**1.553**	0.154	**1.873**	0.042	**0.850**	0.040	**0.348**	0.041
6.5	**1.079**	0.047	**1.361**	0.038	no sample *	no sample *	**2.386**	0.118	**0.962**	0.058	**0.455**	0.036
7.5	**1.047**	0.027	**1.221**	0.066	no sample *	no sample *	**2.185**	0.120	**0.830**	0.027	**0.553**	0.036
8.5	**0.913**	0.032	**1.223**	0.074	no sample *	no sample *	**2.092**	0.075	**0.834**	0.047	**0.641**	0.011
9.5	**0.929**	0.087	**1.145**	0.038	**0.861**	0.074	**1.703**	0.130	**0.713**	0.047	**0.618**	0.035
10.5	**0.893**	0.041	**1.062**	0.048	**1.167**	0.109	**1.376**	0.051	**0.712**	0.049	**0.639**	0.043
11.5	**0.918**	0.073	**1.008**	0.056	**1.016**	0.082	**1.294**	0.074	**0.629**	0.012	**0.593**	0.026
12.5	**0.880**	0.045	**0.923**	0.067	**1.077**	0.054	**1.214**	0.056	**0.672**	0.039	**0.588**	0.022
13.5	**0.871**	0.048	**0.863**	0.064	**1.009**	0.035	**1.275**	0.124	**0.658**	0.023	**0.566**	0.019
14.5	**0.888**	0.064	**0.835**	0.060	**0.756**	0.059	**1.087**	0.050	**0.674**	0.009	no sample **	no sample **
15.5	**0.879**	0.066	**0.808**	0.056	**0.832**	0.077	**0.975**	0.043	**0.718**	0.039	**0.577**	0.030
blank 1	<LoD		<LoD		<LoD		<LoD		0.040	0.030	<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		0.027	0.012	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
correction value	0.000		0.000		0.005		0.000		0.008		0.000	
LoD	0.020		0.020		0.017		0.039		0.039		0.038	
LoQ	0.050		0.050		0.046		0.094		0.094		0.095	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 21: Arsenic concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.430**	0.024	**0.355**	0.024	**0.486**	0.032	**2.190**	0.122	**0.726**	0.047	**0.528**	0.027
-4.5	**0.417**	0.016	**0.314**	0.023	**0.591**	0.037	**1.673**	0.049	**1.232**	0.071	**0.521**	0.021
-3.5	**0.436**	0.010	**0.250**	0.008	**0.527**	0.011	**1.403**	0.061	**1.116**	0.048	0.439	0.048
-2.5	**0.464**	0.018	**0.334**	0.028	**0.540**	0.021	**1.340**	0.075	**1.065**	0.053	0.427	0.048
-1.5	**0.449**	0.022	**0.304**	0.023	**0.550**	0.033	**1.325**	0.050	**0.845**	0.048	0.409	0.036
-0.5	**0.417**	0.015	**0.530**	0.051	**0.715**	0.052	**1.145**	0.057	**0.624**	0.036	0.384	0.037
0.5	**0.931**	0.035	**0.685**	0.028	**1.106**	0.064	**1.165**	0.040	**0.886**	0.076	<LoD	
1.5	**1.306**	0.102	**0.803**	0.035	**1.152**	0.021	**1.199**	0.017	**1.785**	0.011	0.387	0.034
2.5	**1.209**	0.072	**0.958**	0.050	**0.737**	0.022	**1.712**	0.045	**2.050**	0.128	**1.185**	0.093
3.5	**0.986**	0.036	**0.939**	0.041	**0.793**	0.033	**2.090**	0.101	**1.348**	0.038	**1.242**	0.095
4.5	**0.996**	0.039	**0.813**	0.057	**0.842**	0.041	**1.691**	0.062	**1.203**	0.080	**1.075**	0.063
5.5	**1.134**	0.046	**0.871**	0.045	**0.666**	0.019	**1.164**	0.076	**1.241**	0.177	**0.954**	0.047
6.5	**0.915**	0.076	**0.796**	0.022	**0.710**	0.044	no sample ***	no sample ***	**1.071**	0.031	**0.870**	0.062
7.5	**0.773**	0.058	**0.737**	0.055	**0.656**	0.038	no sample ***	no sample ***	**0.973**	0.060	**0.774**	0.029
8.5	**0.819**	0.064	**0.694**	0.028	**0.525**	0.008	no sample ***	no sample ***	**1.012**	0.043	**0.665**	0.029
9.5	**0.873**	0.019	**0.706**	0.034	**0.409**	0.029	no sample ***	no sample ***	**1.013**	0.042	**0.649**	0.034
10.5	**0.858**	0.054	**0.698**	0.051	**0.478**	0.018	**1.019**	0.038	**1.065**	0.061	**0.644**	0.033
11.5	**0.834**	0.044	**0.784**	0.045	**0.418**	0.017	**0.863**	0.015	**0.837**	0.044	**0.609**	0.029
12.5	**0.760**	0.051	**0.732**	0.011	**0.626**	0.027	**0.930**	0.020	**0.839**	0.042	**0.588**	0.037
13.5	**0.806**	21.474	**0.693**	0.044	**0.725**	0.061	**0.855**	0.031	**0.922**	0.034	**0.573**	0.027
14.5	**0.771**	0.032	**0.570**	0.031	**0.611**	0.021	**0.933**	0.041	**0.935**	0.048	**0.525**	0.028
15.5	**0.842**	0.056	**0.709**	0.040	**0.592**	0.041	no sample ***	no sample ***	**0.927**	0.083	**0.507**	0.015
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		<LoD				<LoD	
correction value	0.000		0.000		0.000		0.000		0.000		0.000	
LoD	0.014		0.014		0.014		0.039		0.039		0.177	
LoQ	0.038		0.038		0.038		0.101		0.101		0.471	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**1.003**	0.039	**0.971**	0.054	**1.480**	0.067	**1.388**	0.146	**1.177**	0.034	**1.725**	0.020
-4.5	**0.774**	0.030	**0.981**	0.047	**1.195**	0.120	**1.144**	0.067	**1.076**	0.051	**1.070**	0.041
-3.5	**0.755**	0.039	**0.924**	0.047	**1.201**	0.080	**0.977**	0.071	**1.167**	0.055	**0.920**	0.077
-2.5	**0.783**	0.040	**0.853**	0.046	**1.002**	0.116	**1.025**	0.030	**1.031**	0.068	**0.755**	0.081
-1.5	**0.742**	0.021	**0.765**	0.060	**1.044**	0.086	**1.011**	0.072	**0.751**	0.042	**0.677**	0.010
-0.5	**0.644**	0.044	**0.707**	0.040	**1.234**	0.106	**1.094**	0.055	**0.659**	0.018	**0.659**	0.053
0.5	**0.621**	0.047	**0.599**	0.044	**1.216**	0.095	**1.018**	0.076	**1.137**	0.046	**0.899**	0.077
1.5	**0.864**	0.069	**0.411**	0.027	**1.144**	0.102	**0.714**	0.040	**0.567**	0.034	**0.530**	0.020
2.5	**1.508**	0.059	**0.818**	0.077	**1.677**	0.137	**0.658**	0.057	**0.771**	0.041	**0.531**	0.058
3.5	**1.674**	0.049	**1.238**	0.091	**1.930**	0.150	**1.769**	0.120	**0.851**	0.042	**0.422**	0.034
4.5	**1.854**	0.150	**1.494**	0.084	**1.697**	0.138	**2.180**	0.112	**1.156**	0.049	**0.428**	0.030
5.5	**1.482**	0.029	**1.551**	0.105	**1.600**	0.097	**2.330**	0.190	**1.064**	0.055	no sample **	no sample **
6.5	**1.358**	0.026	**1.507**	0.069	no sample *	no sample *	**2.798**	0.160	**0.937**	0.059	**0.453**	0.041
7.5	**1.146**	0.036	**1.397**	0.085	no sample *	no sample *	**1.870**	0.220	**0.874**	0.059	**0.546**	0.006
8.5	**1.528**	0.026	**1.315**	0.053	no sample *	no sample *	**1.677**	0.063	**0.844**	0.040	**0.595**	0.016
9.5	**1.438**	0.035	**1.171**	0.065	**1.035**	0.093	**1.639**	0.042	**0.667**	0.051	**0.658**	0.018
10.5	**1.222**	0.030	**1.094**	0.072	**1.183**	0.102	**1.691**	0.097	**0.641**	0.054	**0.610**	0.061
11.5	**1.197**	0.016	**1.022**	0.059	**0.980**	0.042	**1.540**	0.080	**0.666**	0.024	no sample **	no sample **
12.5	**1.147**	0.022	**0.950**	0.051	**0.994**	0.064	**1.424**	0.117	**0.604**	0.051	no sample **	no sample **
13.5	**1.275**	0.035	**0.884**	0.040	**0.962**	0.064	**1.518**	0.092	**0.596**	0.020	no sample **	no sample **
14.5	**1.159**	0.025	**0.852**	0.054	**1.054**	0.073	**1.371**	0.075	**0.591**	0.015	no sample **	no sample **
15.5	**1.286**	0.021	**0.807**	0.057	**0.753**	0.026	**1.177**	0.044	**0.574**	0.014	no sample **	no sample **
blank 1	<LoD		<LoD		0.035	0.025	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		<LoD		0.019	0.020	<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		<LoD				<LoD	
correction value	0.000		0.000		0.007		0.004		0.000		0.000	
LoD	0.177		0.146		0.034		0.017		0.039		0.038	
LoQ	0.471		0.380		0.087		0.046		0.094		0.095	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 22: Arsenic concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.461**	0.020	**0.438**	0.040	**0.878**	0.134	**1.916**	0.089	**0.697**	0.036	**1.496**	0.067
-4.5	**0.471**	0.069	**0.380**	0.024	**0.951**	0.068	**1.968**	0.112	**0.678**	0.060	**1.570**	0.061
-3.5	**0.403**	0.012	**0.386**	0.039	**0.849**	0.091	**1.036**	0.076	**0.971**	0.028	**1.469**	0.060
-2.5	**0.441**	0.034	**0.457**	0.038	**0.828**	0.066	**1.449**	0.028	**0.626**	0.034	**1.646**	0.076
-1.5	**0.485**	0.061	**0.864**	0.096	**1.032**	0.045	**0.925**	0.057	**1.397**	0.101	**1.583**	0.009
-0.5	**0.551**	0.048	**1.364**	0.195	**1.623**	0.071	**1.302**	0.090	**1.040**	0.049	**1.823**	0.033
0.5	**0.474**	0.016	**0.742**	0.029	**1.588**	0.358	**1.134**	0.079	**1.725**	0.080	**1.537**	0.060
1.5	**0.645**	0.050	**0.769**	0.032	**1.366**	0.047	**1.370**	0.052	**1.166**	0.038	**1.407**	0.065
2.5	**0.642**	0.054	**0.663**	0.042	**1.002**	0.088	**1.855**	0.094	**1.290**	0.034	**1.127**	0.060
3.5	**0.588**	0.055	**0.527**	0.011	**1.035**	0.017	**1.676**	0.042	**0.795**	0.040	**1.240**	0.041
4.5	**0.899**	0.082	**0.521**	0.027	**0.916**	0.034	**1.467**	0.040	**0.921**	0.081	**0.568**	0.039
5.5	**1.193**	0.073	**0.453**	0.062	**0.837**	0.031	**1.261**	0.091	**1.008**	0.057	**1.402**	0.029
6.5	**0.793**	0.025	**0.459**	0.066	**0.830**	0.114	**1.093**	0.040	**1.323**	0.058	**0.729**	0.073
7.5	**0.830**	0.055	**0.467**	0.023	**0.885**	0.078	**1.117**	0.061	**0.966**	0.041	**1.222**	0.024
8.5	**0.789**	0.034	**0.707**	0.033	**0.695**	0.083	**0.994**	0.045	**0.846**	0.025	**0.548**	0.041
9.5	**1.228**	0.212	**0.314**	0.036	**0.648**	0.023	**1.015**	0.047	**0.942**	0.025	**1.185**	0.040
10.5	**0.754**	0.100	**0.440**	0.027	**0.659**	0.101	**0.947**	0.036	**0.784**	0.052	**0.983**	0.053
11.5	**0.838**	0.062	**0.366**	0.021	**0.604**	0.038	**0.943**	0.036	**0.894**	0.058	**1.017**	0.031
12.5	**0.722**	0.059	**0.485**	0.052	**0.516**	0.012	**0.978**	0.026	**0.542**	0.026	**0.881**	0.022
13.5	**0.597**	0.057	**0.460**	0.025	**0.510**	0.038	**1.026**	0.047	**0.668**	0.018	**0.798**	0.044
14.5	**0.693**	0.079	**0.467**	0.067	**0.550**	0.016	**0.945**	0.029	**0.888**	0.053	**0.756**	0.049
15.5	**0.799**	0.107	**0.333**	0.012	**0.562**	0.057	**0.981**	0.074	**0.688**	0.049	**0.781**	0.061
blank 1	0.003	0.002	<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	0.005	0.003	0.004	0.002	<LoD		<LoD		<LoD		<LoD	
blank 3	0.004	0.002	0.003	0.002	0.003	0.001	<LoD		<LoD		<LoD	
blank 4	0.005	0.003	0.005	0.001	<LoD		<LoD		<LoD		<LoD	
blank 5	0.005	0.003	<LoD		<LoD		<LoD		<LoD		<LoD	
correction value	0.004		0.002		0.001		0.000		0.000		0.000	
LoD	0.002		0.002		0.002		0.051		0.051		0.034	
LoQ	0.006		0.006		0.006		0.142		0.142		0.087	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**1.359**	0.079	**0.734**	0.021	**3.717**	0.127	**3.082**	0.167	**2.944**	0.189	**1.739**	0.079
-4.5	**1.079**	0.038	**0.665**	0.061	**3.266**	0.111	**4.000**	0.272	**2.661**	0.054	**1.719**	0.111
-3.5	**0.984**	0.029	**0.682**	0.062	**2.959**	0.196	**3.560**	0.117	**3.111**	0.083	**1.509**	0.090
-2.5	**0.855**	0.061	**0.704**	0.029	**2.571**	0.172	**3.595**	0.100	**2.725**	0.121	**1.694**	0.125
-1.5	**0.851**	0.070	**0.668**	0.061	**1.994**	0.136	**3.198**	0.143	**2.781**	0.044	**1.738**	0.042
-0.5	**0.747**	0.048	**0.763**	0.033	**2.289**	0.117	**3.341**	0.241	**2.201**	0.063	**1.690**	0.125
0.5	**0.919**	0.061	**2.603**	0.102	**4.652**	0.167	**8.644**	0.343	**2.111**	0.087	**4.114**	0.193
1.5	**1.358**	0.063	**2.934**	0.080	**5.213**	0.274	**6.438**	0.154	**2.549**	0.130	**3.335**	0.112
2.5	**1.633**	0.070	**2.380**	0.093	**3.861**	0.266	**4.433**	0.253	**1.959**	0.063	**2.995**	0.109
3.5	**1.623**	0.081	**2.839**	0.282	**3.287**	0.133	**2.785**	0.087	**3.144**	0.089	**3.054**	0.096
4.5	**1.619**	0.061	**2.578**	0.093	**3.062**	0.162	**2.663**	0.085	**3.066**	0.122	**3.027**	0.142
5.5	**1.573**	0.048	**2.398**	0.105	**2.469**	0.292	**2.357**	0.155	**2.981**	0.096	**2.861**	0.183
6.5	**1.527**	0.077	**2.172**	0.047	**1.386**	0.045	**2.049**	0.091	**3.547**	0.177	**2.588**	0.077
7.5	**1.463**	0.044	**2.040**	0.066	**1.839**	0.069	**1.893**	0.138	**3.721**	0.129	**2.217**	0.102
8.5	**1.355**	0.061	**1.893**	0.053	**2.073**	0.066	**1.793**	0.067	**3.388**	0.226	**2.081**	0.043
9.5	**1.283**	0.043	**1.803**	0.096	**1.304**	0.037	**1.622**	0.032	**2.714**	0.082	**1.850**	0.081
10.5	no sample**	no sample**	**1.543**	0.096	**1.241**	0.094	**1.432**	0.069	**2.438**	0.084	**1.724**	0.112
11.5	**1.273**	0.036	**1.431**	0.042	**0.976**	0.080	**1.297**	0.073	**2.422**	0.067	**1.578**	0.133
12.5	no sample**	no sample**	**1.272**	0.060	**0.888**	0.060	**1.357**	0.055	**2.375**	0.136	**1.463**	0.097
13.5	**1.066**	0.062	**1.256**	0.068	**1.038**	0.082	**1.221**	0.090	**2.412**	0.121	**0.675**	0.046
14.5	no sample**	no sample**	**1.235**	0.062	**0.684**	0.022	**1.144**	0.045	**1.985**	0.048	**0.611**	0.032
15.5	**0.979**	0.065	**1.227**	0.056	no sample**	no sample**	**1.158**	0.048	**2.209**	0.123	**1.128**	0.051
blank 1	0.025	0.019	<LoD		<LoD		<LoD		<LoD		0.019	0.008
blank 2	<LoD		<LoD		0.022	0.027	<LoD		<LoD		0.016	0.006
blank 3	<LoD		<LoD		0.031	0.021	<LoD		<LoD		0.016	0.005
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		0.012	0.008
blank 5	<LoD		<LoD		<LoD		<LoD		<LoD		0.011	0.008
correction value	0.005		0.000		0.011		0.000		0.000		0.015	
LoD	0.020		0.020		0.017		0.039		0.039		0.038	
LoQ	0.050		0.050		0.046		0.094		0.094		0.095	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 23: Arsenic concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.524**	0.032	**0.364**	0.010	**0.726**	0.039	**1.696**	0.110	**1.588**	0.088	**1.208**	0.059
-4.5	**0.740**	0.022	**0.526**	0.032	**0.945**	0.053	**1.330**	0.022	**1.153**	0.056	**0.856**	0.034
-3.5	**0.614**	0.019	**0.562**	0.025	**0.744**	0.042	**1.491**	0.080	**1.802**	0.080	**1.201**	0.040
-2.5	**0.633**	0.022	**0.627**	0.048	**0.729**	0.027	**0.947**	0.074	**1.961**	0.097	**1.413**	0.040
-1.5	**0.595**	0.032	**1.006**	0.040	**0.904**	0.035	**0.936**	0.057	**1.864**	0.078	**1.313**	0.036
-0.5	**0.625**	0.011	**1.220**	0.043	**1.455**	0.053	**0.974**	0.059	**1.615**	0.059	**1.154**	0.071
0.5	**0.775**	0.026	**0.996**	0.045	**1.128**	0.058	**0.999**	0.070	**2.312**	0.114	**1.479**	0.066
1.5	**1.050**	0.042	**0.782**	0.048	**1.081**	0.025	**1.365**	0.059	**1.176**	0.072	**1.433**	0.038
2.5	**0.945**	0.036	**0.617**	0.022	**0.895**	0.031	no sample ***	no sample ***	**0.983**	0.065	**1.357**	0.054
3.5	**1.188**	0.038	**0.608**	0.015	**0.801**	0.025	no sample ***	no sample ***	**0.888**	0.047	**1.400**	0.016
4.5	**1.507**	0.117	**0.593**	0.044	**0.830**	0.017	**1.639**	0.109	**0.955**	0.078	**1.618**	0.027
5.5	**1.288**	0.043	**0.521**	0.014	**0.713**	0.048	**1.264**	0.043	**1.002**	0.057	**1.465**	0.043
6.5	**1.366**	0.089	**0.642**	0.058	**0.902**	0.013	**1.152**	0.045	**0.772**	0.063	**1.187**	0.031
7.5	**1.348**	0.089	**0.511**	0.006	**0.700**	0.033	**1.127**	0.055	**0.720**	0.052	**1.031**	0.024
8.5	**1.118**	0.045	**0.437**	0.029	**0.622**	0.032	**1.310**	0.044	**0.857**	0.034	**1.079**	0.050
9.5	**1.011**	0.034	**0.386**	0.030	**0.692**	0.037	**1.300**	0.076	**0.792**	0.054	**1.032**	0.028
10.5	**1.203**	0.063	**0.415**	0.021	**0.681**	0.056	**1.200**	0.032	**0.697**	0.045	**0.761**	0.022
11.5	**1.041**	0.047	**0.395**	0.024	**0.728**	0.055	**1.157**	0.062	**0.722**	0.098	**0.824**	0.022
12.5	**0.892**	0.050	**0.401**	0.044	**0.742**	0.034	no sample ***	no sample ***	**0.627**	0.031	**0.699**	0.021
13.5	**0.904**	0.063	**0.439**	0.015	**0.688**	0.032	**1.055**	0.036	**0.631**	0.036	**0.779**	0.019
14.5	**0.948**	0.068	**0.421**	0.011	**0.599**	0.059	no sample ***	no sample ***	**0.621**	0.017	**0.539**	0.021
15.5	**0.723**	0.033	**0.401**	0.020	**0.710**	0.061	no sample ***	no sample ***	**0.559**	0.060	**0.614**	0.021
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD						<LoD	
correction value	0.000		0.000		0.000		0.000		0.000		0.000	
LoD	0.014		0.014		0.014		0.039		0.039		0.177	
LoQ	0.038		0.038		0.038		0.101		0.101		0.471	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**1.054**	0.070	**1.000**	0.051	**3.093**	0.116	**2.528**	0.171	**2.591**	0.127	**1.621**	0.055
-4.5	**1.319**	0.081	**0.703**	0.046	**2.977**	0.306	**2.033**	0.117	**2.303**	0.037	**1.583**	0.102
-3.5	**1.241**	0.049	**0.735**	0.052	**2.795**	0.157	**2.481**	0.067	**2.797**	0.464	**1.599**	0.059
-2.5	**1.002**	0.061	**0.711**	0.051	**2.240**	0.100	**2.662**	0.253	**1.913**	0.106	**1.543**	0.100
-1.5	**0.977**	0.071	**0.691**	0.040	**2.087**	0.069	**2.733**	0.097	**1.596**	0.063	**1.527**	0.082
-0.5	**0.925**	0.080	**0.952**	0.040	**2.257**	0.098	**3.294**	0.097	**1.588**	0.072	**1.802**	0.133
0.5	**1.094**	0.074	**2.813**	0.063	**9.369**	0.569	**6.994**	0.290	**1.618**	0.049	**4.622**	0.175
1.5	**1.569**	0.079	**3.251**	0.114	**6.803**	0.239	**5.851**	0.125	**1.782**	0.051	**3.869**	0.053
2.5	**2.064**	0.113	**4.484**	0.190	**4.876**	0.429	**5.097**	0.236	**5.652**	0.150	**3.446**	0.090
3.5	**1.925**	0.093	**3.718**	0.061	**2.879**	0.267	**4.460**	0.326	**3.694**	0.150	**3.325**	0.085
4.5	**1.831**	0.059	**3.044**	0.103	**2.091**	0.063	**3.443**	0.200	**3.042**	0.195	**3.114**	0.124
5.5	**1.808**	0.062	**2.569**	0.077	**1.976**	0.135	**2.598**	0.135	**3.038**	0.133	**2.801**	0.020
6.5	**1.693**	0.070	**2.259**	0.073	**1.699**	0.108	**2.207**	0.075	no sample**	no sample**	**2.564**	0.190
7.5	**1.660**	0.050	**2.007**	0.036	**1.604**	0.063	**1.940**	0.048	no sample**	no sample**	**2.176**	0.058
8.5	**1.544**	0.056	**1.805**	0.055	**1.748**	0.109	**1.828**	0.091	no sample**	no sample**	**2.023**	0.100
9.5	**1.436**	0.030	**1.897**	0.064	**0.930**	0.020	**1.784**	0.142	no sample**	no sample**	**1.853**	0.059
10.5	**1.311**	0.052	**1.676**	0.039	**1.027**	0.016	**1.718**	0.072	no sample**	no sample**	**1.733**	0.114
11.5	**1.273**	0.071	**1.426**	0.036	**0.825**	0.072	**1.580**	0.036	no sample**	no sample**	**1.553**	0.034
12.5	**1.221**	0.064	**1.280**	0.018	**0.762**	0.032	**0.063**	0.009	no sample**	no sample**	no sample**	no sample**
13.5	**1.152**	0.045	**1.174**	0.049	**0.917**	0.058	no sample ***	no sample ***	no sample**	no sample**	**1.363**	0.095
14.5	**1.102**	0.032	**1.126**	0.031	**0.831**	0.049	no sample ***	no sample ***	no sample**	no sample**	**1.164**	0.076
15.5	**1.045**	0.046	**1.090**	0.053	**0.682**	0.053	no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
correction value	0.000		0.000		0.000		0.000		0.000		0.000	
LoD	0.146		0.146		0.034		0.017		0.039		0.038	
LoQ	0.380		0.380		0.087		0.046		0.094		0.095	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 24: Cadmium concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.018**	0.001	**0.002**	0.001	**0.005**	0.003	<LoD		0.013	0.001	0.010	0.003
-4.5	**0.024**	0.002	**0.002**	0.001	**0.028**	0.004	<LoD		0.014	0.001	0.006	0.004
-3.5	**0.028**	0.006	**0.003**	0.001	**0.033**	0.005	<LoD		<LoD		0.007	0.006
-2.5	**0.019**	0.002	**0.002**	0.000	**0.036**	0.002	<LoD		<LoD		0.006	0.001
-1.5	**0.026**	0.004	**0.008**	0.002	**0.041**	0.008	<LoD		<LoD		0.005	0.002
-0.5	**0.036**	0.015	**0.017**	0.005	**0.047**	0.001	<LoD		<LoD		0.031	0.005
0.5	**0.028**	0.001	**0.019**	0.003	**0.006**	0.002	<LoD		<LoD		**0.049**	0.007
1.5	**0.003**	0.000	**0.007**	0.003	**0.003**	0.001	<LoD		<LoD		0.003	0.002
2.5	0.001	0.000	**0.008**	0.002	**0.005**	0.000	<LoD		<LoD		0.003	0.002
3.5	0.001	0.000	**0.006**	0.001	**0.001**	0.002	0.020	0.002	<LoD		0.002	0.002
4.5	0.001	0.002	**0.012**	0.002	**0.005**	0.002	<LoD		<LoD		0.004	0.002
5.5	**0.002**	0.001	**0.015**	0.007	**0.003**	0.001	<LoD		<LoD		0.004	0.002
6.5	0.001	0.000	**0.010**	0.001	**0.028**	0.004	<LoD		<LoD		0.009	0.003
7.5	0.001	0.001	**0.007**	0.002	**0.003**	0.001	<LoD		<LoD		0.004	0.001
8.5	**0.005**	0.003	**0.005**	0.000	**0.003**	0.001	<LoD		<LoD		<LoD	
9.5	**0.001**	0.001	**0.002**	0.002	**0.002**	0.001	<LoD		<LoD		0.002	0.002
10.5	0.001	0.000	**0.004**	0.002	<LoD		<LoD		<LoD		0.002	0.002
11.5	0.001	0.001	**0.001**	0.001	<LoD		<LoD		<LoD		<LoD	
12.5	<LoD		**0.002**	0.002	<LoD		<LoD		<LoD		0.004	0.001
13.5	0.001	0.000	<LoD		<LoD		0.050	0.004	<LoD		<LoD	
14.5	<LoD		**0.002**	0.001	0.001	0.001	<LoD		<LoD		<LoD	
15.5	0.001	0.001	0.001	0.001	<LoD		<LoD		<LoD		<LoD	
blank 1	0.001	0.000	0.001	0.000	0.002	0.000	<LoD		<LoD		<LoD	
blank 2	0.001	0.001	0.001	0.000	0.002	0.001	<LoD		<LoD		<LoD	
blank 3	0.001	0.000	0.001	0.001	0.002	0.001	<LoD		<LoD		<LoD	
blank 4	0.001	0.000	0.001	0.001	0.002	0.000	<LoD		<LoD		<LoD	
blank 5	0.001	0.001	<LoD		0.002	0.001	<LoD		<LoD		<LoD	
correction value	0.001		0.001		0.002		0.000		0.000		0.000	
LoD	0.001		0.001		0.001		0.013		0.013		0.016	
LoQ	0.001		0.001		0.001		0.036		0.036		0.047	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.078**	0.006	**0.376**	0.018	**0.217**	0.009	**0.330**	0.016	**0.458**	0.021	**0.653**	0.037
-4.5	0.065	0.002	**0.357**	0.014	**0.203**	0.012	**0.326**	0.014	**0.512**	0.025	**0.638**	0.053
-3.5	0.059	0.002	**0.334**	0.013	**0.230**	0.025	**0.313**	0.020	**0.496**	0.040	**0.476**	0.018
-2.5	0.050	0.003	**0.329**	0.010	**0.295**	0.032	**0.188**	0.011	**0.650**	0.020	**0.395**	0.039
-1.5	0.054	0.004	**0.314**	0.012	**0.174**	0.014	**0.287**	0.021	**0.549**	0.031	**0.385**	0.014
-0.5	0.054	0.003	**0.327**	0.009	**0.198**	0.013	**0.278**	0.014	**0.577**	0.020	**0.384**	0.017
0.5	0.051	0.002	**0.515**	0.012	0.020	0.014	**0.042**	0.002	**0.513**	0.040	**0.207**	0.005
1.5	<LoD		**0.077**	0.004	<LoD		0.004	0.002	<LoD		**0.013**	0.004
2.5	<LoD		<LoD		<LoD	0.023	<LoD		0.002	0.004	0.005	0.002
3.5	<LoD		<LoD		<LoD	0.016	<LoD		<LoD		**0.011**	0.004
4.5	<LoD		<LoD		<LoD	0.010	<LoD		<LoD		0.006	0.002
5.5	<LoD		<LoD		<LoD	0.010	<LoD		<LoD		0.005	0.004
6.5	<LoD		<LoD		no sample *	no sample *	<LoD		<LoD		<LoD	
7.5	<LoD		<LoD		no sample *	no sample *	<LoD		<LoD		0.004	0.004
8.5	**0.099**	0.003	<LoD		no sample *	no sample *	0.006	0.004	0.004	0.002	0.004	0.000
9.5	<LoD		<LoD		<LoD	0.008	<LoD		<LoD		0.007	0.001
10.5	<LoD		<LoD		<LoD	0.013	<LoD		<LoD		0.005	0.001
11.5	<LoD		<LoD		0.012	0.004	<LoD		<LoD		0.002	0.001
12.5	<LoD		<LoD		<LoD	0.008	<LoD		0.002	0.004	0.005	0.003
13.5	**0.379**	0.021	<LoD		<LoD	0.015	<LoD		<LoD		0.004	0.002
14.5	<LoD		<LoD		<LoD	0.004	<LoD		<LoD		no sample **	no sample **
15.5	<LoD		<LoD		<LoD	0.007	<LoD		<LoD		0.002	0.001
blank 1	<LoD		<LoD		0.130	0.006	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.164	0.018	<LoD		0.005	0.002	<LoD	
blank 3	<LoD		<LoD		0.135	0.011	0.005	0.003	0.024	0.004	<LoD	
blank 4	<LoD		<LoD		0.162	0.014	<LoD		<LoD		<LoD	
blank 5	<LoD		0.045	0.002	0.126	0.012	<LoD		<LoD		0.013	0.002
correction value	0.000		0.009		0.143		0.001		0.006		0.003	
LoD	0.023		0.023		0.008		0.004		0.004		0.004	
LoQ	0.068		0.068		0.021		0.009		0.009		0.011	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 25: Cadmium concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. Identified outliers are grayed out. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.032**	0.003	<LoD	#WERT!	0.009	0.001	<LoD		<LoD		**0.035**	0.005
-4.5	**0.031**	0.002	<LoD	#WERT!	**0.034**	0.007	<LoD		<LoD		**0.052**	0.005
-3.5	**0.034**	0.003	<LoD	#WERT!	**0.040**	0.005	<LoD		<LoD		**0.047**	0.003
-2.5	**0.040**	0.003	<LoD	#WERT!	**0.044**	0.005	<LoD		<LoD		**0.049**	0.003
-1.5	**0.037**	0.003	0.007	0.001	**0.044**	0.004	<LoD		<LoD		**0.049**	0.004
-0.5	**0.041**	0.003	**0.023**	0.002	**0.039**	0.004	<LoD		<LoD		**0.038**	0.002
0.5	**0.061**	0.006	**0.045**	0.004	0.017	0.002	<LoD		<LoD		0.014	0.001
1.5	0.016	0.002	**0.035**	0.003	0.009	0.002	<LoD		<LoD		0.016	0.003
2.5	0.007	0.003	**0.023**	0.002	<LoD		<LoD		<LoD		**0.072**	0.008
3.5	<LoD		**0.019**	0.003	<LoD		<LoD		<LoD		<LoD	
4.5	<LoD		**0.019**	0.003	<LoD		<LoD		<LoD		<LoD	
5.5	<LoD		0.017	0.002	<LoD		<LoD		<LoD		<LoD	
6.5	<LoD		0.016	0.002	0.034	0.003	no sample ***	no sample ***	0.366	0.023	<LoD	
7.5	<LoD		0.014	0.002	<LoD		no sample ***	no sample ***	<LoD		<LoD	
8.5	<LoD		0.011	0.002	<LoD		no sample ***	no sample ***	<LoD		<LoD	
9.5	0.007	0.001	0.013	0.003	<LoD		no sample ***	no sample ***	<LoD		<LoD	
10.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
11.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
12.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
13.5	<LoD	21.474	<LoD		<LoD		<LoD		0.075	0.009	<LoD	
14.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
15.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		<LoD				<LoD	
correction value	0.000		0.000		0.000		0.000		0.000		0.000	
LoD	0.006		0.006		0.006		0.024		0.024		0.012	
LoQ	0.017		0.017		0.017		0.063		0.063		0.031	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.097**	0.008	**0.442**	0.012	**0.319**	0.035	**0.350**	0.027	**0.498**	0.028	**0.556**	0.021
-4.5	**0.073**	0.003	**0.416**	0.006	**0.188**	0.017	**0.275**	0.021	**0.482**	0.016	**0.578**	0.020
-3.5	**0.072**	0.002	**0.399**	0.012	**0.227**	0.021	**0.247**	0.010	**0.575**	0.023	**0.435**	0.037
-2.5	**0.075**	0.001	**0.393**	0.016	**0.174**	0.031	**0.269**	0.023	**0.564**	0.032	**0.419**	0.046
-1.5	**0.089**	0.004	**0.385**	0.011	**0.211**	0.015	**0.255**	0.013	**0.399**	0.007	**0.402**	0.019
-0.5	**0.061**	0.003	**0.371**	0.010	**0.214**	0.012	**0.246**	0.021	**0.356**	0.020	**0.404**	0.008
0.5	**0.066**	0.003	**0.598**	0.017	**0.079**	0.019	**0.046**	0.007	**0.437**	0.024	**0.220**	0.013
1.5	<LoD		**0.123**	0.009	<LoD		<LoD		<LoD		0.011	0.005
2.5	<LoD		<LoD		<LoD		<LoD		0.007	0.002	<LoD	
3.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
4.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
5.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
6.5	<LoD		0.238	0.023	no sample *	no sample *	<LoD		<LoD		<LoD	
7.5	<LoD		<LoD		no sample *	no sample *	<LoD		<LoD		<LoD	
8.5	<LoD		0.025	0.003	no sample *	no sample *	<LoD		<LoD		<LoD	
9.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
10.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
11.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
12.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
13.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
14.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
15.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
blank 1	<LoD		<LoD		0.151	0.011	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.148	0.007	<LoD		0.005	0.001	<LoD	
blank 3	<LoD		2.161	0.069	0.149	0.013	<LoD		0.042	0.012	<LoD	
blank 4	<LoD		<LoD		0.116	0.008	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		0.150	0.011	<LoD				0.013	0.002
correction value	0.000		0.000		0.143		0.000		0.002		0.003	
LoD	0.012		0.016		0.002		0.008		0.004		0.004	
LoQ	0.031		0.047		0.006		0.021		0.009		0.011	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 26: Cadmium concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. Identified outliers are grayed out. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.019**	0.003	**0.003**	0.000	**0.006**	0.002	<LoD		<LoD		<LoD	
-4.5	**0.019**	0.002	**0.004**	0.002	**0.021**	0.004	<LoD		<LoD		<LoD	
-3.5	**0.018**	0.004	**0.005**	0.001	**0.028**	0.001	<LoD		<LoD		<LoD	
-2.5	**0.018**	0.001	**0.014**	0.003	**0.035**	0.004	<LoD		<LoD		<LoD	
-1.5	**0.025**	0.004	**0.032**	0.007	**0.036**	0.003	<LoD		<LoD		<LoD	
-0.5	**0.036**	0.004	**0.059**	0.008	**0.015**	0.000	<LoD		<LoD		**0.106**	0.003
0.5	**0.015**	0.002	**0.016**	0.001	**0.009**	0.000	<LoD		<LoD		**0.077**	0.004
1.5	**0.002**	0.001	**0.013**	0.001	**0.006**	0.002	<LoD		<LoD		<LoD	
2.5	**0.002**	0.002	**0.009**	0.001	**0.005**	0.001	<LoD		<LoD		<LoD	
3.5	<LoD		**0.005**	0.001	**0.003**	0.002	<LoD		**0.075**	0.010	<LoD	
4.5	**0.005**	0.002	**0.005**	0.001	**0.002**	0.000	<LoD		<LoD		<LoD	
5.5	**0.002**	0.000	**0.004**	0.002	**0.002**	0.001	<LoD		<LoD		<LoD	
6.5	**0.001**	0.001	**0.003**	0.000	**0.002**	0.002	<LoD		<LoD		<LoD	
7.5	**0.003**	0.000	**0.004**	0.001	**0.003**	0.001	<LoD		<LoD		<LoD	
8.5	**0.001**	0.001	**0.006**	0.003	**0.004**	0.002	<LoD		<LoD		<LoD	
9.5	**0.003**	0.001	**0.003**	0.000	<NWG	0.001	<LoD		<LoD		<LoD	
10.5	<LoD		**0.003**	0.001	0.001	0.000	<LoD		0.019	0.002	<LoD	
11.5	0.001	0.001	**0.003**	0.001	0.001	0.000	<LoD		<LoD		<LoD	
12.5	**0.002**	0.000	**0.002**	0.001	0.001	0.001	<LoD		0.022	0.002	<LoD	
13.5	<LoD		**0.002**	0.001	0.001	0.000	<LoD		<LoD		<LoD	
14.5	**0.002**	0.001	**0.003**	0.002	<NWG	0.000	<LoD		<LoD		<LoD	
15.5	**0.001**	0.001	**0.002**	0.001	<NWG	0.001	<LoD		<LoD		<LoD	
blank 1	0.002	0.001	<LoD		0.001	0.001	<LoD		<LoD		<LoD	
blank 2	0.001	0.001	<LoD		0.002	0.001	<LoD		<LoD		<LoD	
blank 3	<LoD		0.001	0.001	0.001	0.000	<LoD		<LoD		<LoD	
blank 4	0.001	0.000	0.001	0.000	<LoD		<LoD		<LoD		<LoD	
blank 5	0.002	0.001	0.001	0.001	0.001	0.001	<LoD		<LoD		0.003	0.004
correction value	0.001		0.000		0.001		0.000		0.000		0.001	
LoD	0.001		0.001		0.001		0.013		0.013		0.002	
LoQ	0.001		0.001		0.001		0.036		0.036		0.006	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	<LoD		<LoD		0.011	0.014	**0.017**	0.004	**0.009**	0.004	**0.093**	0.008
-4.5	<LoD		<LoD		<LoD		**0.020**	0.004	**0.009**	0.005	0.004	0.003
-3.5	<LoD		<LoD		0.013	0.008	**0.020**	0.006	**0.009**	0.005	0.001	0.001
-2.5	<LoD		<LoD		<LoD		**0.021**	0.007	**0.012**	0.003	0.002	0.002
-1.5	<LoD		<LoD		<LoD		**0.022**	0.005	**0.011**	0.003	0.004	0.002
-0.5	<LoD		<LoD		<LoD		**0.021**	0.003	**0.010**	0.003	0.005	0.002
0.5	<LoD		<LoD		<LoD		**0.017**	0.002	**0.019**	0.005	0.002	0.002
1.5	<LoD		<LoD		0.010	0.024	**0.013**	0.002	**0.011**	0.004	<LoD	
2.5	<LoD		<LoD		0.003	0.013	0.007	0.003	<LoD		<LoD	
3.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
4.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
5.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
6.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
7.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
8.5	<LoD		<LoD		<LoD		<LoD		0.005	0.003	<LoD	
9.5	<LoD		<LoD		<LoD		0.002	0.003	0.009	0.004	0.002	0.001
10.5	no sample**	no sample**	<LoD		<LoD		<LoD		0.003	0.003	**0.011**	0.004
11.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
12.5	no sample**	no sample**	<LoD		<LoD		<LoD		0.006	0.001	0.001	0.001
13.5	<LoD		**0.491**	0.028	0.003	0.012	<LoD		<LoD		<LoD	
14.5	no sample**	no sample**	**3.281**	0.226	<LoD		<LoD		<LoD		0.003	0.002
15.5	<LoD		<LoD		no sample**	no sample**	<LoD		<LoD		0.004	0.001
blank 1	<LoD		<LoD		0.173	0.009	0.008	0.004	<LoD		0.007	0.001
blank 2	<LoD		<LoD		0.146	0.022	<LoD		0.006	0.002	0.006	0.001
blank 3	<LoD		<LoD		0.150	0.013	0.005	0.003	<LoD		0.006	0.001
blank 4	<LoD		<LoD		0.128	0.009	<LoD		<LoD		0.004	0.001
blank 5	<LoD		<LoD		0.104	0.010	<LoD		<LoD		0.004	0.001
correction value	0.000		0.000		0.132		0.003		0.002		0.005	
LoD	0.023		0.023		0.008		0.004		0.004		0.004	
LoQ	0.068		0.068		0.021		0.009		0.009		0.011	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 27: Cadmium concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.024**	0.001	<LoD		0.008	0.001	<LoD		<LoD		<LoD	
-4.5	**0.034**	0.002	<LoD		**0.026**	0.002	<LoD		<LoD		<LoD	
-3.5	**0.033**	0.002	0.007	0.002	**0.021**	0.001	<LoD		<LoD		<LoD	
-2.5	**0.030**	0.002	0.013	0.003	**0.029**	0.001	<LoD		<LoD		<LoD	
-1.5	**0.039**	0.003	**0.045**	0.002	**0.032**	0.002	<LoD		<LoD		<LoD	
-0.5	**0.037**	0.003	**0.078**	0.003	**0.024**	0.004	<LoD		<LoD		**0.214**	0.009
0.5	**0.038**	0.003	**0.054**	0.005	0.013	0.004	<LoD		0.033	0.005	**0.169**	0.011
1.5	0.011	0.001	0.017	0.002	0.008	0.001	<LoD		<LoD		<LoD	
2.5	<LoD		0.008	0.002	<LoD		no sample ***	no sample ***	<LoD		<LoD	
3.5	<LoD		0.009	0.003	<LoD		no sample ***	no sample ***	<LoD		<LoD	
4.5	0.014	0.002	0.007	0.004	<LoD		<LoD		<LoD		<LoD	
5.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
6.5	<LoD		0.008	0.002	<LoD		<LoD		<LoD		0.021	0.001
7.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
8.5	0.007	0.001	<LoD		<LoD		<LoD		<LoD		<LoD	
9.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
10.5	<LoD		<LoD		<LoD		<LoD		0.025	0.003	<LoD	
11.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
12.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
13.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
14.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
15.5	0.006	0.002	<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		0.011	0.002	<LoD		<LoD		<LoD		0.018	0.002
blank 5	<LoD		<LoD		<LoD						<LoD	
correction value	0.000		0.002		0.000		0.000		0.000		0.004	
LoD	0.006		0.006		0.006		0.024		0.024		0.012	
LoQ	0.017		0.017		0.017		0.063		0.063		0.031	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	<LoD		<LoD		<LoD		0.009	0.004	0.006	0.004	<LoD	
-4.5	<LoD		<LoD		<LoD		<LoD		0.005	0.002	<LoD	
-3.5	0.017	0.002	<LoD		<LoD		0.011	0.003	0.005	0.003	<LoD	
-2.5	<LoD		<LoD		<LoD		0.017	0.003	0.005	0.002	<LoD	
-1.5	<LoD		<LoD		<LoD		0.016	0.005	0.006	0.003	0.005	0.002
-0.5	<LoD		<LoD		<LoD		0.016	0.003	0.006	0.003	0.007	0.004
0.5	<LoD		<LoD		<LoD		0.009	0.003	**0.015**	0.004	<LoD	
1.5	<LoD		<LoD		<LoD		0.008	0.003	0.007	0.004	<LoD	
2.5	0.018	0.002	<LoD		<LoD		0.008	0.005	<LoD		<LoD	
3.5	<LoD		<LoD		<LoD		<LoD		**0.011**	0.003	<LoD	
4.5	<LoD		<LoD		<LoD		**0.075**	0.019	<LoD		<LoD	
5.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
6.5	0.046	0.003	<LoD		<LoD		<LoD		no sample**	no sample**	<LoD	
7.5	<LoD		<LoD		<LoD		<LoD		no sample**	no sample**	<LoD	
8.5	<LoD		<LoD		<LoD		<LoD		no sample**	no sample**	<LoD	
9.5	<LoD		<LoD		<LoD		<LoD		no sample**	no sample**	0.009	0.002
10.5	<LoD		<LoD		<LoD		<LoD		no sample**	no sample**	<LoD	
11.5	<LoD		0.054	0.005	<LoD		<LoD		no sample**	no sample**	<LoD	
12.5	<LoD		<LoD		<LoD		<LoD		no sample**	no sample**	<LoD	
13.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
14.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	no sample**	no sample**	**0.017**	0.005
15.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	<LoD		<LoD		0.115	0.007	<LoD		<LoD		0.007	0.002
blank 2	<LoD		<LoD		0.123	0.010	<LoD		<LoD		<LoD	
blank 3	<LoD		0.040	0.004	0.138	0.013	<LoD		<LoD		0.008	0.002
blank 4	0.017	0.002	<LoD		0.135	0.011	<LoD		<LoD		0.005	0.001
blank 5	<LoD		<LoD		0.153	0.016	0.010	0.001	<LoD		0.005	0.001
correction value	0.003		0.008		0.133		0.002		0.000		0.005	
LoD	0.016		0.016		0.002		0.008		0.004		0.004	
LoQ	0.047		0.047		0.006		0.021		0.009		0.011	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 28: Cobalt concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. Identified outliers are grayed out. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.350**	0.036	**0.258**	0.039	**0.421**	0.031	**0.392**	0.035	**0.967**	0.038	**0.658**	0.071
-4.5	**0.433**	0.041	**0.346**	0.024	**0.501**	0.047	**0.555**	0.047	**1.149**	0.081	**0.743**	0.032
-3.5	**0.437**	0.020	**0.418**	0.066	**0.466**	0.057	**0.693**	0.033	**1.238**	0.038	**0.750**	0.051
-2.5	**0.324**	0.021	**0.302**	0.008	**0.438**	0.036	**0.651**	0.039	**0.585**	0.023	**0.810**	0.075
-1.5	**0.323**	0.044	**0.337**	0.057	**0.438**	0.082	**0.682**	0.045	**0.614**	0.030	**0.893**	0.079
-0.5	**0.388**	0.047	**0.898**	0.074	**1.292**	0.029	**0.764**	0.042	**1.131**	0.124	**0.709**	0.061
0.5	**0.839**	0.033	**1.986**	0.316	**1.991**	0.132	**0.989**	0.042	**0.730**	0.027	**1.223**	0.106
1.5	**1.186**	0.119	**1.082**	0.099	**1.398**	0.049	**1.271**	0.041	**2.390**	0.086	**0.949**	0.058
2.5	**1.098**	0.137	**1.042**	0.021	**1.468**	0.090	**1.561**	0.056	**1.840**	0.066	**1.477**	0.069
3.5	**1.114**	0.149	**1.128**	0.023	**1.125**	0.053	**1.108**	0.040	**1.478**	0.078	**1.133**	0.101
4.5	**1.320**	0.265	**1.018**	0.031	**1.467**	0.168	**0.950**	0.064	**1.591**	0.094	**1.838**	0.127
5.5	**1.443**	0.114	**1.204**	0.148	**1.167**	0.144	**0.892**	0.075	**1.365**	0.056	**1.297**	0.092
6.5	**1.380**	0.083	**1.151**	0.167	**1.546**	0.196	**0.833**	0.038	**1.374**	0.063	**1.332**	0.083
7.5	**1.643**	0.145	**1.458**	0.242	**1.490**	0.104	**0.920**	0.049	**1.768**	0.076	**1.204**	0.088
8.5	**2.418**	0.262	**1.338**	0.032	**1.805**	0.125	**0.927**	0.052	**1.383**	0.063	**1.155**	0.081
9.5	**1.328**	0.152	**1.475**	0.089	**2.360**	0.347	**0.868**	0.064	**1.519**	0.097	**1.129**	0.091
10.5	**1.895**	0.186	**1.889**	0.015	**2.107**	0.070	**0.848**	0.050	**1.340**	0.091	**2.159**	0.149
11.5	**1.736**	0.149	**1.674**	0.104	**2.500**	0.066	**0.912**	0.041	**1.313**	0.090	**1.288**	0.115
12.5	**2.222**	0.255	**1.807**	0.134	**2.021**	0.182	**0.896**	0.033	**1.290**	0.049	**1.282**	0.043
13.5	**1.680**	0.075	**1.617**	0.061	**2.294**	0.292	**0.934**	0.025	**1.329**	0.071	**1.535**	0.110
14.5	**1.902**	0.373	**2.483**	0.268	**2.145**	0.116	**0.901**	0.049	**1.318**	0.072	**1.128**	0.076
15.5	**1.649**	0.110	**1.654**	0.112	**2.141**	0.070	**0.957**	0.040	**1.342**	0.056	**1.275**	0.123
blank 1	0.005	0.005	<LoD		0.023	0.005	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.014	0.004	<LoD		<LoD		<LoD	
blank 3	0.012	0.005	0.004	0.002	0.020	0.007	<LoD		<LoD		<LoD	
blank 4	0.003	0.001	0.009	0.003	0.012	0.005	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		0.016	0.006	<LoD		<LoD		<LoD	
correction value	0.004		0.003		0.017		0.000		0.000		0.000	
LoD	0.002		0.002		0.002		0.022		0.022		0.016	
LoQ	0.006		0.006		0.006		0.058		0.058		0.045	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**2.377**	0.134	**4.914**	0.145	**6.216**	0.333	**9.605**	0.847	**10.658**	0.442	**9.704**	0.277
-4.5	**2.170**	0.067	**4.838**	0.225	**6.074**	0.166	**10.262**	0.504	**11.514**	0.253	**8.413**	0.268
-3.5	**2.049**	0.072	**4.613**	0.060	**6.618**	0.321	**10.762**	0.663	**11.427**	0.434	**30.515**	1.148
-2.5	**1.761**	0.062	**4.540**	0.080	**7.562**	0.181	**5.778**	0.305	**14.523**	0.694	**8.131**	0.312
-1.5	**1.810**	0.073	**4.435**	0.170	**5.462**	0.268	**10.020**	0.477	**12.647**	0.475	**7.098**	0.228
-0.5	**2.045**	0.075	**4.460**	0.123	**5.447**	0.251	**9.804**	0.437	**13.069**	0.238	**6.843**	0.268
0.5	**2.414**	0.083	**4.135**	0.114	**1.991**	0.120	**2.758**	0.073	**7.802**	0.160	**3.905**	0.240
1.5	**2.082**	0.063	**1.406**	0.027	**0.426**	0.021	**0.236**	0.018	**0.795**	0.056	**0.480**	0.038
2.5	**1.591**	0.075	**0.491**	0.025	**0.865**	0.076	**0.620**	0.039	**0.400**	0.031	**0.668**	0.038
3.5	**1.861**	0.073	**0.894**	0.036	**1.394**	0.026	**1.302**	0.093	**0.874**	0.043	**0.605**	0.034
4.5	**1.395**	0.083	**1.090**	0.061	**1.718**	0.140	**1.751**	0.149	**1.427**	0.103	**0.601**	0.016
5.5	**1.442**	0.088	**1.237**	0.034	**1.828**	0.211	**1.686**	0.136	**1.618**	0.087	**0.858**	0.053
6.5	**1.548**	0.103	**1.254**	0.055	no sample *	no sample *	**2.184**	0.156	**1.913**	0.117	**1.076**	0.114
7.5	**1.614**	0.021	**1.295**	0.103	no sample *	no sample *	**2.360**	0.068	**1.817**	0.105	**1.336**	0.073
8.5	**1.453**	0.026	**1.307**	0.095	no sample *	no sample *	**2.731**	0.143	**1.922**	0.063	**1.457**	0.075
9.5	**1.387**	0.112	**1.337**	0.030	**1.429**	0.109	**2.414**	0.172	**1.869**	0.121	**1.518**	0.135
10.5	**1.372**	0.089	**1.296**	0.080	**2.340**	0.118	**2.549**	0.239	**2.072**	0.130	**1.644**	0.141
11.5	**1.404**	0.057	**1.311**	0.081	**1.941**	0.168	**2.487**	0.216	**1.876**	0.096	**1.728**	0.134
12.5	**1.365**	0.075	**1.277**	0.086	**2.208**	0.089	**2.347**	0.149	**2.225**	0.093	**1.786**	0.090
13.5	**1.348**	0.066	**1.303**	0.069	**2.230**	0.035	**2.366**	0.123	**2.104**	0.096	**1.768**	0.135
14.5	**1.355**	0.109	**1.282**	0.078	**1.717**	0.063	**2.257**	0.115	**2.194**	0.115	no sample **	no sample **
15.5	**1.333**	0.060	**1.276**	0.081	**2.040**	0.137	**2.225**	0.155	**2.585**	0.100	**1.868**	0.133
blank 1	<LoD		<LoD		0.028	0.017	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.038	0.011	<LoD		0.028	0.003	<LoD	
blank 3	<LoD		<LoD		0.026	0.016	<LoD		0.014	0.009	<LoD	
blank 4	<LoD		<LoD		0.031	0.008	0.036	0.011	0.007	0.006	<LoD	
blank 5	<LoD		<LoD		0.030	0.009	0.007	0.007	<LoD		<LoD	
correction value	0.000		0.000		0.031		0.009		0.010		0.000	
LoD	0.007		0.007		0.009		0.006		0.006		0.012	
LoQ	0.019		0.019		0.024		0.014		0.014		0.028	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 29: Cobalt concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.502**	0.018	**0.347**	0.018	**0.363**	0.016	**0.693**	0.054	**0.364**	0.030	**0.474**	0.046
-4.5	**0.446**	0.033	**0.384**	0.032	**0.529**	0.014	**0.580**	0.031	**0.733**	0.032	**0.597**	0.016
-3.5	**0.502**	0.031	**0.353**	0.022	**0.541**	0.015	**0.517**	0.033	**0.700**	0.062	**0.503**	0.039
-2.5	**0.533**	0.045	**0.349**	0.020	**0.491**	0.013	**0.541**	0.015	**0.666**	0.060	**0.551**	0.044
-1.5	**0.481**	0.019	**0.311**	0.015	**0.515**	0.023	**0.594**	0.026	**0.485**	0.040	**0.583**	0.023
-0.5	**0.452**	0.025	**1.060**	0.071	**1.119**	0.049	**0.555**	0.030	**0.319**	0.015	**0.604**	0.039
0.5	**1.503**	0.034	**1.859**	0.075	**2.693**	0.073	**0.462**	0.033	**0.821**	0.098	**0.127**	0.010
1.5	**2.224**	0.155	**1.424**	0.053	**1.993**	0.059	**0.959**	0.047	**2.301**	0.065	**0.876**	0.080
2.5	**1.909**	0.074	**1.390**	0.113	**1.094**	0.055	**1.083**	0.020	**1.568**	0.084	**2.052**	0.163
3.5	**1.478**	0.058	**1.338**	0.048	**1.249**	0.044	**0.896**	0.033	**1.201**	0.042	**1.750**	0.133
4.5	**1.267**	0.051	**1.233**	0.083	**1.554**	0.066	**0.855**	0.071	**1.136**	0.101	**1.709**	0.131
5.5	**1.714**	0.112	**1.618**	0.138	**1.414**	0.086	**0.822**	0.039	**1.268**	0.193	**1.662**	0.122
6.5	**1.708**	0.126	**1.629**	0.055	**1.806**	0.076	no sample ***	no sample ***	**1.240**	0.093	**1.633**	0.103
7.5	**1.712**	0.073	**1.702**	0.104	**1.927**	0.127	no sample ***	no sample ***	**1.167**	0.055	**1.626**	0.070
8.5	**1.815**	0.053	**1.870**	0.060	**1.851**	0.050	no sample ***	no sample ***	**1.222**	0.062	**1.577**	0.062
9.5	**2.069**	0.081	**2.065**	0.041	**1.400**	0.060	no sample ***	no sample ***	**1.226**	0.060	**1.573**	0.047
10.5	**2.117**	0.098	**1.807**	0.042	**1.759**	0.095	**1.029**	0.049	**1.347**	0.024	**1.523**	0.069
11.5	**2.265**	0.187	**2.065**	0.068	**1.681**	0.063	**0.894**	0.046	**1.274**	0.062	**1.463**	0.060
12.5	**2.034**	0.119	**1.964**	0.051	**2.182**	0.111	**0.916**	0.061	**1.324**	0.100	**1.519**	0.080
13.5	**2.317**	21.474	**1.996**	0.111	**2.432**	0.099	**0.917**	0.029	**1.241**	0.056	**1.510**	0.023
14.5	**2.062**	0.074	**1.512**	0.040	**2.122**	0.076	**1.015**	0.024	**1.307**	0.062	**1.499**	0.039
15.5	**2.331**	0.122	**2.089**	0.049	**2.209**	0.087	no sample ***	no sample ***	**1.299**	0.070	**1.471**	0.069
blank 1	<LoD		0.009	0.004	0.031	0.008	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.032	0.003	<LoD		<LoD		<LoD	
blank 3	<LoD		0.007	0.006	0.018	0.003	<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		0.032	0.008	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		0.021	0.005	<LoD				<LoD	
correction value	0.000		0.003		0.027		0.000		0.000		0.000	
LoD	0.007		0.007		0.007		0.022		0.022		0.030	
LoQ	0.019		0.019		0.019		0.057		0.057		0.081	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**3.154**	0.079	**5.095**	0.133	**8.071**	0.480	**9.045**	0.322	**10.730**	0.262	**8.022**	0.534
-4.5	**2.488**	0.022	**4.909**	0.142	**6.844**	0.639	**8.912**	0.305	**10.388**	0.419	**7.231**	0.476
-3.5	**2.622**	0.079	**4.748**	0.169	**6.906**	0.350	**7.540**	0.273	**12.851**	0.711	**27.352**	0.710
-2.5	**2.903**	0.107	**4.785**	0.132	**5.695**	0.287	**7.975**	0.396	**13.132**	0.626	**7.772**	0.766
-1.5	**2.939**	0.046	**4.634**	0.125	**6.242**	0.389	**8.359**	0.529	**8.890**	0.550	**7.278**	0.481
-0.5	**2.547**	0.064	**4.592**	0.164	**6.016**	0.585	**7.805**	0.291	**8.368**	0.268	**6.909**	0.444
0.5	**3.166**	0.053	**4.335**	0.113	**2.186**	0.191	**2.486**	0.163	**7.989**	0.141	**3.929**	0.188
1.5	**2.257**	0.148	**1.535**	0.123	**0.426**	0.051	**0.247**	0.017	**0.812**	0.060	**0.453**	0.035
2.5	**1.997**	0.088	**0.498**	0.042	**0.881**	0.061	**0.383**	0.041	**0.394**	0.049	**0.654**	0.044
3.5	**1.810**	0.061	**0.866**	0.080	**1.325**	0.137	**1.176**	0.073	**0.741**	0.080	**0.590**	0.045
4.5	**2.487**	0.175	**1.139**	0.075	**1.493**	0.115	**1.196**	0.038	**1.297**	0.070	**0.663**	0.040
5.5	**2.129**	0.045	**1.227**	0.110	**1.634**	0.076	**1.938**	0.104	**1.439**	0.099	no sample **	no sample **
6.5	**1.979**	0.054	**1.356**	0.089	no sample *	no sample *	**1.940**	0.149	**1.664**	0.081	**1.107**	0.049
7.5	**1.678**	0.042	**1.349**	0.093	no sample *	no sample *	**1.788**	0.156	**1.817**	0.184	**1.390**	0.121
8.5	**2.460**	0.023	**1.405**	0.090	no sample *	no sample *	**1.792**	0.129	**1.891**	0.160	**1.585**	0.117
9.5	**2.338**	0.031	**1.371**	0.127	**1.381**	0.060	**2.023**	0.085	**1.612**	0.049	**1.587**	0.105
10.5	**1.990**	0.042	**1.373**	0.093	**2.058**	0.195	**2.198**	0.052	**1.695**	0.097	**1.803**	0.151
11.5	**2.041**	0.017	**1.355**	0.071	**1.796**	0.124	**2.221**	0.106	**1.906**	0.107	no sample **	no sample **
12.5	**1.930**	0.062	**1.348**	0.097	**1.877**	0.024	**2.171**	0.130	**1.780**	0.191	no sample **	no sample **
13.5	**2.240**	0.100	**1.361**	0.088	**2.016**	0.112	**2.626**	0.092	**1.785**	0.172	no sample **	no sample **
14.5	**1.954**	0.042	**1.391**	0.061	**2.259**	0.075	**2.342**	0.101	**1.708**	0.112	no sample **	no sample **
15.5	**2.322**	0.069	**1.331**	0.088	**1.742**	0.140	**2.127**	0.163	**1.777**	0.101	no sample **	no sample **
blank 1	<LoD		<LoD		0.034	0.009	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.036	0.004	0.013	0.007	<LoD		<LoD	
blank 3	<LoD		<LoD		0.024	0.014	<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		0.022	0.011	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		0.021	0.003	0.010	0.003			<LoD	
correction value	0.000		0.000		0.027		0.005		0.000		0.000	
LoD	0.030		0.016		0.005		0.009		0.006		0.012	
LoQ	0.081		0.045		0.010		0.024		0.014		0.028	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 30: Cobalt concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.697**	0.072	**0.424**	0.044	**1.184**	0.136	**0.740**	0.087	**0.409**	0.023	**1.176**	0.055
-4.5	**0.684**	0.085	**0.654**	0.023	**1.692**	0.072	**1.031**	0.093	**0.424**	0.014	**1.439**	0.046
-3.5	**0.581**	0.027	**0.928**	0.100	**1.554**	0.096	**0.627**	0.036	**0.640**	0.030	**1.515**	0.060
-2.5	**0.613**	0.012	**1.087**	0.096	**1.582**	0.113	**0.959**	0.051	**0.392**	0.021	**1.794**	0.049
-1.5	**0.773**	0.040	**1.369**	0.183	**2.188**	0.120	**0.595**	0.050	**0.864**	0.030	**1.702**	0.068
-0.5	**0.918**	0.125	**1.716**	0.190	**1.996**	0.069	**0.800**	0.070	**0.584**	0.034	**2.086**	0.066
0.5	**1.459**	0.110	**0.758**	0.047	**1.640**	0.311	**0.680**	0.052	**1.593**	0.122	**1.642**	0.062
1.5	**2.677**	0.102	**1.027**	0.067	**1.434**	0.086	**0.784**	0.057	**1.146**	0.031	**1.408**	0.044
2.5	**1.605**	0.063	**1.118**	0.068	**1.207**	0.095	**0.931**	0.051	**1.559**	0.057	**1.282**	0.074
3.5	**1.117**	0.084	**1.110**	0.088	**1.536**	0.021	**0.717**	0.067	**1.102**	0.032	**1.564**	0.080
4.5	**1.435**	0.153	**1.203**	0.066	**1.505**	0.021	**0.720**	0.060	**1.403**	0.063	**1.311**	0.047
5.5	**1.492**	0.155	**1.220**	0.131	**1.626**	0.053	**0.756**	0.047	**1.543**	0.082	**1.984**	0.034
6.5	**1.232**	0.078	**1.495**	0.309	**1.732**	0.200	**0.778**	0.021	**2.166**	0.179	**1.896**	0.143
7.5	**1.491**	0.067	**1.614**	0.085	**2.349**	0.169	**0.868**	0.051	**1.617**	0.105	**1.734**	0.029
8.5	**1.615**	0.115	**2.667**	0.156	**1.888**	0.269	**0.823**	0.038	**1.331**	0.024	**1.422**	0.056
9.5	**2.528**	0.345	**1.361**	0.183	**1.906**	0.107	**0.851**	0.049	**1.566**	0.044	**1.921**	0.068
10.5	**1.811**	0.229	**1.813**	0.079	**2.189**	0.220	**0.872**	0.024	**1.572**	0.063	**1.797**	0.115
11.5	**2.008**	0.221	**1.635**	0.035	**1.900**	0.050	**0.879**	0.073	**1.802**	0.059	**2.016**	0.037
12.5	**1.888**	0.254	**2.045**	0.199	**1.903**	0.095	**0.909**	0.038	**1.235**	0.053	**1.831**	0.034
13.5	**1.710**	0.172	**2.148**	0.017	**2.019**	0.241	**0.988**	0.044	**1.634**	0.054	**1.707**	0.065
14.5	**1.982**	0.190	**2.050**	0.133	**2.020**	0.192	**0.942**	0.030	**2.144**	0.139	**1.715**	0.095
15.5	**2.097**	0.181	**1.775**	0.044	**2.186**	0.290	**0.967**	0.034	**1.787**	0.051	**1.801**	0.066
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	0.002	0.003	0.004	0.002	0.002	0.004	<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		0.004	0.003	<LoD		<LoD		<LoD	
blank 4	0.005	0.002	<LoD		<LoD		<LoD		<LoD		<LoD	
blank 5	0.006	0.001	0.003	0.002	0.002	0.002	<LoD		<LoD		<LoD	
correction value	0.003		0.001		0.002		0.000		0.000		0.000	
LoD	0.002		0.002		0.002		0.022		0.022		0.005	
LoQ	0.006		0.006		0.006		0.058		0.058		0.010	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**1.324**	0.053	**1.095**	0.040	**0.504**	0.009	**0.445**	0.061	**1.242**	0.087	**0.456**	0.054
-4.5	**1.097**	0.053	**0.962**	0.036	**0.442**	0.055	**0.635**	0.078	**0.692**	0.036	**0.467**	0.063
-3.5	**1.060**	0.033	**0.906**	0.055	**0.457**	0.038	**0.659**	0.042	**0.845**	0.058	**0.393**	0.024
-2.5	**0.823**	0.047	**0.858**	0.040	**0.458**	0.052	**0.731**	0.063	**0.865**	0.087	**0.478**	0.052
-1.5	**0.929**	0.038	**0.784**	0.039	**0.423**	0.027	**0.710**	0.058	**0.921**	0.058	**0.491**	0.022
-0.5	**0.850**	0.035	**0.602**	0.010	**0.504**	0.036	**0.727**	0.086	**0.870**	0.054	**0.542**	0.049
0.5	**1.294**	0.057	**0.388**	0.020	**0.650**	0.056	**1.124**	0.119	**0.937**	0.023	**0.817**	0.039
1.5	**1.157**	0.059	**0.643**	0.023	**1.317**	0.084	**1.673**	0.112	**0.802**	0.030	**1.161**	0.053
2.5	**1.062**	0.046	**0.880**	0.063	**1.599**	0.060	**1.293**	0.055	**0.678**	0.068	**1.642**	0.067
3.5	**1.070**	0.075	**1.006**	0.071	**1.754**	0.101	**1.544**	0.051	**1.011**	0.083	**1.594**	0.054
4.5	**1.141**	0.057	**1.076**	0.053	**2.086**	0.197	**1.601**	0.114	**1.316**	0.137	**1.755**	0.174
5.5	**1.174**	0.075	**1.199**	0.052	**2.036**	0.153	**1.548**	0.086	**1.614**	0.085	**1.934**	0.155
6.5	**1.237**	0.089	**1.204**	0.041	**2.016**	0.160	**1.508**	0.085	**1.948**	0.079	**1.792**	0.151
7.5	**1.226**	0.069	**1.270**	0.022	**2.193**	0.110	**1.656**	0.080	**1.790**	0.112	**1.820**	0.157
8.5	**1.242**	0.096	**1.241**	0.057	**2.212**	0.147	**1.613**	0.034	**1.658**	0.095	**1.759**	0.136
9.5	**1.234**	0.063	**1.235**	0.061	**2.130**	0.164	**1.600**	0.046	**1.612**	0.105	**1.800**	0.042
10.5	no sample**	no sample**	**1.260**	0.062	**2.300**	0.054	**1.635**	0.096	**1.502**	0.115	**1.881**	0.039
11.5	**1.324**	0.028	**1.249**	0.039	**2.121**	0.133	**1.620**	0.125	**1.585**	0.124	**1.861**	0.174
12.5	no sample**	no sample**	**1.259**	0.038	**2.374**	0.067	**1.873**	0.107	**1.568**	0.149	**1.867**	0.158
13.5	**1.254**	0.062	**1.271**	0.045	**2.784**	0.136	**1.592**	0.068	**1.626**	0.127	**0.879**	0.101
14.5	no sample**	no sample**	**1.286**	0.040	**2.055**	0.127	**1.610**	0.068	**1.512**	0.174	**0.872**	0.066
15.5	**1.237**	0.102	**1.276**	0.061	no sample**	no sample**	**1.499**	0.077	**1.528**	0.081	**1.795**	0.138
blank 1	<LoD		<LoD		0.037	0.008	<LoD		<LoD		0.007	0.000
blank 2	<LoD		<LoD		0.030	0.003	<LoD		<LoD		0.006	0.000
blank 3	<LoD		<LoD		0.030	0.008	<LoD		0.006	0.006	0.017	0.000
blank 4	<LoD		<LoD		0.017	0.005	<LoD		<LoD		0.008	0.000
blank 5	<LoD		<LoD		0.022	0.005	<LoD		<LoD		0.007	0.000
correction value	0.000		0.000		0.027		0.000		0.000		0.009	
LoD	0.007		0.007		0.009		0.006		0.006		0.012	
LoQ	0.019		0.019		0.024		0.014		0.014		0.028	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 31: Cobalt concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.773**	0.033	**0.325**	0.018	**1.052**	0.072	**0.671**	0.042	**0.783**	0.061	**1.207**	0.049
-4.5	**1.099**	0.045	**0.953**	0.033	**1.781**	0.121	**0.638**	0.019	**0.601**	0.026	**0.925**	0.017
-3.5	**0.958**	0.020	**1.307**	0.085	**1.456**	0.056	**0.951**	0.081	**1.074**	0.094	**1.450**	0.093
-2.5	**0.936**	0.043	**1.489**	0.042	**1.483**	0.032	**0.621**	0.026	**1.182**	0.047	**1.758**	0.058
-1.5	**0.902**	0.065	**1.629**	0.089	**1.805**	0.103	**0.568**	0.034	**1.184**	0.067	**1.531**	0.066
-0.5	**1.026**	0.046	**1.620**	0.042	**1.954**	0.099	**0.542**	0.028	**1.074**	0.055	**1.396**	0.072
0.5	**2.476**	0.103	**1.083**	0.034	**1.253**	0.045	**0.580**	0.020	**2.150**	0.048	**1.722**	0.061
1.5	**3.702**	0.235	**1.161**	0.055	**1.325**	0.055	**0.751**	0.046	**1.156**	0.071	**1.474**	0.064
2.5	**1.902**	0.116	**1.049**	0.027	**1.130**	0.049	no sample ***	no sample ***	**1.082**	0.056	**1.683**	0.092
3.5	**1.590**	0.051	**1.304**	0.060	**1.251**	0.040	no sample ***	no sample ***	**1.139**	0.033	**1.948**	0.045
4.5	**1.548**	0.066	**1.429**	0.042	**1.526**	0.044	**0.709**	0.024	**1.332**	0.067	**2.323**	0.071
5.5	**1.518**	0.067	**1.439**	0.060	**1.603**	0.115	**0.717**	0.038	**1.446**	0.035	**2.121**	0.067
6.5	**1.974**	0.094	**2.057**	0.101	**2.212**	0.096	**0.739**	0.022	**1.141**	0.048	**1.932**	0.088
7.5	**1.803**	0.150	**1.806**	0.096	**1.911**	0.051	**0.756**	0.040	**1.154**	0.079	**1.705**	0.053
8.5	**1.871**	0.085	**1.784**	0.124	**1.804**	0.063	**0.751**	0.035	**1.375**	0.033	**2.139**	0.063
9.5	**1.773**	0.068	**1.717**	0.143	**2.162**	0.096	**0.794**	0.053	**1.231**	0.062	**2.110**	0.085
10.5	**2.337**	0.113	**1.793**	0.115	**2.330**	0.135	**0.865**	0.014	**1.223**	0.061	**1.669**	0.030
11.5	**2.133**	0.127	**1.727**	0.080	**2.760**	0.164	**0.880**	0.069	**1.247**	0.163	**2.002**	0.074
12.5	**1.957**	0.164	**1.936**	0.089	**2.701**	0.147	no sample ***	no sample ***	**1.262**	0.054	**1.846**	0.051
13.5	**1.897**	0.141	**2.132**	0.090	**2.535**	0.090	**0.879**	0.031	**1.254**	0.042	**2.091**	0.035
14.5	**2.290**	0.071	**1.900**	0.144	**2.213**	0.199	no sample ***	no sample ***	**1.257**	0.094	**1.528**	0.040
15.5	**1.773**	0.136	**2.138**	0.140	**2.781**	0.097	no sample ***	no sample ***	**1.239**	0.093	**1.837**	0.030
blank 1	<LoD		<LoD		<LoD						<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		0.014		<LoD		<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
correction value	0.000		0.003		0.000		0.000		0.000		0.000	
LoD	0.007		0.007		0.007		0.022		0.022		0.030	
LoQ	0.019		0.019		0.019		0.057		0.057		0.081	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.828**	0.055	**1.123**	0.024	**0.392**	0.033	**0.323**	0.041	**1.173**	0.151	**0.447**	0.063
-4.5	**1.196**	0.054	**1.012**	0.054	**0.397**	0.058	**0.318**	0.068	**0.722**	0.071	**0.432**	0.048
-3.5	**1.162**	0.048	**0.935**	0.039	**0.453**	0.015	**0.378**	0.033	**0.830**	0.170	**0.389**	0.027
-2.5	**0.863**	0.035	**0.889**	0.039	**0.352**	0.025	**0.481**	0.059	**0.638**	0.039	**0.446**	0.063
-1.5	**0.904**	0.038	**0.810**	0.008	**0.381**	0.024	**0.523**	0.024	**0.591**	0.030	**0.439**	0.035
-0.5	**0.876**	0.048	**0.626**	0.022	**0.475**	0.046	**0.550**	0.026	**0.620**	0.018	**0.491**	0.045
0.5	**1.358**	0.071	**0.388**	0.021	**1.022**	0.020	**0.701**	0.043	**0.766**	0.065	**0.833**	0.020
1.5	**1.259**	0.081	**0.619**	0.046	**1.334**	0.079	**1.114**	0.054	**0.629**	0.038	**1.174**	0.031
2.5	**1.153**	0.084	**0.891**	0.060	**1.599**	0.138	**1.358**	0.108	**0.736**	0.058	**1.423**	0.100
3.5	**1.119**	0.070	**1.018**	0.009	**1.485**	0.071	**1.389**	0.132	**1.155**	0.076	**1.669**	0.147
4.5	**1.179**	0.055	**1.090**	0.058	**1.340**	0.058	**1.473**	0.131	**1.400**	0.051	**1.862**	0.093
5.5	**1.258**	0.056	**1.189**	0.037	**1.595**	0.093	**1.432**	0.146	**1.626**	0.073	**1.871**	0.061
6.5	**1.261**	0.062	**1.231**	0.031	**1.759**	0.122	**1.491**	0.151	no sample**	no sample**	**1.866**	0.180
7.5	**1.319**	0.066	**1.215**	0.048	**1.756**	0.064	**1.473**	0.057	no sample**	no sample**	**1.854**	0.076
8.5	**1.313**	0.059	**1.230**	0.053	**2.394**	0.142	**1.418**	0.134	no sample**	no sample**	**1.885**	0.116
9.5	**1.331**	0.015	**1.213**	0.052	**1.424**	0.122	**1.451**	0.141	no sample**	no sample**	**1.916**	0.096
10.5	**1.380**	0.070	**1.238**	0.061	**1.868**	0.160	**1.542**	0.155	no sample**	no sample**	**1.889**	0.115
11.5	**1.302**	0.066	**1.242**	0.026	**1.616**	0.051	**1.470**	0.090	no sample**	no sample**	**1.909**	0.200
12.5	**1.303**	0.064	**1.257**	0.024	**1.702**	0.092	**0.072**	0.011	no sample**	no sample**	no sample**	no sample**
13.5	**1.315**	0.062	**1.254**	0.048	**2.325**	0.190	no sample ***	no sample ***	no sample**	no sample**	**2.051**	0.207
14.5	**1.298**	0.067	**1.266**	0.048	**2.221**	0.103	no sample ***	no sample ***	no sample**	no sample**	**1.993**	0.180
15.5	**1.294**	0.060	**1.276**	0.067	**2.172**	0.168	no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	<LoD		<LoD		0.030		<LoD		0.001		<LoD	
blank 2	<LoD		<LoD		0.019		<LoD		0.001		<LoD	
blank 3	<LoD		<LoD		0.024		<LoD		0.001		<LoD	
blank 4	<LoD		<LoD		0.033		<LoD		0.004		<LoD	
blank 5	<LoD		<LoD		0.018		<LoD		0.001		<LoD	
correction value	0.000		0.000		0.025		0.000		0.001		0.000	
LoD	0.016		0.016		0.005		0.009		0.006		0.012	
LoQ	0.045		0.045		0.010		0.024		0.014		0.028	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 32: Chromium concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	<LoD		<LoD	0.015	<LoD		**0.236**	0.011	**0.150**	0.016	<LoD	
-4.5	<LoD		0.019	0.007	<LoD		**0.168**	0.021	**0.213**	0.027	<LoD	
-3.5	0.032	0.003	0.031	0.015	<LoD		**0.144**	0.027	**0.151**	0.020	<LoD	
-2.5	<LoD		**0.215**	0.029	<LoD		**0.106**	0.017	**0.091**	0.030	<LoD	
-1.5	<LoD		0.029	0.019	<LoD		**0.107**	0.018	0.049	0.009	<LoD	
-0.5	<LoD		**0.053**	0.019	<LoD		**0.078**	0.016	**0.095**	0.024	<LoD	
0.5	<LoD		**0.219**	0.039	**1.242**	0.163	**0.178**	0.036	0.037	0.008	**0.133**	0.031
1.5	**0.229**	0.014	**0.149**	0.025	<LoD		**0.064**	0.030	**0.130**	0.019	**0.093**	0.032
2.5	<LoD		**0.137**	0.025	<LoD		**0.129**	0.016	**0.229**	0.019	**0.192**	0.049
3.5	0.037	0.048	**0.266**	0.031	<LoD		**0.133**	0.036	**0.137**	0.011	**0.164**	0.035
4.5	**0.061**	0.056	**0.236**	0.028	<LoD		**0.114**	0.024	**0.200**	0.015	**0.237**	0.081
5.5	**0.117**	0.014	**0.751**	0.092	<LoD		**0.122**	0.017	**0.174**	0.028	**0.157**	0.031
6.5	**0.066**	0.014	**0.204**	0.044	<LoD		**0.131**	0.020	**0.214**	0.024	**0.180**	0.050
7.5	**0.542**	0.067	**2.028**	0.337	<LoD		**0.155**	0.023	**0.255**	0.032	**0.104**	0.031
8.5	**4.735**	0.608	**0.126**	0.032	<LoD		**0.111**	0.010	**0.185**	0.028	**0.126**	0.050
9.5	**0.041**	0.019	**0.129**	0.010	<LoD		**0.107**	0.027	**0.283**	0.044	**0.121**	0.018
10.5	**0.179**	0.049	**0.532**	0.028	<LoD		**0.089**	0.012	**0.173**	0.022	**0.346**	0.072
11.5	**0.081**	0.038	**0.087**	0.032	<LoD		**0.114**	0.014	**0.183**	0.030	**0.170**	0.015
12.5	**0.132**	0.067	**0.143**	0.010	<LoD		**0.140**	0.009	**0.187**	0.034	**0.132**	0.050
13.5	**0.082**	0.024	**1.936**	0.163	<LoD		**0.118**	0.022	**0.177**	0.022	**0.207**	0.047
14.5	**0.063**	0.073	**0.145**	0.039	<LoD		**0.098**	0.029	**0.177**	0.018	**0.122**	0.038
15.5	**0.091**	0.039	**0.081**	0.028	<LoD		**0.134**	0.015	**0.170**	0.018	**0.198**	0.028
blank 1	0.082	0.018	<LoD		1.236	0.165	<LoD		0.029	0.008	0.105	0.008
blank 2	0.094	0.025	0.026	0.019	0.249	0.020	<LoD		<LoD		0.030	0.005
blank 3	0.255	0.046	0.125	0.023	0.276	0.002	0.045	0.021	0.025	0.009	<LoD	
blank 4	0.076	0.020	0.130	0.032	0.216	0.010	0.025	0.007	0.022	0.008	0.039	0.004
blank 5	0.160	0.042	0.021	0.003	0.515	0.017	0.059	0.015	0.023	0.012	0.047	0.004
correction value	0.133		0.060		0.498		0.026		0.020		0.044	
LoD	0.015		0.015		0.015		0.020		0.020		0.026	
LoQ	0.039		0.039		0.039		0.051		0.051		0.064	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	0.049	0.006	**0.131**	0.009	0.101	0.127	**1.084**	0.142	**2.172**	0.109	**1.130**	0.119
-4.5	0.042	0.011	**0.349**	0.031	0.026	0.093	**1.551**	0.146	**2.740**	0.141	**1.160**	0.164
-3.5	<LoD		**0.192**	0.013	**0.220**	0.083	**2.190**	0.226	**3.903**	0.159	**7.795**	0.328
-2.5	0.045	0.005	**0.160**	0.012	**0.397**	0.184	0.503	0.117	**4.377**	0.215	**5.724**	0.302
-1.5	<LoD		**0.140**	0.006	<LoD		**0.931**	0.116	**4.449**	0.294	**4.750**	0.254
-0.5	<LoD		**0.161**	0.010	<LoD		**0.798**	0.030	**4.647**	0.171	**3.805**	0.240
0.5	0.038	0.010	**0.105**	0.005	<LoD		0.053	0.022	**1.734**	0.048	**1.876**	0.066
1.5	0.050	0.007	**0.077**	0.006	<LoD		<LoD		0.313	0.047	0.309	0.082
2.5	**0.108**	0.017	**0.315**	0.025	<LoD		<LoD		<LoD		0.317	0.043
3.5	**0.166**	0.012	**0.247**	0.016	**0.201**	0.073	0.131	0.061	0.305	0.049	0.381	0.025
4.5	**0.151**	0.021	**0.221**	0.013	<LoD		<LoD		0.363	0.048	0.229	0.038
5.5	**0.150**	0.017	**0.280**	0.010	<LoD		0.106	0.076	0.415	0.081	0.220	0.044
6.5	**0.176**	0.024	**0.340**	0.015	no sample *	no sample *	0.121	0.032	0.513	0.063	0.262	0.060
7.5	**0.147**	0.007	**0.337**	0.026	no sample *	no sample *	0.291	0.033	0.397	0.052	0.226	0.032
8.5	**0.148**	0.009	**0.257**	0.021	no sample *	no sample *	0.309	0.052	0.476	0.030	0.362	0.038
9.5	**0.121**	0.007	**0.354**	0.016	<LoD		0.237	0.085	0.471	0.077	0.403	0.048
10.5	**0.131**	0.016	**0.251**	0.017	<LoD		0.032	0.064	0.538	0.041	0.413	0.036
11.5	**0.117**	0.008	**0.263**	0.019	<LoD		0.141	0.069	0.602	0.092	0.365	0.030
12.5	**0.116**	0.015	**0.233**	0.011	<LoD		0.055	0.086	0.505	0.037	0.360	0.036
13.5	**0.108**	0.012	**0.323**	0.018	<LoD		0.097	0.028	0.471	0.033	0.285	0.024
14.5	**0.127**	0.014	**0.340**	0.030	<LoD		0.139	0.025	0.530	0.049	no sample **	no sample **
15.5	**0.108**	0.014	**0.205**	0.003	<LoD		0.225	0.075	0.665	0.091	0.316	0.038
blank 1	0.062	0.009	<LoD		1.602	0.105	<LoD		<LoD		<LoD	
blank 2	0.044	0.017	<LoD		2.087	0.138	<LoD		<LoD		<LoD	
blank 3	0.066	0.013	0.032	0.007	1.779	0.183	<LoD		<LoD		<LoD	
blank 4	0.052	0.005	<LoD		2.473	0.111	1.346	0.122	<LoD		<LoD	
blank 5	0.099	0.010	<LoD		1.944	0.109	<LoD		<LoD		<LoD	
correction val	0.065		0.006		1.775		0.269		0.000		0.000	
LoD	0.029		0.029		0.057		0.297		0.297		0.178	
LoQ	0.076		0.076		0.156		0.751		0.751		0.458	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 33: Chromium concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	0.021	0.008	**0.101**	0.016	<LoD		**0.085**	0.016	**0.084**	0.025	<LoD	
-4.5	**0.059**	0.008	<LoD		<LoD		0.062	0.031	**0.117**	0.007	<LoD	
-3.5	0.052	0.014	<LoD		<LoD		0.036	0.007	**0.106**	0.011	<LoD	
-2.5	**0.075**	0.018	<LoD		<LoD		**0.096**	0.032	**0.153**	0.028	<LoD	
-1.5	0.033	0.015	<LoD		<LoD		0.040	0.021	0.076	0.028	<LoD	
-0.5	0.022	0.013	<LoD		<LoD		<LoD		0.062	0.012	<LoD	
0.5	**0.076**	0.018	**0.795**	0.037	<LoD		<LoD		**0.109**	0.013	**0.500**	0.039
1.5	**0.179**	0.033	**0.167**	0.023	**0.171**	0.032	0.039	0.005	**0.109**	0.017	<LoD	
2.5	**0.242**	0.008	**0.365**	0.042	<LoD		**0.110**	0.015	**0.194**	0.022	0.222	0.026
3.5	**0.236**	0.031	**0.375**	0.029	**0.083**	0.028	**0.342**	0.026	**0.211**	0.017	0.253	0.019
4.5	**0.213**	0.027	**0.536**	0.032	**0.240**	0.023	**0.158**	0.011	**0.173**	0.035	0.210	0.020
5.5	**0.293**	0.020	**0.264**	0.043	**0.072**	0.018	**0.176**	0.025	**0.190**	0.025	0.226	0.017
6.5	**0.265**	0.024	**0.305**	0.044	**0.094**	0.014	no sample ***	no sample ***	**0.196**	0.029	0.227	0.021
7.5	**0.265**	0.028	**0.228**	0.035	**0.073**	0.018	no sample ***	no sample ***	**0.176**	0.013	0.280	0.011
8.5	**0.381**	0.033	**0.234**	0.028	**0.028**	0.028	no sample ***	no sample ***	**0.359**	0.024	0.239	0.012
9.5	**0.653**	0.026	**0.244**	0.036	<LoD	0.037	no sample ***	no sample ***	**0.189**	0.016	0.248	0.011
10.5	**0.337**	0.042	**0.187**	0.021	**0.066**	0.048	**0.154**	0.019	**0.250**	0.017	**0.647**	0.031
11.5	**0.456**	0.041	**0.251**	0.026	<LoD	0.025	**0.143**	0.030	**0.234**	0.011	0.289	0.010
12.5	**0.425**	0.047	**0.323**	0.038	**0.140**	0.030	**0.133**	0.018	**0.254**	0.017	0.301	0.021
13.5	**0.548**	21.474	**0.292**	0.046	**0.286**	0.034	**0.101**	0.022	**0.226**	0.026	0.301	0.008
14.5	**0.482**	0.041	**0.301**	0.021	**0.218**	0.015	**0.145**	0.012	**0.255**	0.021	0.299	0.013
15.5	**0.479**	0.033	**0.679**	0.075	**0.168**	0.048	no sample ***	no sample ***	**0.230**	0.019	**0.339**	0.011
blank 1	0.038	0.015	0.482	0.064	0.294	0.022	0.198	0.034	<LoD		<LoD	
blank 2	0.036	0.004	0.091	0.016	0.281	0.027	0.049	0.017	0.039	0.012	<LoD	
blank 3	0.064	0.013	0.194	0.031	0.216	0.029	<LoD		0.035	0.019	<LoD	
blank 4	0.065	0.006	0.150	0.014	0.284	0.018	<LoD		<LoD		<LoD	
blank 5	0.040	0.008	0.053	0.010	0.207	0.017	<LoD				<LoD	
correction value	0.049		0.194		0.256		0.049		0.015		0.000	
LoD	0.021		0.021		0.021		0.032		0.032		0.129	
LoQ	0.053		0.053		0.053		0.076		0.076		0.331	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	0.085	0.011	0.059	0.007	**0.610**	0.109	**1.046**	0.058	**1.751**	0.060	**1.025**	0.057
-4.5	**0.518**	0.017	0.035	0.013	0.057	0.258	**1.411**	0.081	**2.375**	0.086	**1.033**	0.123
-3.5	0.108	0.007	**0.138**	0.011	0.309	0.175	**1.014**	0.072	**3.828**	0.316	**59.497**	4.218
-2.5	0.120	0.003	<LoD		<LoD		**0.904**	0.063	**4.407**	0.290	**7.782**	0.604
-1.5	0.097	0.004	0.029	0.012	0.234	0.056	**0.911**	0.117	**2.966**	0.197	**6.250**	0.229
-0.5	0.072	0.005	<LoD		<LoD	0.112	**0.650**	0.072	**2.808**	0.181	**4.738**	0.371
0.5	0.078	0.014	<LoD		**0.367**	0.142	0.132	0.046	**1.679**	0.111	**3.887**	0.257
1.5	0.133	0.009	<LoD		<LoD		0.044	0.053	0.355	0.060	**0.985**	0.028
2.5	0.199	0.016	0.036	0.017	<LoD		0.033	0.028	<LoD		**0.385**	0.095
3.5	0.308	0.013	**0.113**	0.022	<LoD		**0.173**	0.044	0.302	0.048	**14.128**	0.894
4.5	**0.392**	0.039	**0.163**	0.023	<LoD		**0.169**	0.022	0.380	0.045	**1.022**	0.070
5.5	**0.333**	0.014	**0.173**	0.030	<LoD		**0.429**	0.048	0.446	0.061	no sample **	no sample **
6.5	0.324	0.015	**0.207**	0.028	no sample *	no sample *	**0.370**	0.057	0.504	0.100	0.279	0.016
7.5	0.271	0.014	**0.176**	0.030	no sample *	no sample *	**0.421**	0.033	0.660	0.162	0.285	0.027
8.5	**0.503**	0.024	**0.237**	0.022	no sample *	no sample *	**0.371**	0.037	0.566	0.103	0.432	0.115
9.5	**0.500**	0.008	**0.175**	0.017	<LoD		**0.380**	0.055	0.473	0.040	0.365	0.090
10.5	**0.364**	0.009	**0.176**	0.017	**0.409**	0.123	**0.888**	0.114	0.496	0.058	0.290	0.051
11.5	**0.397**	0.009	**0.181**	0.019	0.086	0.077	**0.669**	0.074	0.530	0.055	no sample **	no sample **
12.5	**0.341**	0.019	**0.191**	0.014	0.080	0.057	**0.578**	0.042	0.690	0.128	no sample **	no sample **
13.5	**0.406**	0.008	**0.157**	0.014	0.077	0.099	**0.623**	0.067	0.630	0.111	no sample **	no sample **
14.5	**0.352**	0.013	**0.162**	0.020	**2.904**	0.402	**0.543**	0.049	0.640	0.094	no sample **	no sample **
15.5	**0.401**	0.016	**0.146**	0.018	**0.992**	0.207	**0.440**	0.083	0.626	0.071	no sample **	no sample **
blank 1	0.330	0.024	0.039	0.004	1.927	0.129	<LoD		<LoD		<LoD	
blank 2	<LoD		0.134	0.008	1.856	0.129	0.066	0.023	<LoD		<LoD	
blank 3	<LoD		0.048	0.002	1.812	0.114	<LoD		<LoD		<LoD	
blank 4	<LoD		0.386	0.015	1.535	0.075	0.122	0.057	<LoD		<LoD	
blank 5	<LoD		0.068	0.004	1.931	0.091	0.133	0.021			<LoD	
correction value	0.066		0.135		1.734		0.064		0.000		0.000	
LoD	0.129		0.026		0.135		0.057		0.297		0.178	
LoQ	0.331		0.064		0.354		0.156		0.751		0.458	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 34: Chromium concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.126**	0.023	**0.111**	0.030	**0.071**	0.033	**0.077**	0.018	0.033	0.016	0.172	0.016
-4.5	<LoD		**0.069**	0.016	**0.059**	0.027	**0.098**	0.015	0.033	0.025	0.115	0.011
-3.5	**0.294**	0.027	**0.063**	0.022	**0.045**	0.013	**0.057**	0.024	0.034	0.006	0.105	0.013
-2.5	<LoD		0.022	0.011	**0.054**	0.015	**0.099**	0.012	0.031	0.007	0.116	0.013
-1.5	**0.040**	0.045	**0.239**	0.046	**0.074**	0.018	**0.073**	0.011	**0.126**	0.029	0.113	0.006
-0.5	**0.063**	0.025	**0.180**	0.020	**0.158**	0.013	**0.277**	0.035	0.047	0.019	0.206	0.022
0.5	<LoD		**0.167**	0.015	**0.272**	0.084	**0.196**	0.035	**0.071**	0.022	0.171	0.009
1.5	**1.617**	0.056	**0.334**	0.074	**0.324**	0.005	**0.055**	0.014	**0.084**	0.018	0.174	0.016
2.5	<LoD		**0.367**	0.067	**0.291**	0.014	**0.114**	0.022	**0.114**	0.017	0.174	0.014
3.5	<LoD		**0.274**	0.014	**0.569**	0.061	**0.105**	0.012	**0.069**	0.020	0.241	0.020
4.5	**0.074**	0.010	**0.289**	0.010	**0.293**	0.005	**0.079**	0.018	**0.124**	0.034	0.206	0.009
5.5	**0.183**	0.020	**0.311**	0.041	**0.309**	0.015	**0.125**	0.019	**0.133**	0.014	0.308	0.021
6.5	**0.285**	0.035	**0.316**	0.086	**0.322**	0.055	**0.095**	0.020	**0.971**	0.105	0.253	0.012
7.5	**0.072**	0.028	**0.273**	0.016	**0.539**	0.048	**0.102**	0.029	**0.105**	0.019	0.293	0.018
8.5	**0.120**	0.015	**0.388**	0.016	**0.354**	0.037	**0.103**	0.010	**0.191**	0.015	0.223	0.011
9.5	**0.292**	0.085	**0.195**	0.044	**0.241**	0.019	**0.120**	0.010	**0.169**	0.026	0.315	0.011
10.5	**0.114**	0.043	**0.239**	0.025	**0.233**	0.003	**0.105**	0.018	**0.157**	0.019	0.223	0.017
11.5	**0.077**	0.012	**0.212**	0.020	**0.223**	0.040	**0.106**	0.021	**0.204**	0.025	0.342	0.018
12.5	**0.248**	0.048	**0.280**	0.040	**0.188**	0.011	**0.149**	0.010	**0.117**	0.023	0.274	0.015
13.5	**0.185**	0.030	**0.302**	0.026	**0.451**	0.011	**0.127**	0.027	**0.156**	0.033	0.271	0.015
14.5	**0.133**	0.029	**0.246**	0.028	**0.212**	0.011	**0.158**	0.026	**0.216**	0.019	0.276	0.023
15.5	**0.124**	0.020	**0.176**	0.012	**0.389**	0.037	**0.119**	0.018	**0.197**	0.021	0.262	0.018
blank 1	0.031	0.012	0.019	0.011	<LoD		<LoD		<LoD		0.138	0.056
blank 2	0.062	0.011	<LoD		0.015	0.009	0.064	0.014	<LoD		<LoD	
blank 3	0.052	0.010	0.030	0.007	0.333	0.051	0.059	0.010	0.093	0.008	<LoD	
blank 4	0.297	0.057	0.023	0.002	0.022	0.005	0.020	0.010	0.059	0.010	<LoD	
blank 5	0.150	0.022	0.045	0.011	0.059	0.010	0.147	0.019	0.074	0.017	<LoD	
correction value	0.118		0.023		0.024		0.036		0.045		0.028	
LoD	0.015		0.015		0.015		0.020		0.020		0.135	
LoQ	0.039		0.039		0.039		0.051		0.051		0.354	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	0.059	0.009	**0.084**	0.005	<LoD		0.346	0.051	<LoD		0.109	0.021
-4.5	0.033	0.008	<LoD		<LoD		0.399	0.074	<LoD		<LoD	
-3.5	0.028	0.012	<LoD		<LoD		0.403	0.039	0.350	0.029	0.149	0.034
-2.5	0.020	0.008	<LoD		<LoD		0.428	0.060	<LoD		<LoD	
-1.5	0.024	0.006	<LoD		<LoD		0.360	0.055	<LoD		0.119	0.041
-0.5	0.043	0.012	<LoD		<LoD		0.423	0.058	0.359	0.058	**0.459**	0.086
0.5	0.032	0.014	<LoD		<LoD		0.490	0.111	<LoD		0.186	0.052
1.5	**0.087**	0.006	0.036	0.007	<LoD		0.534	0.050	<LoD		0.233	0.071
2.5	**0.131**	0.011	0.050	0.010	<LoD		0.338	0.044	<LoD		0.306	0.034
3.5	**0.208**	0.022	0.072	0.009	<LoD		<LoD		0.337	0.073	0.299	0.022
4.5	**0.254**	0.021	**0.109**	0.016	**0.171**	0.109	<LoD		0.314	0.046	0.377	0.049
5.5	**0.199**	0.015	**0.132**	0.005	<LoD		<LoD		0.397	0.054	0.337	0.095
6.5	**0.237**	0.011	**0.116**	0.010	<LoD		<LoD		0.447	0.079	0.346	0.055
7.5	**0.210**	0.010	**0.162**	0.009	0.091	0.112	<LoD		0.395	0.045	0.269	0.031
8.5	**0.200**	0.010	**0.175**	0.023	0.018	0.146	0.317	0.061	0.394	0.056	0.270	0.034
9.5	**0.192**	0.020	**0.111**	0.015	0.116	0.073	0.356	0.046	0.411	0.071	0.382	0.065
10.5	no sample**	no sample**	**0.103**	0.015	0.100	0.102	<LoD		0.402	0.032	0.275	0.037
11.5	**0.163**	0.007	**0.116**	0.010	<LoD		<LoD		0.449	0.050	0.275	0.043
12.5	no sample**	no sample**	**0.132**	0.013	0.026	0.121	0.334	0.031	0.403	0.040	0.229	0.048
13.5	**0.158**	0.008	**0.143**	0.011	**0.513**	0.141	<LoD		0.449	0.063	0.139	0.039
14.5	no sample**	no sample**	**0.167**	0.015	<LoD		0.314	0.033	0.427	0.087	0.125	0.045
15.5	**0.191**	0.021	**0.267**	0.010	no sample**	no sample**	<LoD		0.451	0.051	0.227	0.049
blank 1	0.045	0.005	<LoD		2.256	0.110	<LoD		<LoD		0.083	0.028
blank 2	0.061	0.006	0.056	0.010	2.240	0.224	<LoD		<LoD		<LoD	
blank 3	0.030	0.005	0.342	0.009	2.041	0.213	<LoD		<LoD		0.116	0.018
blank 4	<LoD		0.094	0.014	1.561	0.123	<LoD		<LoD		0.063	0.021
blank 5	<LoD		0.069	0.006	1.292	0.105	<LoD		<LoD		0.081	0.023
correction value	0.027		0.055		1.878		0.000		0.000		0.080	
LoD	0.029		0.029		0.057		0.297		0.297		0.178	
LoQ	0.076		0.076		0.156		0.751		0.751		0.458	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 35: Chromium concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.090**	0.024	<LoD		0.049	0.012	**0.109**	0.016	**0.195**	0.032	0.144	0.008
-4.5	<LoD		<LoD		**0.056**	0.011	**0.109**	0.023	**0.117**	0.022	<LoD	
-3.5	<LoD		**0.098**	0.019	0.037	0.021	**0.130**	0.031	**0.232**	0.027	<LoD	
-2.5	<LoD		**0.323**	0.040	<NWG	0.009	**0.101**	0.018	**0.197**	0.020	0.170	0.008
-1.5	**0.158**	0.024	<LoD		**0.146**	0.017	**0.090**	0.007	**0.196**	0.011	0.142	0.009
-0.5	**0.056**	0.017	**0.801**	0.050	**0.225**	0.028	0.068	0.022	**0.148**	0.014	0.227	0.009
0.5	0.027	0.014	**0.200**	0.047	**0.228**	0.053	**0.111**	0.023	**0.196**	0.039	0.227	0.013
1.5	**0.209**	0.019	**0.183**	0.040	**0.321**	0.017	0.076	0.017	**0.150**	0.019	0.245	0.011
2.5	**0.119**	0.023	**0.237**	0.026	**0.300**	0.016	no sample ***	no sample ***	**0.176**	0.014	**0.343**	0.025
3.5	**0.422**	0.040	**0.184**	0.041	**0.307**	0.012	no sample ***	no sample ***	**0.219**	0.031	**0.415**	0.009
4.5	**0.238**	0.027	**0.233**	0.041	**0.310**	0.041	**0.139**	0.019	**0.291**	0.021	**0.608**	0.013
5.5	**0.257**	0.042	**0.200**	0.025	**0.263**	0.010	**0.230**	0.025	**0.350**	0.039	**0.532**	0.021
6.5	**0.406**	0.052	**0.361**	0.026	**0.348**	0.033	**0.108**	0.012	**0.325**	0.012	**0.549**	0.025
7.5	**0.653**	0.077	**0.399**	0.036	**0.256**	0.025	**0.113**	0.016	**0.303**	0.037	**0.633**	0.008
8.5	**0.524**	0.064	**0.317**	0.063	**0.259**	0.011	**0.133**	0.021	**0.529**	0.054	**0.631**	0.030
9.5	**0.374**	0.019	**0.122**	0.034	**0.276**	0.031	**0.156**	0.017	**0.310**	0.016	**0.667**	0.019
10.5	**0.613**	0.046	**0.324**	0.025	**0.281**	0.032	**0.169**	0.022	**0.388**	0.052	**0.582**	0.019
11.5	**0.515**	0.062	**0.174**	0.022	**0.336**	0.046	**0.200**	0.027	**0.396**	0.051	**0.699**	0.030
12.5	**0.591**	0.054	**0.151**	0.053	**0.373**	0.041	no sample ***	no sample ***	**0.361**	0.042	**0.618**	0.030
13.5	**1.363**	0.088	**0.219**	0.036	**0.487**	0.041	**0.161**	0.032	**0.393**	0.044	**0.700**	0.026
14.5	**0.409**	0.037	**0.192**	0.019	**0.367**	0.044	no sample ***	no sample ***	**0.431**	0.028	**0.533**	0.016
15.5	**0.302**	0.024	**0.267**	0.016	**0.757**	0.058	no sample ***	no sample ***	**0.443**	0.047	**0.573**	0.024
blank 1	0.117	0.012	0.043	0.011	0.042	0.006	0.039	0.016	<LoD		<LoD	
blank 2	0.068	0.021	0.247	0.021	0.074	0.013	<LoD		<LoD		<LoD	
blank 3	0.117	0.025	0.226	0.030	<LoD		0.057	0.010	<LoD		<LoD	
blank 4	0.130	0.010	0.361	0.042	0.162	0.013	<LoD		0.036	0.006	<LoD	
blank 5	0.303	0.031	0.183	0.019	<LoD						<LoD	
correction value	0.147		0.212		0.056		0.019		0.007		0.000	
LoD	0.021		0.021		0.021		0.032		0.032		0.129	
LoQ	0.053		0.053		0.053		0.076		0.076		0.331	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.432**	0.034	**0.438**	0.016	<LoD		0.171	0.034	57.665	3.105	<LoD	
-4.5	0.022	0.004	**0.065**	0.007	0.221	0.283	0.159	0.044	9.637	0.767	<LoD	
-3.5	0.047	0.006	0.058	0.006	0.193	0.149	0.194	0.034	1.916	0.337	<LoD	
-2.5	<NWG	0.005	0.061	0.001	<LoD		0.222	0.060	1.063	0.165	<LoD	
-1.5	<NWG	0.001	0.053	0.004	<LoD		0.272	0.042	0.353	0.060	<LoD	
-0.5	<NWG	0.005	0.063	0.005	<LoD		0.221	0.037	#WERT!	#WERT!	<LoD	
0.5	0.029	0.010	**0.100**	0.006	**0.560**	0.169	0.223	0.030	0.643	0.054	<LoD	
1.5	0.062	0.008	**0.122**	0.011	0.324	0.107	0.289	0.042	0.477	0.094	0.395	0.029
2.5	**0.158**	0.020	**0.241**	0.023	0.210	0.139	0.288	0.027	4.115	0.214	0.295	0.022
3.5	**0.194**	0.009	**0.340**	0.012	<LoD		0.193	0.036	2.623	0.149	0.665	0.039
4.5	**0.204**	0.022	**0.377**	0.024	0.243	0.106	0.194	0.052	0.658	0.061	0.400	0.042
5.5	**0.199**	0.013	**0.439**	0.021	0.087	0.079	0.216	0.019	0.403	0.037	0.371	0.041
6.5	**0.217**	0.011	**0.474**	0.018	0.075	0.106	0.280	0.048	no sample**	no sample**	0.256	0.020
7.5	**0.311**	0.012	**0.439**	0.012	0.035	0.115	0.285	0.013	no sample**	no sample**	0.348	0.020
8.5	**0.233**	0.019	**0.414**	0.003	**0.624**	0.108	0.249	0.017	no sample**	no sample**	0.250	0.030
9.5	**0.214**	0.012	**0.583**	0.022	<LoD		0.292	0.050	no sample**	no sample**	0.250	0.027
10.5	**0.606**	0.029	**0.559**	0.026	0.163	0.103	0.963	0.059	no sample**	no sample**	0.264	0.029
11.5	**0.214**	0.007	**0.640**	0.028	<LoD		0.380	0.054	no sample**	no sample**	0.251	0.042
12.5	**0.259**	0.019	**0.604**	0.021	<LoD		<LoD		no sample**	no sample**	no sample**	no sample**
13.5	**0.333**	0.010	**0.547**	0.018	**0.465**	0.165	no sample ***	no sample ***	no sample**	no sample**	0.706	0.072
14.5	**0.260**	0.020	**0.552**	0.026	0.343	0.150	no sample ***	no sample ***	no sample**	no sample**	0.228	0.025
15.5	**0.322**	0.015	**0.467**	0.046	0.336	0.141	no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	0.068	0.006	<LoD		1.499	0.130	<LoD		0.035	64.799	<LoD	
blank 2	0.038	0.004	<LoD		1.386	0.097	<LoD		0.046	79.385	<LoD	
blank 3	0.068	0.007	0.031	0.008	1.492	0.062	<LoD		0.054	113.569	<LoD	
blank 4	0.118	0.009	<LoD		1.425	0.080	<LoD		0.036	49.003	<LoD	
blank 5	0.074	0.008	<LoD		1.664	0.104	<LoD		0.054	66.374	<LoD	
correction value	0.073		0.006		1.493		0.000		0.045		0.000	
LoD	0.026		0.026		0.135		0.057		0.297		0.178	
LoQ	0.064		0.064		0.354		0.156		0.751		0.458	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 36: Copper concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**1.848**	0.295	**1.581**	0.125	**2.439**	0.060	**1.199**	0.070	**2.951**	0.057	**0.366**	0.060
-4.5	**2.950**	0.195	**1.989**	0.149	**3.263**	0.217	<LoD	0.007	**2.874**	0.171	0.154	0.066
-3.5	**3.246**	0.066	**2.241**	0.350	**1.929**	0.240	**0.616**	0.048	**2.998**	0.071	**0.259**	0.049
-2.5	**2.904**	0.236	**1.671**	0.082	**2.424**	0.197	0.151	0.016	**1.358**	0.020	<LoD	
-1.5	**2.724**	0.390	**2.658**	0.172	**2.942**	0.640	0.145	0.020	**1.510**	0.058	<LoD	
-0.5	**3.086**	0.828	**1.717**	0.096	**2.098**	0.103	0.218	0.018	**2.538**	0.187	**0.406**	0.072
0.5	**1.214**	0.060	<LoD		**0.500**	0.113	**0.363**	0.027	**0.622**	0.024	<LoD	
1.5	<LoD		<LoD		**0.515**	0.029	**0.346**	0.016	<LoD		**0.269**	0.070
2.5	<LoD		<LoD		**1.406**	0.041	<LoD		0.110	0.014	<LoD	
3.5	0.181	0.100	<LoD		<LoD		**5.462**	0.371	<LoD		<LoD	
4.5	<LoD		<LoD		0.156	0.093	<LoD		<LoD		<LoD	
5.5	<LoD		<LoD		**0.682**	0.187	<LoD		<LoD		<LoD	
6.5	<LoD		<LoD		**0.720**	0.171	<LoD		<LoD		<LoD	
7.5	<LoD		<LoD		**0.654**	0.064	<LoD		**0.264**	0.028	<LoD	
8.5	<LoD		**0.292**	0.089	0.187	0.084	<LoD		<LoD		<LoD	
9.5	<LoD		<LoD		**0.269**	0.151	<LoD		0.951	0.037	<LoD	
10.5	<LoD		<LoD		0.115	0.033	<LoD		<LoD		<LoD	
11.5	<LoD		<LoD		<LoD		<LoD		0.208	0.013	<LoD	
12.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
13.5	**0.369**	0.088	<LoD		<LoD		0.139	0.018	0.120	0.012	<LoD	
14.5	<LoD		<LoD		**0.293**	0.032	<LoD		<LoD		<LoD	
15.5	<LoD		<LoD		<LoD		0.203	0.017	<LoD		<LoD	
blank 1	0.711	0.150	0.442	0.051	5.484	0.811	0.146	0.010	0.251	0.016	1.858	0.086
blank 2	0.626	0.085	0.258	0.059	5.744	0.211	0.207	0.007	<LoD		0.178	0.003
blank 3	1.115	0.138	0.518	0.074	6.562	0.337	<LoD		0.149	0.005	0.130	0.003
blank 4	0.956	0.105	0.295	0.133	5.521	0.307	0.109	0.006	0.086	0.010	0.205	0.003
blank 5	0.825	0.043	0.379	0.037	5.992	0.666	0.394	0.039	0.381	0.021	0.221	0.007
correction value	0.847		0.378		5.861		0.171		0.173		0.518	
LoD	0.101		0.101		0.101		0.080		0.080		0.062	
LoQ	0.251		0.251		0.251		0.220		0.220		0.182	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**22.882**	1.646	**50.891**	1.589	**176.299**	7.080	**38.825**	1.605	**71.238**	2.545	**108.275**	5.452
-4.5	**10.454**	0.321	**48.445**	1.875	**43.320**	1.663	**38.117**	1.061	**78.391**	2.904	**129.000**	3.371
-3.5	**6.652**	0.179	**44.863**	0.617	**37.309**	0.951	**39.496**	0.701	**79.948**	2.930	**124.417**	4.377
-2.5	**4.233**	0.171	**43.837**	0.475	**44.147**	2.449	**26.091**	2.465	**99.077**	1.775	**96.544**	2.187
-1.5	**3.214**	0.102	**42.803**	0.538	**30.516**	1.943	**35.535**	1.203	**86.608**	3.622	**81.079**	3.690
-0.5	**3.075**	0.120	**44.112**	0.831	**31.422**	2.332	**32.822**	1.351	**92.651**	5.868	**77.556**	2.270
0.5	**1.952**	0.081	**44.331**	1.302	<LoD		**0.457**	0.069	**58.932**	2.612	**18.336**	0.482
1.5	**1.566**	0.023	**0.476**	0.023	<LoD		<LoD		0.273	0.072	**0.158**	0.039
2.5	<LoD		**2.954**	0.118	<LoD		<LoD		0.189	0.023	**0.173**	0.062
3.5	<LoD		**1.310**	0.054	<LoD		<LoD		<LoD		**0.339**	0.049
4.5	<LoD		**0.571**	0.046	<LoD		<LoD		0.138	0.057	**0.292**	0.070
5.5	<LoD		**0.340**	0.015	no sample *	no sample *	<LoD		<LoD		0.151	0.039
6.5	**1.827**	0.081	**0.449**	0.024	no sample *	no sample *	<LoD		**0.604**	0.095	**0.242**	0.021
7.5	<LoD		<LoD	0.023	no sample *	no sample *	<LoD		<LoD		**0.213**	0.032
8.5	<LoD		**0.354**	0.024	<LoD		<LoD		0.111	0.061	**0.272**	0.020
9.5	**0.396**	0.075	**0.211**	0.015	<LoD		<LoD		<LoD		**0.277**	0.054
10.5	<LoD		<LoD	0.014	<LoD		<LoD		<LoD		**0.306**	0.029
11.5	<LoD		<LoD	0.011	<LoD		<LoD		0.274	0.069	**0.270**	0.041
12.5	**0.117**	0.030	**0.536**	0.037	<LoD		<LoD		0.147	0.032	**0.239**	0.028
13.5	**0.111**	0.028	<LoD	0.013	<LoD		<LoD		<LoD		**0.343**	0.045
14.5	<LoD		**0.241**	0.025	<LoD		<LoD		0.183	0.046	no sample **	no sample **
15.5	<LoD		<LoD	0.017	**36.196**	1.605	<LoD		<LoD		0.145	0.032
blank 1	0.765	0.016	0.273	0.013	2.578	0.091	0.187	0.013	0.162	0.048	0.247	0.030
blank 2	0.457	0.014	48.595	1.685	3.314	0.221	0.201	0.020	0.247	0.038	0.107	0.024
blank 3	0.857	0.016	0.395	0.012	3.560	0.099	0.234	0.030	0.292	0.060	0.199	0.024
blank 4	0.614	0.026	3.989	0.126	3.034	0.166	0.703	0.084	<LoD		0.109	0.024
blank 5	0.607	0.020	0.185	0.007	2.301	0.137	0.318	0.037	<LoD		0.208	0.036
correction value	0.660		0.284		2.957		0.329		0.140		0.174	
LoD	0.021		0.021		0.074		0.109		0.109		0.061	
LoQ	0.044		0.044		0.203		0.296		0.296		0.166	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 37: Copper concentration across the **SWI (<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. Identified outliers are grayed out. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**3.704**	0.089	**3.158**	0.051	**2.412**	0.060	**0.443**	0.025	**2.621**	0.090	**1.415**	0.122
-4.5	**3.801**	0.116	**3.385**	0.177	**3.170**	0.086	**0.373**	0.013	**4.695**	0.118	**1.584**	0.061
-3.5	**4.158**	0.158	**2.984**	0.113	**2.717**	0.214	**0.606**	0.020	**4.083**	0.187	**1.476**	0.097
-2.5	**4.811**	0.147	**2.747**	0.095	**2.733**	0.161	**0.584**	0.019	**4.314**	0.216	**1.328**	0.117
-1.5	**4.325**	0.180	**2.581**	0.139	**2.750**	0.096	**0.682**	0.043	**3.458**	0.134	**1.117**	0.062
-0.5	**4.351**	0.186	**2.463**	0.123	**1.504**	0.080	**0.852**	0.013	**2.514**	0.068	**1.429**	0.098
0.5	**3.941**	0.167	**1.436**	0.038	**0.908**	0.034	0.320	0.030	**2.857**	0.198	**0.957**	0.068
1.5	**0.961**	0.109	**0.810**	0.057	**0.522**	0.042	**0.759**	0.017	**1.084**	0.043	**0.596**	0.055
2.5	**0.592**	0.047	**0.521**	0.053	<LoD		**0.691**	0.041	**1.004**	0.053	**0.779**	0.067
3.5	**0.980**	0.071	**0.400**	0.028	0.333	0.017	**0.731**	0.005	**0.739**	0.026	**0.821**	0.065
4.5	**0.419**	0.028	0.203	0.014	<LoD		**1.046**	0.054	**0.696**	0.030	**0.702**	0.044
5.5	0.262	0.031	0.245	0.025	<LoD		**0.707**	0.031	**0.393**	0.071	**0.185**	0.020
6.5	<LoD		0.160	0.015	**1.414**	0.097	no sample ***	no sample ***	0.335	0.019	<LoD	
7.5	<LoD		<LoD		0.341	0.057	no sample ***	no sample ***	**1.692**	0.046	**0.183**	0.014
8.5	<LoD		**6.191**	0.156	0.194	0.005	no sample ***	no sample ***	0.284	0.009	<LoD	
9.5	0.290	0.017	0.163	0.018	<LoD		no sample ***	no sample ***	0.361	0.015	<LoD	
10.5	<LoD		0.285	0.025	<LoD		**0.514**	0.021	**1.196**	0.026	<LoD	
11.5	<LoD		0.208	0.029	<LoD		0.374	0.015	**1.208**	0.026	<LoD	
12.5	0.230	0.037	<LoD	0.003	<LoD		0.363	0.020	**0.781**	0.028	<LoD	
13.5	0.149	21.474	**0.437**	0.066	<LoD		0.358	0.010	**1.196**	0.037	<LoD	
14.5	<LoD		0.193	0.016	<LoD		**0.556**	0.011	**0.398**	0.010	<LoD	
15.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	0.273	0.018	<LoD	
blank 1	8.985	0.200	5.961	0.102	6.985	0.215	3.152	0.447	<LoD		0.092	0.004
blank 2	6.765	0.203	6.513	0.278	6.590	0.238	<LoD		<LoD		0.060	0.007
blank 3	6.879	0.418	6.436	0.611	4.886	0.136	<LoD		<LoD		0.130	0.010
blank 4	8.134	0.124	7.642	0.195	7.535	0.273	<LoD		<LoD		0.062	0.005
blank 5	8.494	0.325	5.389	0.109	4.759	0.109	<LoD				0.241	0.023
correction value	0.205		0.284		0.284		0.000		0.000		0.117	
LoD	0.142		0.142		0.142		0.152		0.152		0.049	
LoQ	0.374		0.374		0.374		0.388		0.388		0.095	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**34.210**	0.836	**50.479**	1.092	**195.183**	3.020	**41.641**	2.362	**73.164**	1.791	**94.590**	2.438
-4.5	**13.837**	0.097	**46.703**	1.970	**33.791**	4.399	**32.528**	0.895	**72.514**	1.336	**113.449**	1.273
-3.5	**10.587**	0.307	**44.469**	2.315	**37.099**	3.773	**28.499**	1.152	**84.555**	3.739	**122.591**	3.938
-2.5	**10.439**	0.281	**44.480**	1.595	**33.640**	3.007	**29.822**	1.286	**87.719**	4.333	**95.482**	1.991
-1.5	**6.773**	0.048	**44.585**	2.549	**30.027**	1.756	**32.483**	0.661	**65.972**	2.633	**82.147**	2.975
-0.5	**5.755**	0.049	**44.940**	2.332	**26.668**	4.764	**27.118**	0.694	**60.022**	2.556	**77.179**	2.217
0.5	**4.394**	0.054	**45.652**	2.422	**4.417**	4.914	**4.305**	0.288	**57.968**	0.819	**18.719**	0.274
1.5	**3.378**	0.234	**3.824**	0.049	<LoD		**0.244**	0.046	**0.602**	0.059	**0.767**	0.068
2.5	**4.645**	0.129	**4.636**	0.258	<LoD		<LoD	0.005	**0.538**	0.047	**1.492**	0.085
3.5	**2.844**	0.076	**2.198**	0.143	<LoD		<LoD	0.030	<LoD		**0.625**	0.047
4.5	**1.283**	0.130	**0.590**	0.054	<LoD		<LoD	0.010	<LoD		**0.458**	0.033
5.5	**0.492**	0.015	<LoD		<LoD		<LoD	0.016	<LoD		no sample **	no sample **
6.5	**0.515**	0.032	<LoD		no sample *	no sample *	<LoD	0.029	<LoD		**0.277**	0.059
7.5	<LoD		<LoD		no sample *	no sample *	**1.565**	0.075	0.188	0.032	<LoD	
8.5	**0.572**	0.027	<LoD		no sample *	no sample *	<LoD	0.013	<LoD		**0.400**	0.043
9.5	**1.342**	0.014	<LoD		<LoD		**0.218**	0.030	<LoD		**0.901**	0.109
10.5	**0.173**	0.008	<LoD		<LoD		<LoD	0.013	0.230	0.081	**0.223**	0.023
11.5	**0.568**	0.007	<LoD		**0.264**	4.094	<LoD	0.030	<LoD		no sample **	no sample **
12.5	**0.348**	0.009	<LoD		<LoD		<LoD	0.013	<LoD		no sample **	no sample **
13.5	<LoD		<LoD		<LoD		<LoD	0.018	<LoD		no sample **	no sample **
14.5	<LoD		<LoD		<LoD		<LoD	0.014	<LoD		no sample **	no sample **
15.5	<LoD		<LoD		<LoD		<LoD	0.022	<LoD		no sample **	no sample **
blank 1	0.138	0.013	0.145	0.002	2.362	0.095	0.347	0.043	0.210	0.013	0.247	0.030
blank 2	0.057	0.008	2.341	0.102	2.225	0.054	0.338	0.022	<LoD		0.107	0.024
blank 3	0.527	0.032	0.160	0.010	1.981	0.102	0.240	0.018	0.180	0.021	0.199	0.024
blank 4	0.506	0.021	0.141	0.006	1.661	0.158	0.348	0.039	<LoD		0.109	0.024
blank 5	0.618	0.037	0.134	0.006	2.055	0.138	0.330	0.040			0.208	0.036
correction value	0.369		0.584		2.057		0.321		0.078		0.174	
LoD	0.049		0.062		0.075		0.074		0.109		0.061	
LoQ	0.095		0.182		0.195		0.203		0.296		0.166	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 38: Copper concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**2.406**	0.276	**1.612**	0.194	**1.376**	0.398	<LoD		**0.965**	0.021	**2.210**	0.069
-4.5	**2.249**	0.334	**1.368**	0.054	**3.780**	0.240	**1.980**	0.159	**1.603**	0.062	**1.958**	0.038
-3.5	**1.654**	0.187	**1.716**	0.135	**1.611**	0.135	**0.348**	0.048	**1.882**	0.036	**2.162**	0.061
-2.5	**1.949**	0.114	**2.074**	0.291	**1.578**	0.146	**0.818**	0.031	**0.878**	0.030	**2.068**	0.039
-1.5	**2.167**	0.472	**2.120**	0.337	**0.941**	0.088	**0.630**	0.032	**1.724**	0.090	**1.895**	0.047
-0.5	**2.657**	0.277	**1.310**	0.284	<LoD		**0.780**	0.059	**1.378**	0.070	**2.750**	0.079
0.5	**0.598**	0.156	**0.366**	0.010	<LoD		**0.803**	0.067	**0.729**	0.052	**1.076**	0.040
1.5	<LoD		<LoD		<LoD		**0.631**	0.051	**1.214**	0.043	**1.657**	0.028
2.5	<LoD		<LoD		<LoD		<LoD		<NWG	0.024	**0.218**	0.010
3.5	<LoD		<LoD		<LoD		<LoD		<NWG	0.009	**0.622**	0.019
4.5	<LoD		<LoD		<LoD		<LoD		0.131	0.021	0.128	0.004
5.5	<LoD		<LoD		<LoD		<LoD		**0.498**	0.011	**0.264**	0.006
6.5	<LoD		<LoD		<LoD		<LoD		<NWG	0.012	0.169	0.003
7.5	<LoD		<LoD		<LoD		<LoD		<NWG	0.012	0.187	0.006
8.5	<LoD		<LoD		<LoD		<LoD		<NWG	0.014	0.146	0.007
9.5	<LoD		<LoD		<LoD		<LoD		<NWG	0.012	**0.209**	0.003
10.5	<LoD		<LoD		<LoD		<LoD		<NWG	0.008	0.157	0.008
11.5	<LoD		<LoD		<LoD		<LoD		<NWG	0.008	**0.292**	0.007
12.5	<LoD		<LoD		**0.784**	0.107	<LoD		0.113	0.016	**0.277**	0.011
13.5	<LoD		<LoD		<LoD		<LoD		<NWG	0.005	0.121	0.004
14.5	<LoD		<LoD		<LoD		0.153	0.011	<NWG	0.010	0.148	0.006
15.5	<LoD		<LoD		<LoD		<LoD		**0.711**	0.028	0.160	0.005
blank 1	0.513	0.097	0.371	0.038	0.801	0.083	0.302	0.016	0.156	0.013	1.333	0.055
blank 2	0.851	0.028	0.292	0.080	0.589	0.044	0.302	0.024	0.193	0.013	0.080	0.028
blank 3	0.903	0.085	0.564	0.080	1.644	0.150	0.914	0.019	0.169	0.012	<LoD	
blank 4	0.762	0.176	0.474	0.070	1.138	0.180	0.159	0.010	0.241	0.015	0.129	0.024
blank 5	1.747	0.216	0.915	0.074	1.216	0.191	0.226	0.015	0.158	0.012	0.106	0.031
correction value	0.955		0.523		1.078		0.247		0.183		0.079	
LoD	0.101		0.101		0.101		0.080		0.080		0.075	
LoQ	0.251		0.251		0.251		0.220		0.220		0.195	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**1.622**	0.084	**2.732**	0.053	**0.655**	0.181	**0.335**	0.038	**0.338**	0.052	**0.313**	0.057
-4.5	**0.610**	0.033	<LoD		<LoD		**0.391**	0.060	**0.838**	0.040	**0.203**	0.064
-3.5	**0.425**	0.028	**0.273**	0.022	<LoD		**0.480**	0.078	**0.470**	0.109	<LoD	
-2.5	**0.288**	0.031	<LoD		0.109	0.085	**0.423**	0.080	**0.339**	0.044	<LoD	
-1.5	**0.721**	0.048	**0.169**	0.035	<LoD		**0.395**	0.077	0.201	0.024	<LoD	
-0.5	**0.192**	0.028	<LoD		<LoD		**0.687**	0.044	**0.303**	0.027	<LoD	
0.5	**0.309**	0.033	<LoD		<LoD		0.279	0.074	**0.462**	0.039	<LoD	
1.5	<LoD		**0.139**	0.006	<LoD		0.284	0.036	0.184	0.021	<LoD	
2.5	<LoD		<LoD		**2.919**	0.253	0.159	0.019	0.240	0.026	<LoD	
3.5	<LoD		<LoD		<LoD		<LoD		0.255	0.058	<LoD	
4.5	<LoD		<LoD		**0.488**	0.108	0.105	0.057	**0.319**	0.027	<LoD	
5.5	<LoD		**0.846**	0.030	0.154	0.234	0.170	0.046	0.210	0.016	0.144	0.053
6.5	<LoD		<LoD		<LoD		0.288	0.079	0.296	0.080	**0.167**	0.020
7.5	**2.924**	0.104	**1.034**	0.014	<LoD		0.116	0.025	0.172	0.013	<LoD	
8.5	**1.163**	0.072	<LoD		<LoD		<LoD		**0.376**	0.026	0.122	0.038
9.5	**0.576**	0.036	<LoD		<LoD		**0.447**	0.049	**1.030**	0.030	0.128	0.044
10.5	no sample**	no sample**	**0.682**	0.035	**0.422**	0.146	<LoD		**0.763**	0.052	**0.230**	0.014
11.5	**9.122**	0.166	<LoD		<LoD		<LoD		0.217	0.032	**0.876**	0.073
12.5	no sample**	no sample**	<LoD		<LoD		<LoD		**0.359**	0.046	**0.713**	0.052
13.5	**16.846**	0.573	**0.163**	0.013	**0.316**	0.074	0.121	0.059	<LoD		**1.044**	0.034
14.5	no sample**	no sample**	<LoD		no sample**	no sample**	<LoD		**0.337**	0.030	**0.231**	0.030
15.5	**0.389**	0.048	**2.886**	0.092	<LoD		<LoD		0.173	0.031	<LoD	
blank 1	2.142	0.107	0.235	0.012	4.824	0.386	0.242	0.039	<LoD		0.147	0.018
blank 2	0.673	0.031	0.154	0.006	2.933	0.173	0.232	0.038	1.256	0.091	0.083	0.028
blank 3	0.510	0.031	0.537	0.018	3.005	0.076	0.213	0.027	0.125	0.022	0.133	0.020
blank 4	0.539	0.015	0.216	0.014	2.487	0.194	0.222	0.020	0.150	0.014	0.199	0.027
blank 5	1.060	0.065	0.225	0.011	1.942	0.159	0.391	0.055	0.856	0.066	0.199	0.020
correction value	0.574		0.273		2.454		0.260		0.000		0.152	
LoD	0.021		0.021		0.074		0.109		0.109		0.061	
LoQ	0.044		0.044		0.203		0.296		0.296		0.166	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 39: Copper concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	<LoD		<LoD		**0.710**	0.115	**0.648**	0.052	**4.312**	0.289	**1.979**	0.075
-4.5	<LoD		**0.443**	0.154	**1.644**	0.196	**0.751**	0.033	**2.803**	0.140	**1.091**	0.025
-3.5	<LoD		**1.094**	0.227	**1.088**	0.156	**1.615**	0.136	**4.812**	0.196	**3.426**	0.179
-2.5	<LoD		**1.502**	0.156	**1.363**	0.059	**1.682**	0.037	**4.863**	0.202	**1.830**	0.065
-1.5	<LoD		**2.148**	0.237	**1.113**	0.075	**1.671**	0.031	**4.568**	0.231	**1.535**	0.070
-0.5	<LoD		**1.906**	0.147	**1.224**	0.093	**2.040**	0.053	**3.971**	0.131	**2.214**	0.092
0.5	<LoD		<LoD		<LoD		**2.434**	0.042	**5.827**	0.278	**3.044**	0.131
1.5	<LoD		<LoD		<LoD		**1.565**	0.035	**1.049**	0.043	**0.552**	0.022
2.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	0.264	0.025	**0.264**	0.014
3.5	<LoD		<LoD		**2.510**	0.476	no sample ***	no sample ***	<LoD		<LoD	
4.5	<LoD		<LoD		<LoD		**0.397**	0.024	<LoD		**0.147**	0.004
5.5	<LoD		<LoD		<LoD		<LoD		**0.647**	0.032	<LoD	
6.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
7.5	<LoD		<LoD		<LoD		<LoD		0.277	0.016	**0.201**	0.009
8.5	<LoD		<LoD		<LoD		<LoD		0.188	0.019	<LoD	
9.5	<LoD		<LoD		<LoD		0.153	0.012	<LoD		<LoD	
10.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
11.5	<LoD		<LoD		<LoD		<LoD		0.235	0.057	**0.143**	0.015
12.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	0.198	0.009	<LoD	
13.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
14.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
15.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
blank 1	14.777	0.353	2.655	0.043	1.363	0.061	<LoD		0.210	0.012	<LoD	
blank 2	4.449	0.154	1.975	0.026	2.835	0.089	0.255	0.001	0.393	0.028	0.210	0.018
blank 3	5.194	0.138	3.032	0.142	2.167	0.060	0.152	0.016	0.264	0.016	0.235	0.011
blank 4	4.665	0.126	2.840	0.072	2.246	0.060	0.425	0.008	0.195	0.013	0.313	0.013
blank 5	4.198	0.036	3.709	0.128	2.374	0.045					<LoD	
correction value	6.657		2.842		2.197		0.167		0.212		0.152	
LoD	0.142		0.142		0.142		0.152		0.152		0.049	
LoQ	0.374		0.374		0.374		0.388		0.388		0.095	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**1.400**	0.096	**4.686**	0.031	**0.333**	0.043	<LoD		**1.302**	0.051	<LoD	
-4.5	**0.803**	0.047	**0.534**	0.032	**0.279**	0.090	<LoD		<LoD		<LoD	
-3.5	**0.473**	0.030	**0.457**	0.018	**0.641**	0.094	<LoD		<LoD		<LoD	
-2.5	**0.294**	0.050	**0.488**	0.024	<LoD		<LoD		<LoD		<LoD	
-1.5	0.155	0.035	**0.565**	0.011	**0.224**	0.067	<LoD		<LoD		<LoD	
-0.5	<NWG	0.051	**0.502**	0.012	**0.522**	0.092	0.173	0.066	<LoD		<LoD	
0.5	**2.205**	0.147	**0.459**	0.012	**2.025**	0.149	**0.622**	0.071	<LoD		<LoD	
1.5	**0.262**	0.042	**0.348**	0.009	**0.331**	0.068	<NWG	0.034	<LoD		<LoD	
2.5	**1.609**	0.094	**0.233**	0.011	**0.484**	0.097	<NWG	0.041	0.243	0.011	<LoD	
3.5	**0.244**	0.039	**0.233**	0.005	**0.782**	0.137	<NWG	0.014	0.277	0.026	<LoD	
4.5	0.149	0.030	**0.782**	0.015	**0.347**	0.096	**25.331**	0.500	<LoD		<LoD	
5.5	<LoD		0.162	0.005	<LoD		<LoD		**1.795**	0.112	**5.752**	0.408
6.5	<LoD		**0.646**	0.009	<LoD		<LoD		no sample**	no sample**	<LoD	
7.5	<LoD		**6.073**	0.169	<LoD		<LoD		no sample**	no sample**	<LoD	
8.5	0.155	0.025	**0.842**	0.025	**0.205**	0.113	<LoD		no sample**	no sample**	<LoD	
9.5	<LoD		**0.309**	0.006	<LoD		<LoD		no sample**	no sample**	0.162	0.010
10.5	<LoD		**0.336**	0.013	<LoD		<LoD		no sample**	no sample**	<LoD	
11.5	<LoD		**0.617**	0.010	**37.608**	0.791	<LoD		no sample**	no sample**	<LoD	
12.5	<LoD		**5.225**	0.026	<LoD		<LoD		no sample**	no sample**	no sample**	no sample**
13.5	1.322	0.037	**6.145**	0.115	<LoD		no sample ***	no sample ***	no sample**	no sample**	<LoD	
14.5	<LoD		**0.266**	0.010	<LoD		no sample ***	no sample ***	no sample**	no sample**	**0.182**	0.038
15.5	<LoD		**30.623**	0.474	<LoD		no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	0.797	0.043	84.213	1.880	1.490	0.005	0.177	0.021	0.127	18.692	0.209	0.007
blank 2	2.415	0.102	0.150	0.012	1.525	0.045	0.814	0.017	0.102	23.582	0.072	0.016
blank 3	0.776	0.033	4.034	0.172	1.832	0.099	0.552	0.036	0.056	14.136	1.809	0.076
blank 4	0.808	0.039	0.170	0.005	1.985	0.101	0.215	0.017	0.083	28.427	0.161	0.033
blank 5	1.670	0.087	0.169	0.005	1.862	0.078	0.385	0.020	0.063	22.247	0.191	0.025
correction value	0.794		0.163		1.739		0.429		0.097		0.158	
LoD	0.062		0.062		0.075		0.074		0.109		0.061	
LoQ	0.182		0.182		0.195		0.203		0.296		0.166	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 40: Iron concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**45**	5.83	**29**	1.76	**162**	5.85	**35**	2.07	**364**	10.60	**103**	3.53
-4.5	**50**	2.52	**27**	2.07	**110**	4.49	**20**	0.93	**336**	24.79	**83**	2.31
-3.5	**46**	0.45	**35**	4.81	**98**	9.70	**22**	1.36	**342**	17.19	**75**	1.78
-2.5	**37**	2.38	**20**	1.38	**94**	2.15	**20**	1.50	**173**	3.82	**65**	2.49
-1.5	**39**	4.62	**28**	1.99	**99**	16.51	**20**	1.82	**122**	5.25	**79**	0.82
-0.5	**37**	8.45	**38**	2.43	**102**	3.51	**22**	1.49	**247**	7.06	**79**	0.83
0.5	**84**	2.98	**65**	10.44	**45**	3.86	**30**	1.87	**36**	1.39	**171**	5.59
1.5	**823**	79.15	**57**	8.08	**41**	1.82	**39**	0.78	**284**	11.45	**37**	1.11
2.5	**2,381**	376.91	**93**	12.35	**54**	1.35	**455**	22.59	**392**	17.59	**24**	0.78
3.5	**519**	65.52	**78**	2.88	**50**	2.40	**128**	4.42	**190**	13.65	**42**	1.03
4.5	**2,275**	488.75	**88**	2.85	**66**	7.25	**168**	10.66	**124**	7.80	**609**	16.21
5.5	**6,284**	613.13	**62**	6.36	**57**	6.80	**90**	1.69	**54**	2.87	**1,363**	36.69
6.5	**123**	7.10	**62**	10.60	**57**	6.47	**33**	0.82	**46**	1.05	**2,320**	106.28
7.5	**60**	4.63	**45**	7.42	**48**	2.05	**20**	0.98	**60**	4.07	**13**	0.81
8.5	**679**	65.19	**83**	4.15	**77**	7.86	**14**	0.68	**46**	2.14	**15**	0.34
9.5	**2,380**	191.17	**499**	22.32	**95**	15.30	**12**	0.52	**59**	3.49	**14**	0.71
10.5	**2,332**	193.22	**598**	19.78	**73**	2.56	**9**	0.53	**59**	3.30	**32**	0.82
11.5	**691**	59.90	**1,640**	99.33	**59**	1.70	**18**	0.75	**67**	2.22	**19**	0.48
12.5	**4,219**	432.05	**3,685**	274.91	**1,171**	88.91	**8**	0.20	**33**	0.76	**25**	0.56
13.5	**280**	11.12	**5,242**	464.31	**2,608**	328.05	**9**	0.93	**35**	0.62	**32**	0.52
14.5	**2,880**	590.99	**10,386**	1,239.61	**9,159**	476.56	**7**	0.32	**22**	0.51	**26**	0.82
15.5	**5,614**	597.63	**6,672**	730.82	**12,544**	876.38	**9**	0.11	**25**	1.01	**35**	0.96
blank 1	1.43	0.22	0.99	0.04	5.56	0.79	3.07	0.41	1.30	0.12	2.45	0.05
blank 2	1.80	0.18	0.82	0.01	3.54	0.09	0.74	0.08	0.93	0.06	1.31	0.04
blank 3	2.67	0.22	37.69	1.17	3.60	0.09	0.65	0.03	1.47	0.06	1.02	0.06
blank 4	2.34	0.26	1.41	0.25	3.12	0.18	0.89	0.04	0.77	0.04	1.33	0.05
blank 5	1.69	0.15	0.99	0.07	4.30	0.40	4.16	0.67	1.57	0.11	2.16	0.03
correction value	1.99		8.38		4.02		1.90		1.21		1.65	
LoD	0.47		0.47		0.47		0.07		0.07		0.30	
LoQ	1.23		1.23		1.23		0.20		0.20		0.84	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**111**	2.52	**39**	0.64	**298**	11.65	**1,496**	34.63	**1,816**	24.52	**1,378**	60.23
-4.5	**78**	1.68	**37**	0.64	**391**	17.90	**1,011**	21.13	**1,684**	36.47	**1,329**	43.90
-3.5	**45**	0.88	**35**	0.78	**368**	10.21	**993**	25.83	**1,378**	22.61	**5,052**	289.44
-2.5	**32**	0.67	**33**	0.49	**431**	25.93	**581**	7.13	**1,910**	23.92	**1,253**	19.21
-1.5	**29**	0.59	**34**	3.51	**283**	21.16	**798**	13.09	**1,418**	18.24	**1,091**	40.98
-0.5	**59**	1.51	**44**	0.45	**7,360**	312.45	**8,319**	220.21	**1,465**	20.42	**1,261**	36.17
0.5	**10**	0.21	**2,123**	43.11	**42,925**	2,979.93	**85,059**	3,285.90	**25,711**	814.28	**28,658**	569.80
1.5	**17**	0.20	**2,683**	70.74	**20,511**	1,036.95	**81,671**	3,902.17	**73,621**	1,104.68	**50,382**	2,004.23
2.5	**56**	0.44	**17**	0.75	**4,246**	112.54	**45,790**	1,319.03	**34,555**	1,512.68	**31,878**	1,164.68
3.5	**68**	1.47	**19**	0.27	**1,075**	11.69	**8,803**	391.38	**7,220**	101.76	**15,819**	1,000.42
4.5	**77**	3.28	**23**	0.56	**640**	30.85	**4,467**	146.27	**1,231**	22.56	**927**	24.42
5.5	**81**	1.32	**42**	0.86	**2,020**	74.68	**5,593**	222.58	**1,568**	15.05	**38**	1.39
6.5	**170**	6.09	**35**	0.35	no sample *	no sample *	**7,888**	297.98	**3,065**	57.49	**73**	2.32
7.5	**141**	4.58	**34**	3.12	no sample *	no sample *	**8,689**	217.99	**3,024**	57.33	**77**	2.14
8.5	**63**	3.92	**38**	0.59	no sample *	no sample *	**12,712**	356.80	**4,737**	163.37	**65**	1.74
9.5	**68**	1.73	**62**	1.93	**3,146**	52.59	**14,419**	655.73	**6,353**	79.77	**63**	2.68
10.5	**32**	0.36	**52**	0.74	**5,035**	211.48	**4,809**	112.58	**9,233**	219.51	**36**	0.74
11.5	**50**	0.72	**60**	0.82	**8,381**	369.98	**6,717**	230.48	**11,183**	445.36	**30**	2.50
12.5	**73**	2.30	**61**	0.35	**9,412**	642.73	**8,938**	349.27	**6,521**	321.61	**35**	1.10
13.5	**108**	1.45	**86**	1.32	**12,002**	1,137.34	**12,519**	849.89	**9,202**	455.93	**27**	2.00
14.5	**232**	4.10	**105**	1.20	**11,465**	382.62	**14,338**	406.74	**12,493**	306.09	no sample **	no sample **
15.5	**655**	20.00	**269**	2.69	**14,207**	961.65	**16,303**	621.20	**15,669**	501.83	**27**	0.98
blank 1	0.97	0.03	0.97	0.04	18.34	0.89	21.50	0.46	1.09	0.04	2.85	0.40
blank 2	1.17	0.01	1.20	0.03	21.48	1.03	23.59	0.18	2.82	0.14	<LoD	
blank 3	1.27	0.02	4.48	0.08	22.52	0.97	22.72	1.06	2.12	0.05	1.73	0.19
blank 4	1.06	0.02	1.14	0.02	19.67	1.01	35.27	0.86	1.18	0.12	1.32	0.19
blank 5	1.99	0.03	0.69	0.03	15.20	1.30	22.79	0.84	<LoD		3.30	0.21
correction value	1.29		1.70		19.44		25.17		1.44		1.84	
LoD	0.31		0.31		0.31		1.08		1.08		1.07	
LoQ	0.89		0.89		0.86		2.92		2.92		2.26	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 41: Iron concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**95**	4.02	**282**	12.99	**750**	28.57	**184**	12.34	**262**	11.28	**77**	1.63
-4.5	**89**	3.53	**115**	6.69	**291**	10.42	**36**	1.41	**489**	30.80	**59**	0.29
-3.5	**96**	4.06	**72**	2.21	**205**	15.78	**58**	2.73	**405**	19.16	**30**	0.52
-2.5	**107**	1.99	**54**	2.34	**166**	9.09	**43**	2.55	**334**	17.81	**25**	0.14
-1.5	**96**	3.13	**42**	1.90	**168**	6.27	**65**	4.36	**251**	12.11	**8**	0.38
-0.5	**81**	3.04	**76**	3.57	**169**	10.19	**65**	2.63	**151**	4.65	**24**	0.45
0.5	**385**	19.69	**2,454**	47.42	**1,256**	45.61	**13**	0.91	**195**	7.34	**13**	0.24
1.5	**5,869**	492.53	**6,298**	202.58	**2,968**	120.43	**155**	5.19	**1,618**	45.53	**56**	0.40
2.5	**10,519**	531.75	**8,440**	480.53	**2,193**	53.01	**1,398**	61.38	**3,416**	279.07	**271**	14.15
3.5	**8,627**	324.87	**6,824**	234.41	**2,250**	93.43	**6,509**	247.28	**2,482**	43.03	**397**	15.47
4.5	**10,630**	326.33	**1,569**	88.92	**1,190**	58.93	**6,576**	235.16	**1,160**	42.93	**371**	5.80
5.5	**11,659**	491.66	**652**	30.74	**425**	11.23	**1,458**	70.52	**530**	54.23	**649**	17.31
6.5	**6,048**	327.80	**434**	14.44	**393**	20.10	no sample ***	no sample ***	**434**	12.70	**2,223**	30.74
7.5	**3,180**	213.83	**311**	16.72	**336**	22.87	no sample ***	no sample ***	**226**	11.98	**4,026**	112.08
8.5	**7,383**	162.04	**797**	29.30	**289**	7.08	no sample ***	no sample ***	**135**	2.39	**1,958**	29.55
9.5	**11,452**	276.90	**4,685**	154.77	**1,179**	20.63	no sample ***	no sample ***	**135**	3.17	**3,292**	73.08
10.5	**13,201**	968.79	**13,872**	334.83	**1,892**	132.09	**154**	6.40	**599**	27.07	**4,907**	140.48
11.5	**15,316**	1,156.70	**21,430**	939.95	**3,250**	81.34	**180**	5.84	**495**	22.69	**6,633**	181.95
12.5	**16,012**	1,332.25	**20,544**	324.22	**13,290**	545.61	**162**	5.80	**203**	7.40	**6,898**	112.74
13.5	**19,379**	21.47	**17,573**	721.58	**19,671**	651.28	**118**	1.62	**345**	14.37	**7,302**	103.12
14.5	**19,498**	672.74	**14,678**	316.39	**16,454**	677.87	**90**	1.59	**134**	3.31	**7,898**	161.93
15.5	**20,195**	1,005.23	**16,179**	710.88	**15,838**	961.43	no sample ***	no sample ***	**106**	4.48	**9,981**	218.58
blank 1	<LoD		4.52	0.36	7.14	0.24	9.25	1.18	<LoD		4.65	0.08
blank 2	<LoD		<LoD		6.61	0.24	42.32	1.10	48.22	8.16	4.51	0.10
blank 3	<LoD		<LoD		5.22	0.09	<LoD		<LoD		6.61	0.07
blank 4	<LoD		<LoD		7.01	0.23	<LoD		<LoD		6.67	0.06
blank 5	<LoD		<LoD		5.06	0.12	<LoD				8.15	0.09
correction value	0.00		0.90		6.21		10.31		9.64		6.12	
LoD	2.71		2.71		2.71		4.35		4.35		0.71	
LoQ	8.33		8.33		8.33		13.11		13.11		1.97	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**291**	5.84	**38**	0.91	**313**	6.87	**1,630**	100.80	**1,649**	20.15	**1,195**	28.19
-4.5	**176**	4.26	**29**	2.35	**302**	19.33	**850**	28.53	**1,721**	11.07	**1,182**	18.96
-3.5	**107**	1.81	**38**	0.64	**378**	12.97	**670**	29.75	**1,853**	44.41	**5,210**	81.85
-2.5	**105**	2.30	**31**	0.27	**276**	6.99	**670**	38.69	**1,648**	28.86	**1,271**	26.30
-1.5	**97**	2.15	**32**	0.77	**284**	6.00	**652**	9.36	**1,193**	13.16	**1,146**	55.93
-0.5	**54**	1.05	**44**	0.38	**6,870**	392.48	**6,522**	494.68	**1,031**	13.59	**1,279**	28.26
0.5	**63**	1.72	**3,781**	71.76	**39,951**	1,562.33	**78,532**	7,595.00	**27,393**	349.80	**30,567**	1,387.66
1.5	**200**	1.48	**4,815**	89.26	**28,187**	1,240.42	**83,841**	4,138.56	**72,298**	2,704.12	**54,853**	3,859.03
2.5	**1,344**	34.89	**131**	3.03	**14,879**	332.91	**36,856**	2,485.97	**59,340**	1,661.38	**37,272**	608.20
3.5	**1,954**	50.19	**124**	1.63	**5,411**	91.56	**25,001**	634.64	**32,668**	1,000.07	**17,623**	694.33
4.5	**1,737**	86.18	**87**	2.12	**2,834**	99.90	**14,248**	80.48	**19,789**	585.56	**11,906**	310.60
5.5	**1,459**	61.80	**77**	1.24	**5,686**	185.92	**10,103**	649.00	**10,781**	143.41	no sample **	no sample **
6.5	**2,617**	80.55	**74**	0.68	no sample *	no sample *	**13,361**	501.01	**7,992**	245.11	**1,071**	54.12
7.5	**2,342**	84.89	**60**	1.49	no sample *	no sample *	**8,055**	147.83	**7,960**	214.68	**308**	160.82
8.5	**9,137**	178.73	**65**	0.86	no sample *	no sample *	**9,951**	508.70	**8,848**	152.07	**290**	4.53
9.5	**11,724**	264.19	**69**	0.59	**14,065**	317.46	**13,660**	683.21	**9,928**	220.34	**178**	17.86
10.5	**7,402**	146.91	**74**	2.72	**13,843**	941.31	**16,435**	1,420.96	**11,720**	262.07	**155**	3.41
11.5	**8,463**	401.35	**90**	1.37	**13,585**	428.41	**21,326**	1,198.54	**13,835**	500.16	no sample **	no sample **
12.5	**6,924**	137.67	**106**	1.37	**13,698**	715.77	**18,133**	841.39	**17,156**	652.91	no sample **	no sample **
13.5	**9,246**	314.05	**140**	2.48	**14,882**	597.05	**18,510**	1,737.60	**18,196**	492.33	no sample **	no sample **
14.5	**8,451**	106.57	**170**	2.18	**16,636**	427.94	**20,321**	847.09	**15,936**	437.52	no sample **	no sample **
15.5	**10,403**	366.84	**341**	3.73	**14,155**	106.31	**17,054**	985.26	**16,955**	423.14	no sample **	no sample **
blank 1	2.12	0.10	2.07	0.08	14.55	0.26	59.56	2.33	2.09	0.23	2.85	0.40
blank 2	1.83	0.07	10.91	0.15	15.42	0.59	189.23	10.17	2.12	0.25	<LoD	
blank 3	1.73	0.05	2.37	0.03	21.40	1.04	49.74	2.83	1.63	0.30	1.73	0.19
blank 4	4.37	0.11	5.69	0.10	10.99	0.64	52.82	1.52	<LoD		1.32	0.19
blank 5	8.23	0.25	1.76	0.04	13.15	0.65	56.40	1.42			3.30	0.21
correction value	3.66		4.56		15.10		81.55		1.17		1.84	
LoD	0.71		0.30		0.72		0.31		1.08		1.07	
LoQ	1.97		0.84		1.91		0.86		2.92		2.26	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 42: Iron concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**56**	4.11	**83**	5.78	**161**	21.98	**50**	4.50	**43**	0.72	**264**	8.00
-4.5	**61**	5.33	**72**	2.43	**166**	12.60	**44**	3.55	**51**	1.42	**232**	7.58
-3.5	**53**	3.31	**73**	3.99	**140**	4.32	**25**	1.99	**66**	2.70	**213**	4.75
-2.5	**48**	1.81	**80**	7.86	**100**	3.50	**47**	1.45	**32**	0.72	**262**	6.71
-1.5	**56**	7.06	**65**	9.03	**72**	3.70	**31**	1.32	**96**	1.48	**246**	6.14
-0.5	**62**	5.19	**85**	8.11	**76**	3.02	**45**	2.61	**62**	3.39	**253**	4.36
0.5	**72**	4.15	**34**	0.34	**68**	14.86	**30**	1.99	**281**	21.04	**364**	6.69
1.5	**226**	2.02	**56**	4.40	**68**	2.77	**33**	1.85	**319**	11.40	**83**	1.64
2.5	**4,615**	228.76	**71**	6.04	**71**	5.99	**146**	9.96	**759**	32.29	**29**	0.29
3.5	**1,885**	127.41	**55**	2.63	**74**	2.21	**194**	13.31	**1,501**	20.50	**83**	1.30
4.5	**4,137**	441.42	**55**	3.65	**63**	1.28	**56**	2.55	**2,784**	174.30	**36**	0.48
5.5	**9,542**	531.68	**48**	5.44	**66**	4.18	**19**	1.07	**4,649**	70.01	**956**	32.18
6.5	**1,047**	53.44	**57**	11.32	**70**	7.70	**20**	0.32	**7,194**	487.61	**56**	1.51
7.5	**229**	13.84	**42**	3.01	**86**	8.06	**43**	1.36	**6,020**	373.30	**2,912**	58.49
8.5	**1,085**	72.88	**70**	2.96	**67**	8.15	**125**	3.37	**5,837**	224.81	**48**	1.03
9.5	**5,215**	748.99	**42**	6.17	**60**	5.48	**71**	2.76	**8,276**	191.07	**5,361**	144.63
10.5	**3,287**	479.87	**83**	4.02	**43**	4.23	**79**	1.74	**58**	1.42	**29**	2.72
11.5	**2,909**	240.89	**671**	19.77	**47**	2.31	**86**	4.32	**84**	2.84	**34**	0.74
12.5	**5,622**	666.59	**3,701**	348.68	**58**	3.31	**58**	1.33	**64**	0.85	**31**	0.84
13.5	**486**	54.20	**7,295**	258.15	**1,175**	58.80	**62**	1.69	**50**	2.07	**38**	0.49
14.5	**2,859**	365.84	**9,202**	842.00	**4,224**	365.46	**111**	4.40	**70**	4.29	**34**	0.50
15.5	**7,885**	924.12	**5,529**	157.17	**8,020**	889.92	**170**	7.15	**59**	2.10	**46**	1.69
blank 1	1.07	0.11	1.99	0.74	1.15	0.02	2.65	0.10	0.92	0.05	1.98	0.19
blank 2	1.25	0.01	0.82	0.10	0.91	0.07	1.60	0.07	7.82	0.70	0.85	0.10
blank 3	1.07	0.07	0.78	0.08	2.05	0.23	5.86	0.32	2.50	0.13	<LoD	
blank 4	1.56	0.25	0.71	0.04	0.49	0.06	1.89	0.07	7.73	0.80	1.32	0.20
blank 5	2.13	0.25	3.35	0.23	0.80	0.13	3.30	0.19	2.28	0.11	1.33	0.11
correction value	1.42		1.53		1.08		3.06		4.25		1.10	
LoD	0.47		0.47		0.47		0.07		0.07		0.72	
LoQ	1.23		1.23		1.23		0.20		0.20		1.91	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**181**	6.24	**1,398**	31.61	**8**	0.99	<NWG	0.18	**32**	1.16	**57**	3.76
-4.5	**101**	2.54	**8**	1.10	**3**	0.64	<NWG	0.24	**12**	0.42	**5**	0.67
-3.5	**59**	1.50	**5**	0.16	**2**	0.81	<NWG	0.45	**16**	0.43	**13**	0.42
-2.5	**36**	1.06	**5**	0.48	**1**	0.85	<NWG	0.37	**11**	0.50	**4**	0.54
-1.5	**201**	4.12	**6**	0.12	<NWG	0.55	<NWG	0.28	**6**	0.34	**4**	0.40
-0.5	**15**	0.25	**2,051**	50.86	**35**	5.14	**2,441**	48.54	**19**	0.30	**625**	33.21
0.5	**24**	0.69	**14,407**	543.88	**2,609**	149.54	**10,653**	303.64	**175**	3.05	**8,017**	571.17
1.5	**16**	0.09	**10,579**	239.32	**2,146**	97.06	**7,526**	366.09	**4,863**	65.71	**3,810**	178.88
2.5	**66**	1.03	**923**	28.05	**89**	3.71	**4,172**	81.01	**58**	3.53	**177**	9.20
3.5	**109**	1.79	**271**	7.32	**63**	4.64	**619**	7.65	**950**	8.79	**78**	1.85
4.5	**128**	1.14	**1,028**	46.21	**93**	5.59	**1,749**	18.23	**327**	2.12	**63**	3.07
5.5	**128**	0.77	**2,640**	93.61	**75**	4.36	**1,685**	5.88	**95**	1.52	**48**	0.95
6.5	**196**	1.80	**2,204**	75.19	**81**	6.40	**1,467**	21.25	**46**	0.60	**36**	0.91
7.5	**210**	0.73	**5,169**	162.84	**85**	5.26	**1,240**	14.41	**40**	0.49	**34**	0.62
8.5	**78**	1.06	**7,378**	134.00	**77**	6.01	**875**	8.44	**38**	1.19	**34**	1.38
9.5	**47**	0.54	**4,245**	174.62	**75**	6.47	**1,161**	19.51	**44**	0.75	**34**	1.44
10.5	no sample**	no sample**	**2,294**	38.07	**107**	5.83	**12**	0.68	**41**	0.49	**30**	0.83
11.5	**165**	3.04	**4,935**	38.09	**105**	5.97	**20**	0.80	**36**	0.47	**28**	1.18
12.5	no sample**	no sample**	**4,878**	100.61	**157**	6.62	**92**	2.51	**35**	0.51	**28**	1.78
13.5	**60**	4.32	**7,186**	256.78	**205**	12.93	**98**	2.06	**6**	4.47	**31**	1.08
14.5	no sample**	no sample**	**8,773**	151.75	**201**	12.93	**159**	3.82	**66**	1.01	**11**	0.35
15.5	**83**	1.49	**10,530**	122.84	no sample**	no sample**	**328**	2.64	**41**	0.65	**40**	1.11
blank 1	2.26	0.02	1.78	0.02	22.88	1.53	28.58	0.51	1.58	0.13	1.04	0.22
blank 2	6.64	0.06	2.51	0.05	18.60	1.00	28.91	0.97	1.94	0.11	0.85	0.13
blank 3	1.73	0.02	3.90	0.02	19.31	0.80	32.08	0.65	2.10	0.15	9.32	0.27
blank 4	1.80	0.03	4.62	0.35	14.61	0.61	30.20	0.96	7.69	0.40	3.72	0.20
blank 5	2.41	0.06	9.09	0.20	12.50	0.75	29.34	0.47	5.54	0.25	1.50	0.17
correction value	2.97		4.38		17.58		29.82		3.02		3.28	
LoD	0.31		0.31		0.31		1.08		1.08		1.07	
LoQ	0.89		0.89		0.86		2.92		2.92		2.26	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 43: Iron concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**123**	5.24	**143**	5.22	**310**	14.07	**215**	10.46	**1,178**	99.12	**529**	16.25
-4.5	**178**	7.86	**316**	15.86	**360**	14.91	**138**	8.32	**800**	30.72	**318**	9.65
-3.5	**154**	8.14	**219**	17.22	**229**	9.02	**262**	22.64	**1,271**	44.54	**455**	25.90
-2.5	**153**	5.78	**232**	9.24	**213**	4.15	**318**	12.67	**1,302**	65.28	**515**	19.05
-1.5	**151**	5.07	**160**	8.22	**171**	10.84	**200**	6.81	**1,238**	84.55	**416**	15.14
-0.5	**152**	8.50	**336**	12.66	**370**	13.36	**218**	9.00	**1,068**	37.06	**350**	3.99
0.5	**424**	16.60	**1,589**	51.09	**1,248**	65.35	**266**	13.40	**1,767**	75.59	**1,020**	35.82
1.5	**5,650**	263.58	**1,648**	57.68	**1,538**	43.35	**532**	11.80	**2,146**	103.13	**1,693**	15.37
2.5	**11,091**	548.41	**855**	39.02	**524**	15.24	no sample ***	no sample ***	**2,967**	166.96	**2,285**	156.55
3.5	**14,882**	403.41	**292**	13.70	**257**	11.42	no sample ***	no sample ***	**4,570**	194.33	**3,722**	97.65
4.5	**20,867**	1,154.87	**169**	5.76	**174**	6.06	**1,187**	24.68	**8,341**	434.38	**6,784**	230.49
5.5	**18,320**	1,029.56	**109**	5.17	**145**	7.42	**271**	7.93	**11,084**	437.98	**8,889**	241.95
6.5	**18,041**	1,465.91	**741**	21.49	**159**	1.21	**385**	18.29	**10,361**	469.47	**10,582**	240.01
7.5	**18,677**	1,529.49	**174**	10.64	**123**	4.94	**641**	11.04	**9,557**	322.40	**12,571**	411.51
8.5	**18,140**	470.49	**145**	8.50	**113**	7.02	**4,838**	249.18	**11,502**	762.91	**9,930**	194.64
9.5	**18,563**	1,025.91	**171**	7.19	**594**	24.65	**4,939**	83.52	**10,763**	729.40	**13,610**	344.55
10.5	**22,553**	1,289.92	**330**	14.10	**583**	33.44	**5,896**	165.91	**8,844**	408.69	**14,394**	265.44
11.5	**23,228**	1,477.04	**1,338**	55.83	**1,662**	131.18	**5,787**	173.70	**8,305**	720.68	**17,512**	956.47
12.5	**18,746**	1,404.50	**4,554**	179.38	**5,755**	360.37	no sample ***	no sample ***	**11,099**	99.42	**15,570**	696.48
13.5	**25,092**	1,502.66	**9,080**	368.02	**10,408**	469.38	**3,329**	62.97	**12,004**	321.90	**15,804**	804.75
14.5	**23,525**	709.20	**10,889**	540.08	**10,796**	909.09	no sample ***	no sample ***	**13,180**	739.33	**13,953**	615.05
15.5	**19,125**	909.79	**12,294**	636.02	**14,740**	808.72	no sample ***	no sample ***	**12,963**	525.49	**16,806**	651.69
blank 1	6.64	0.17	<LoD		<LoD		<LoD		7.39	0.50	8.04	0.29
blank 2	<LoD		<LoD		<LoD		<LoD		7.43	0.53	5.81	0.08
blank 3	<LoD		2.80	0.23	<LoD		7.41	0.40	9.32	0.47	9.87	0.69
blank 4	<LoD		8.14	0.44	<LoD		24.80	1.16	10.63	0.11	12.27	0.24
blank 5	4.41	0.12	5.16	0.31	<LoD						28.54	0.97
correction value	2.21		3.22		0.00		6.44		6.95		12.91	
LoD	2.71		2.71		2.71		4.35		4.35		0.71	
LoQ	8.33		8.33		8.33		13.11		13.11		1.97	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**226**	3.45	**4,388**	40.98	**8**	0.43	<LoD		**725**	19.34	**388**	10.37
-4.5	**178**	2.43	**142**	1.52	**6**	0.26	<LoD		**198**	2.39	**42**	1.55
-3.5	**120**	2.72	**101**	1.45	**7**	0.56	<LoD		**92**	2.14	**26**	0.71
-2.5	**65**	1.64	**53**	1.09	**3**	0.47	<LoD		**57**	0.73	**19**	1.13
-1.5	**27**	0.78	**51**	1.90	<NWG	0.54	<LoD		**41**	0.78	**16**	0.17
-0.5	**20**	0.11	**3,011**	61.09	**131**	4.13	**3,030**	135.24	**74**	1.39	**757**	12.18
0.5	**65**	0.61	**15,812**	305.88	**8,565**	396.92	**7,456**	477.67	**253**	3.51	**9,010**	208.88
1.5	**182**	2.87	**12,913**	444.37	**7,146**	305.01	**6,256**	550.75	**3,902**	136.84	**4,714**	106.95
2.5	**1,397**	45.90	**12,404**	531.26	**2,696**	77.71	**4,268**	159.07	**13,686**	236.30	**1,589**	91.49
3.5	**1,463**	29.71	**11,057**	301.44	**305**	6.32	**6,546**	223.05	**3,017**	38.58	**491**	24.09
4.5	**948**	22.67	**11,228**	350.62	**187**	1.65	**5,285**	319.74	**788**	9.68	**464**	3.82
5.5	**1,277**	125.58	**13,224**	249.12	**128**	2.10	**3,526**	231.88	**438**	5.90	**222**	14.53
6.5	**2,363**	122.77	**13,134**	236.41	**106**	1.38	**3,066**	106.58	no sample**	no sample**	**128**	2.47
7.5	**2,100**	21.69	**13,528**	372.67	**83**	2.72	**2,265**	112.15	no sample**	no sample**	**133**	1.83
8.5	**2,840**	79.69	**13,135**	130.20	**125**	3.13	**1,223**	46.47	no sample**	no sample**	**127**	2.94
9.5	**1,778**	41.01	**21,119**	339.12	**100**	0.59	**1,250**	56.91	no sample**	no sample**	**95**	0.63
10.5	**2,836**	39.86	**20,994**	545.27	**202**	2.90	**2,922**	115.28	no sample**	no sample**	**153**	3.62
11.5	**4,090**	81.68	**19,131**	920.95	**233**	3.73	**3,027**	147.84	no sample**	no sample**	**133**	2.33
12.5	**5,213**	97.79	**20,938**	563.84	**333**	4.94	<LoD		no sample**	no sample**	no sample**	no sample**
13.5	**6,027**	131.10	**18,628**	414.96	**351**	15.15	no sample ***	no sample ***	no sample**	no sample**	**82**	2.66
14.5	**6,446**	259.12	**17,661**	218.08	**324**	13.27	no sample ***	no sample ***	no sample**	no sample**	**87**	2.34
15.5	**7,134**	120.29	**16,932**	257.22	**266**	12.49	no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	5.89	0.08	1.44	0.04	10.80	0.24	38.63	1.24	3.93	4.75	2.08	0.15
blank 2	1.51	0.03	1.59	0.04	9.82	0.58	45.09	1.16	4.87	5.07	<LoD	
blank 3	1.65	0.05	2.69	0.03	12.74	0.47	50.01	1.54	0.74	18.09	1.36	0.10
blank 4	8.23	0.18	2.61	0.09	12.29	0.69	47.57	1.55	0.97	17.63	1.28	0.24
blank 5	3.78	0.06	1.86	0.04	11.88	0.56	53.28	1.68	0.74	12.97	1.61	0.20
correction value	4.21		2.04		11.50		46.91		3.18		1.27	
LoD	0.30		0.30		0.72		0.31		1.08		1.07	
LoQ	0.84		0.84		1.91		0.86		2.92		2.26	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 44: Manganese concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**78**	7.4	**58**	3.0	**81**	3.6	**531**	31.0	**420**	11.6	**168**	6.0
-4.5	**99**	6.4	**76**	4.1	**85**	5.6	**726**	31.5	**437**	12.0	**159**	9.4
-3.5	**99**	2.3	**83**	7.9	**76**	6.6	**770**	7.5	**410**	13.7	**157**	5.6
-2.5	**78**	3.5	**53**	2.4	**73**	6.3	**623**	24.8	**189**	5.3	**134**	5.4
-1.5	**76**	9.5	**69**	4.8	**75**	14.0	**537**	31.8	**183**	6.8	**159**	3.6
-0.5	**83**	17.8	**291**	9.7	**365**	16.7	**551**	19.4	**321**	23.1	**179**	3.5
0.5	**274**	12.3	**886**	115.0	**802**	68.7	**662**	25.0	**138**	3.0	**228**	18.5
1.5	**568**	51.1	**581**	72.0	**809**	48.0	**634**	18.2	**590**	30.3	**252**	8.2
2.5	**676**	91.2	**597**	56.5	**897**	14.0	**813**	49.4	**589**	28.9	**417**	28.8
3.5	**788**	88.9	**626**	24.0	**767**	31.5	**438**	31.9	**540**	17.5	**301**	21.4
4.5	**910**	179.7	**616**	14.3	**952**	103.8	**299**	16.5	**710**	55.8	**489**	13.0
5.5	**926**	101.6	**892**	96.3	**798**	88.4	**261**	7.5	**681**	32.8	**347**	16.8
6.5	**746**	35.1	**874**	134.6	**1,060**	108.7	**195**	6.1	**700**	28.4	**338**	17.0
7.5	**879**	79.5	**413**	54.2	**972**	45.1	**106**	4.9	**877**	42.5	**206**	6.2
8.5	**1,371**	130.7	**302**	10.6	**1,189**	108.8	**69**	2.1	**736**	25.1	**297**	18.7
9.5	**737**	57.3	**604**	31.6	**442**	58.2	**50**	1.0	**835**	13.5	**295**	13.0
10.5	**905**	61.3	**960**	20.7	**362**	17.5	**18**	0.3	**220**	4.4	**476**	41.5
11.5	**717**	50.7	**768**	44.3	**649**	20.2	**13**	0.4	**260**	3.9	**308**	11.2
12.5	**1,117**	100.5	**863**	52.2	**877**	86.7	**12**	0.3	**229**	4.6	**348**	6.9
13.5	**655**	12.5	**747**	58.1	**1,026**	131.9	**12**	0.4	**207**	3.5	**411**	17.8
14.5	**920**	188.7	**1,176**	135.7	**1,043**	39.7	**11**	0.4	**208**	4.0	**288**	16.0
15.5	**770**	74.4	**773**	85.0	**1,105**	72.7	**22**	0.4	**289**	5.0	**365**	13.3
blank 1	0.1	0.0	0.1	0.0	0.2	0.0	0.1	0.0	0.2	0.0	0.1	0.0
blank 2	0.1	0.0	0.1	0.0	0.2	0.0	<LoD		0.1	0.0	0.1	0.0
blank 3	0.2	0.0	2.3	0.1	0.2	0.0	0.1	0.0	0.1	0.0	<LoD	
blank 4	0.1	0.0	0.2	0.0	0.1	0.0	0.1	0.0	0.1	0.0	<LoD	
blank 5	0.1	0.0	0.1	0.0	0.4	0.0	0.2	0.0	0.2	0.0	0.1	0.0
correction value	0.1		0.5		0.2		0.1		0.1		0.1	
LoD	0.0		0.0		0.0		0.1		0.1		0.1	
LoQ	0.1		0.1		0.1		0.2		0.2		0.2	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**448**	5.5	**1,624**	79.1	**3,720**	137.8	**5,284**	183.7	**6,393**	177.7	**6,100**	251.2
-4.5	**433**	7.7	**1,572**	80.6	**3,750**	195.8	**5,876**	172.4	**6,670**	225.2	**5,713**	135.8
-3.5	**380**	7.3	**1,623**	41.4	**3,854**	38.3	**6,342**	132.0	**6,501**	206.6	**6,397**	241.3
-2.5	**324**	4.0	**1,663**	28.0	**4,776**	309.7	**3,948**	345.7	**8,164**	211.9	**5,184**	82.7
-1.5	**318**	5.6	**1,665**	148.3	**3,399**	220.3	**5,690**	242.3	**7,147**	302.2	**4,947**	208.8
-0.5	**343**	3.8	**1,645**	25.7	**3,552**	233.9	**5,920**	210.5	**7,565**	435.8	**5,081**	118.9
0.5	**503**	7.0	**1,560**	132.3	**2,929**	240.1	**4,721**	196.2	**5,343**	160.1	**4,502**	102.1
1.5	**576**	6.6	**1,098**	14.7	**2,076**	69.6	**2,876**	98.2	**3,968**	193.1	**3,410**	176.3
2.5	**463**	3.3	**678**	11.0	**1,382**	33.4	**1,965**	25.4	**2,758**	168.3	**2,547**	57.4
3.5	**478**	8.8	**563**	8.7	**1,141**	30.5	**1,200**	67.1	**1,993**	134.3	**2,032**	109.9
4.5	**431**	16.8	**523**	10.1	**903**	40.1	**1,065**	12.2	**1,132**	20.4	**1,418**	38.1
5.5	**450**	6.2	**539**	6.3	**764**	29.4	**767**	44.2	**872**	40.7	**1,164**	40.4
6.5	**471**	13.9	**585**	5.5	no sample *	no sample *	**858**	22.3	**847**	29.9	**849**	24.0
7.5	**484**	15.0	**628**	60.0	no sample *	no sample *	**834**	28.4	**666**	20.2	**753**	19.3
8.5	**410**	24.5	**646**	7.7	no sample *	no sample *	**1,028**	72.7	**737**	18.2	**711**	19.0
9.5	**463**	7.4	**699**	22.5	**619**	14.0	**981**	58.9	**765**	37.8	**758**	38.0
10.5	**458**	4.7	**723**	10.7	**760**	29.1	**760**	34.6	**846**	31.7	**739**	19.8
11.5	**484**	6.0	**738**	12.5	**825**	35.6	**912**	91.0	**862**	27.2	**808**	37.5
12.5	**529**	15.7	**757**	6.2	**807**	45.2	**796**	21.3	**801**	19.9	**809**	27.5
13.5	**509**	4.6	**761**	7.2	**938**	76.3	**908**	27.6	**849**	30.3	**707**	34.5
14.5	**544**	9.4	**781**	9.3	**807**	20.4	**873**	32.3	**965**	32.1	no sample **	no sample **
15.5	**567**	9.7	**794**	8.5	**960**	51.9	**925**	23.5	**1,021**	41.5	**864**	41.0
blank 1	<LoD		<LoD		0.5	0.0	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.7	0.0	0.3	0.1	5.0	0.3	<LoD	
blank 3	<LoD		0.1	0.0	0.6	0.1	<LoD		0.3	0.1	<LoD	
blank 4	<LoD		0.2	0.0	0.6	0.0	0.3	0.1	<LoD		<LoD	
blank 5	0.1	0.0	<LoD		1.3	0.1	<LoD		<LoD		<LoD	
correction value	0.0		0.1		0.7		0.1		1.1		0.0	
LoD	0.1		0.1		0.1		0.3		0.3		0.3	
LoQ	0.3		0.3		0.4		0.7		0.7		0.7	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 45: Manganese concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**121**	2.37	**72**	2.64	**64**	2.11	**795**	64.65	**64**	1.96	**59**	1.13
-4.5	**114**	6.77	**78**	4.88	**87**	3.44	**599**	14.16	**112**	2.85	**63**	0.59
-3.5	**116**	3.95	**65**	1.56	**83**	7.06	**504**	10.79	**95**	3.79	**66**	1.09
-2.5	**122**	3.92	**66**	3.81	**79**	3.75	**541**	19.74	**86**	4.19	**68**	0.62
-1.5	**111**	3.77	**56**	2.69	**78**	3.44	**505**	19.23	**59**	1.92	**72**	1.62
-0.5	**93**	4.32	**318**	16.40	**303**	15.00	**448**	7.62	**38**	0.72	**82**	1.38
0.5	**464**	24.16	**786**	12.77	**1,031**	29.61	**254**	7.60	**186**	10.31	**23**	0.25
1.5	**988**	71.41	**968**	25.80	**1,033**	35.29	**571**	17.21	**604**	16.30	**256**	1.38
2.5	**1,159**	65.26	**1,036**	68.00	**661**	12.34	**691**	19.00	**661**	43.24	**544**	32.82
3.5	**1,103**	42.31	**1,008**	44.49	**831**	26.41	**1,123**	18.51	**600**	8.46	**491**	4.32
4.5	**938**	26.74	**827**	42.84	**1,000**	36.83	**1,311**	42.88	**643**	24.95	**528**	8.57
5.5	**1,139**	32.86	**1,072**	60.87	**904**	33.18	**1,985**	51.05	**763**	110.65	**567**	3.99
6.5	**1,079**	68.87	**1,162**	46.70	**1,143**	52.94	no sample ***	no sample ***	**751**	27.29	**611**	5.56
7.5	**1,132**	60.86	**2,001**	92.32	**1,365**	105.43	no sample ***	no sample ***	**738**	17.19	**648**	10.27
8.5	**1,261**	36.40	**2,177**	70.95	**1,240**	33.52	no sample ***	no sample ***	**794**	15.16	**627**	9.98
9.5	**1,273**	24.65	**2,014**	68.54	**1,478**	28.29	no sample ***	no sample ***	**807**	26.48	**689**	22.95
10.5	**1,285**	86.54	**1,357**	32.18	**1,760**	120.19	**545**	14.49	**1,626**	23.19	**733**	34.70
11.5	**1,262**	95.26	**1,418**	64.47	**1,470**	37.53	**654**	6.75	**1,598**	51.71	**797**	11.17
12.5	**1,294**	77.92	**1,283**	29.77	**1,391**	54.90	**698**	12.80	**2,010**	36.45	**773**	18.22
13.5	**1,431**	21.47	**1,206**	51.58	**1,370**	50.09	**618**	14.64	**1,439**	20.64	**765**	20.90
14.5	**1,376**	72.33	**975**	20.73	**1,166**	32.55	**484**	10.46	**1,320**	29.64	**762**	13.65
15.5	**1,379**	73.64	**1,194**	48.48	**1,113**	56.02	no sample ***	no sample ***	**1,150**	53.36	**837**	25.77
blank 1	<LoD		0.14	0.00	0.73	0.03	4.18	0.45	<LoD		0.30	0.02
blank 2	<LoD		<LoD		0.67	0.03	<LoD		<LoD		0.29	0.03
blank 3	<LoD		0.12	0.01	0.49	0.01	<LoD		<LoD		0.38	0.02
blank 4	<LoD		0.14	0.01	0.73	0.02	<LoD		<LoD		0.40	0.01
blank 5	<LoD		<LoD		0.49	0.01	0.70	0.03			0.48	0.04
correction value	0.00		0.08		0.62		0.98		0.00		0.37	
LoD	0.12		0.12		0.12		0.68		0.68		0.06	
LoQ	0.32		0.32		0.32		2.04		2.04		0.16	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**562**	9.84	**1,598**	81.50	**3,570**	189.31	**5,772**	414.86	**6,530**	102.59	**5,291**	150.99
-4.5	**465**	8.17	**1,610**	150.73	**2,603**	153.45	**5,060**	133.10	**6,138**	174.71	**5,124**	75.12
-3.5	**468**	5.51	**1,588**	22.52	**3,333**	166.56	**4,589**	229.07	**6,931**	242.91	**6,210**	155.54
-2.5	**497**	10.07	**1,609**	40.16	**2,662**	73.25	**4,839**	279.57	**7,089**	333.96	**5,161**	124.47
-1.5	**499**	9.62	**1,618**	36.18	**2,793**	208.20	**5,190**	27.89	**5,405**	204.91	**5,035**	188.22
-0.5	**399**	5.31	**1,581**	31.29	**2,702**	102.06	**4,837**	147.38	**4,797**	162.23	**5,098**	143.56
0.5	**580**	9.42	**1,540**	33.71	**1,994**	151.99	**4,527**	290.93	**5,264**	169.06	**4,626**	34.55
1.5	**617**	5.49	**1,093**	47.20	**1,474**	41.79	**3,069**	176.21	**3,641**	131.90	**3,427**	104.98
2.5	**518**	7.15	**688**	8.26	**1,112**	81.39	**1,698**	117.70	**2,487**	107.18	**2,587**	98.40
3.5	**479**	4.87	**575**	3.44	**879**	53.72	**1,413**	67.20	**1,761**	49.10	**2,066**	50.27
4.5	**683**	21.14	**537**	11.88	**562**	30.83	**1,000**	178.70	**1,440**	26.48	**1,858**	28.76
5.5	**641**	21.20	**548**	4.63	**587**	34.45	**856**	58.05	**1,029**	17.18	no sample **	no sample **
6.5	**607**	6.64	**591**	3.46	no sample *	no sample *	**1,075**	37.57	**868**	27.38	**1,355**	62.71
7.5	**565**	7.69	**641**	15.65	no sample *	no sample *	**665**	14.79	**806**	23.13	**739**	393.59
8.5	**1,060**	26.92	**675**	3.66	no sample *	no sample *	**732**	33.68	**835**	23.72	**941**	16.05
9.5	**1,189**	70.10	**704**	3.28	**630**	10.39	**916**	38.45	**838**	32.92	**758**	81.19
10.5	**888**	36.98	**725**	23.89	**762**	39.98	**1,066**	75.32	**876**	61.23	**782**	12.93
11.5	**961**	23.02	**749**	7.58	**682**	51.22	**1,180**	53.87	**899**	33.08	no sample **	no sample **
12.5	**949**	24.07	**767**	12.76	**695**	15.14	**1,102**	54.42	**989**	59.31	no sample **	no sample **
13.5	**1,072**	34.11	**780**	7.66	**733**	19.20	**1,093**	108.65	**998**	21.54	no sample **	no sample **
14.5	**976**	24.16	**837**	51.39	**848**	39.56	**1,222**	38.31	**918**	28.11	no sample **	no sample **
15.5	**1,173**	15.30	**838**	11.77	**729**	37.70	**1,015**	58.71	**984**	54.12	no sample **	no sample **
blank 1	0.99	0.06	0.12	0.01	0.45	0.04	0.34	0.09	0.41	0.09	<LoD	
blank 2	0.12	0.01	0.59	0.02	0.38	0.05	1.47	0.19	<LoD		<LoD	
blank 3	0.10	0.01	0.08	0.02	1.42	0.07	0.22	0.04	<LoD		<LoD	
blank 4	0.19	0.01	0.30	0.01	0.29	0.09	0.53	0.03	<LoD		<LoD	
blank 5	0.27	0.02	<LoD		0.30	0.06	0.62	0.07			<LoD	
correction value	0.33		0.22		0.57		0.64		0.08		0.00	
LoD	0.06		0.07		0.15		0.15		0.26		0.27	
LoQ	0.16		0.19		0.38		0.40		0.67		0.66	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 46: Manganese concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**56**	4.11	**83**	5.78	**161**	21.98	**50**	4.50	**43**	0.72	**264**	8.00
-4.5	**61**	5.33	**72**	2.43	**166**	12.60	**44**	3.55	**51**	1.42	**232**	7.58
-3.5	**53**	3.31	**73**	3.99	**140**	4.32	**25**	1.99	**66**	2.70	**213**	4.75
-2.5	**48**	1.81	**80**	7.86	**100**	3.50	**47**	1.45	**32**	0.72	**262**	6.71
-1.5	**56**	7.06	**65**	9.03	**72**	3.70	**31**	1.32	**96**	1.48	**246**	6.14
-0.5	**62**	5.19	**85**	8.11	**76**	3.02	**45**	2.61	**62**	3.39	**253**	4.36
0.5	**72**	4.15	**34**	0.34	**68**	14.86	**30**	1.99	**281**	21.04	**364**	6.69
1.5	**226**	2.02	**56**	4.40	**68**	2.77	**33**	1.85	**319**	11.40	**83**	1.64
2.5	**4,615**	228.76	**71**	6.04	**71**	5.99	**146**	9.96	**759**	32.29	**29**	0.29
3.5	**1,885**	127.41	**55**	2.63	**74**	2.21	**194**	13.31	**1,501**	20.50	**83**	1.30
4.5	**4,137**	441.42	**55**	3.65	**63**	1.28	**56**	2.55	**2,784**	174.30	**36**	0.48
5.5	**9,542**	531.68	**48**	5.44	**66**	4.18	**19**	1.07	**4,649**	70.01	**956**	32.18
6.5	**1,047**	53.44	**57**	11.32	**70**	7.70	**20**	0.32	**7,194**	487.61	**56**	1.51
7.5	**229**	13.84	**42**	3.01	**86**	8.06	**43**	1.36	**6,020**	373.30	**2,912**	58.49
8.5	**1,085**	72.88	**70**	2.96	**67**	8.15	**125**	3.37	**5,837**	224.81	**48**	1.03
9.5	**5,215**	748.99	**42**	6.17	**60**	5.48	**71**	2.76	**8,276**	191.07	**5,361**	144.63
10.5	**3,287**	479.87	**83**	4.02	**43**	4.23	**79**	1.74	**58**	1.42	**29**	2.72
11.5	**2,909**	240.89	**671**	19.77	**47**	2.31	**86**	4.32	**84**	2.84	**34**	0.74
12.5	**5,622**	666.59	**3,701**	348.68	**58**	3.31	**58**	1.33	**64**	0.85	**31**	0.84
13.5	**486**	54.20	**7,295**	258.15	**1,175**	58.80	**62**	1.69	**50**	2.07	**38**	0.49
14.5	**2,859**	365.84	**9,202**	842.00	**4,224**	365.46	**111**	4.40	**70**	4.29	**34**	0.50
15.5	**7,885**	924.12	**5,529**	157.17	**8,020**	889.92	**170**	7.15	**59**	2.10	**46**	1.69
blank 1	1.07	0.11	1.99	0.74	1.15	0.02	2.65	0.10	0.92	0.05	1.98	0.19
blank 2	1.25	0.01	0.82	0.10	0.91	0.07	1.60	0.07	7.82	0.70	0.85	0.10
blank 3	1.07	0.07	0.78	0.08	2.05	0.23	5.86	0.32	2.50	0.13	<LoD	
blank 4	1.56	0.25	0.71	0.04	0.49	0.06	1.89	0.07	7.73	0.80	1.32	0.20
blank 5	2.13	0.25	3.35	0.23	0.80	0.13	3.30	0.19	2.28	0.11	1.33	0.11
correction value	1.42		1.53		1.08		3.06		4.25		1.10	
LoD	0.47		0.47		0.47		0.07		0.07		0.72	
LoQ	1.23		1.23		1.23		0.20		0.20		1.91	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**181**	6.24	**1,398**	31.61	**8**	0.99	<NWG	0.18	**32**	1.16	**57**	3.76
-4.5	**101**	2.54	**8**	1.10	**3**	0.64	<NWG	0.24	**12**	0.42	**5**	0.67
-3.5	**59**	1.50	**5**	0.16	**2**	0.81	<NWG	0.45	**16**	0.43	**13**	0.42
-2.5	**36**	1.06	**5**	0.48	**1**	0.85	<NWG	0.37	**11**	0.50	**4**	0.54
-1.5	**201**	4.12	**6**	0.12	<NWG	0.55	<NWG	0.28	**6**	0.34	**4**	0.40
-0.5	**15**	0.25	**2,051**	50.86	**35**	5.14	**2,441**	48.54	**19**	0.30	**625**	33.21
0.5	**24**	0.69	**14,407**	543.88	**2,609**	149.54	**10,653**	303.64	**175**	3.05	**8,017**	571.17
1.5	**16**	0.09	**10,579**	239.32	**2,146**	97.06	**7,526**	366.09	**4,863**	65.71	**3,810**	178.88
2.5	**66**	1.03	**923**	28.05	**89**	3.71	**4,172**	81.01	**58**	3.53	**177**	9.20
3.5	**109**	1.79	**271**	7.32	**63**	4.64	**619**	7.65	**950**	8.79	**78**	1.85
4.5	**128**	1.14	**1,028**	46.21	**93**	5.59	**1,749**	18.23	**327**	2.12	**63**	3.07
5.5	**128**	0.77	**2,640**	93.61	**75**	4.36	**1,685**	5.88	**95**	1.52	**48**	0.95
6.5	**196**	1.80	**2,204**	75.19	**81**	6.40	**1,467**	21.25	**46**	0.60	**36**	0.91
7.5	**210**	0.73	**5,169**	162.84	**85**	5.26	**1,240**	14.41	**40**	0.49	**34**	0.62
8.5	**78**	1.06	**7,378**	134.00	**77**	6.01	**875**	8.44	**38**	1.19	**34**	1.38
9.5	**47**	0.54	**4,245**	174.62	**75**	6.47	**1,161**	19.51	**44**	0.75	**34**	1.44
10.5	no sample**	no sample**	**2,294**	38.07	**107**	5.83	**12**	0.68	**41**	0.49	**30**	0.83
11.5	**165**	3.04	**4,935**	38.09	**105**	5.97	**20**	0.80	**36**	0.47	**28**	1.18
12.5	no sample**	no sample**	**4,878**	100.61	**157**	6.62	**92**	2.51	**35**	0.51	**28**	1.78
13.5	**60**	4.32	**7,186**	256.78	**205**	12.93	**98**	2.06	**6**	4.47	**31**	1.08
14.5	no sample**	no sample**	**8,773**	151.75	**201**	12.93	**159**	3.82	**66**	1.01	**11**	0.35
15.5	**83**	1.49	**10,530**	122.84	no sample**	no sample**	**328**	2.64	**41**	0.65	**40**	1.11
blank 1	2.26	0.02	1.78	0.02	22.88	1.53	28.58	0.51	1.58	0.13	1.04	0.22
blank 2	6.64	0.06	2.51	0.05	18.60	1.00	28.91	0.97	1.94	0.11	0.85	0.13
blank 3	1.73	0.02	3.90	0.02	19.31	0.80	32.08	0.65	2.10	0.15	9.32	0.27
blank 4	1.80	0.03	4.62	0.35	14.61	0.61	30.20	0.96	7.69	0.40	3.72	0.20
blank 5	2.41	0.06	9.09	0.20	12.50	0.75	29.34	0.47	5.54	0.25	1.50	0.17
correction value	2.97		4.38		17.58		29.82		3.02		3.28	
LoD	0.31		0.31		0.31		1.08		1.08		1.07	
LoQ	0.89		0.89		0.86		2.92		2.92		2.26	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 47: Manganese concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**171**	4.09	**122**	3.69	**246**	9.89	**562**	26.07	**389**	31.18	**385**	7.47
-4.5	**249**	5.92	**238**	13.50	**362**	18.83	**599**	24.03	**272**	12.07	**266**	4.06
-3.5	**217**	9.39	**279**	12.96	**285**	10.48	**894**	67.08	**434**	22.71	**399**	7.97
-2.5	**220**	5.61	**294**	14.10	**302**	4.81	**754**	21.15	**448**	22.02	**462**	12.60
-1.5	**216**	8.01	**292**	12.36	**364**	9.44	**567**	11.80	**421**	25.46	**407**	5.50
-0.5	**230**	14.68	**469**	12.67	**608**	32.11	**516**	10.50	**366**	10.27	**355**	6.64
0.5	**760**	17.61	**640**	22.99	**579**	37.34	**554**	13.13	**754**	38.87	**463**	7.68
1.5	**1,471**	60.51	**750**	18.95	**766**	20.19	**699**	20.95	**569**	15.36	**615**	5.41
2.5	**1,133**	47.66	**721**	33.18	**761**	19.31	no sample ***	no sample ***	**632**	21.77	**704**	36.97
3.5	**1,120**	35.99	**857**	33.23	**838**	23.53	no sample ***	no sample ***	**693**	10.42	**831**	28.36
4.5	**1,100**	62.52	**968**	20.07	**1,022**	15.70	**1,166**	32.87	**877**	28.51	**1,026**	48.12
5.5	**1,081**	53.91	**983**	34.80	**1,034**	38.49	**1,006**	25.19	**982**	37.36	**969**	23.77
6.5	**1,355**	119.48	**1,413**	33.56	**1,435**	36.25	**829**	21.16	**862**	36.22	**966**	27.65
7.5	**1,335**	97.82	**1,873**	79.90	**1,275**	48.41	**519**	2.93	**751**	22.00	**974**	56.58
8.5	**1,328**	43.92	**1,956**	136.66	**1,201**	48.11	**527**	9.43	**879**	29.27	**1,074**	29.38
9.5	**1,238**	85.23	**2,032**	105.38	**1,983**	64.34	**544**	13.59	**795**	19.18	**1,198**	27.51
10.5	**1,561**	73.43	**1,814**	69.30	**2,025**	131.04	**530**	15.72	**771**	27.82	**1,068**	35.00
11.5	**1,428**	91.23	**1,209**	27.70	**1,967**	131.23	**709**	39.99	**880**	98.91	**1,158**	78.44
12.5	**1,287**	85.55	**1,260**	53.45	**1,618**	73.26	no sample ***	no sample ***	**940**	16.95	**1,152**	68.96
13.5	**1,342**	87.10	**1,380**	39.69	**1,387**	48.28	**583**	6.66	**952**	27.89	**1,148**	91.05
14.5	**1,552**	35.56	**1,190**	47.15	**1,226**	92.66	no sample ***	no sample ***	**1,018**	34.47	**896**	44.77
15.5	**1,134**	50.34	**1,154**	53.19	**1,438**	90.03	no sample ***	no sample ***	**987**	33.81	**1,094**	17.91
blank 1	0.17	0.00	<LoD		<LoD		<LoD		<LoD		0.22	0.01
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		0.25	0.02
blank 3	<LoD		0.29	0.02	<LoD		<LoD		<LoD		0.31	0.02
blank 4	<LoD		0.30	0.01	<LoD		<LoD		0.80	0.03	0.57	0.02
blank 5	0.17	0.00	0.59	0.02	<LoD						1.06	0.03
correction value	0.07		0.24		0.00		0.00		0.16		0.48	
LoD	0.12		0.12		0.12		0.68		0.68		0.06	
LoQ	0.32		0.32		0.32		2.04		2.04		0.16	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**377**	4.73	**1,083**	16.49	**708**	25.49	**1,313**	60.51	**1,384**	38.04	**892**	30.03
-4.5	**507**	6.77	**1,086**	19.88	**769**	30.52	**1,018**	23.26	**1,433**	89.24	**995**	22.36
-3.5	**479**	8.48	**1,138**	43.59	**794**	32.82	**1,251**	29.15	**1,718**	79.69	**950**	25.32
-2.5	**411**	7.02	**1,148**	38.98	**592**	48.56	**1,290**	28.54	**1,315**	29.63	**939**	40.52
-1.5	**400**	10.36	**1,115**	20.26	**645**	39.01	**1,462**	57.40	**1,186**	44.23	**944**	14.45
-0.5	**415**	2.75	**1,075**	29.62	**739**	46.46	**1,419**	56.96	**1,167**	48.85	**961**	22.66
0.5	**478**	4.65	**977**	36.85	**1,098**	21.26	**1,056**	51.79	**1,321**	62.69	**935**	16.24
1.5	**437**	5.57	**703**	7.98	**848**	44.33	**870**	58.35	**1,181**	40.23	**744**	16.63
2.5	**398**	2.48	**598**	10.81	**652**	27.91	**749**	24.02	**1,146**	33.02	**647**	36.04
3.5	**405**	4.11	**574**	12.45	**419**	14.50	**632**	26.69	**877**	42.71	**535**	28.84
4.5	**435**	4.42	**599**	7.75	**406**	20.25	**483**	12.49	**755**	54.05	**565**	4.26
5.5	**453**	31.77	**665**	11.38	**466**	16.40	**423**	20.03	**660**	25.65	**520**	26.06
6.5	**506**	6.08	**711**	11.92	**487**	8.84	**383**	13.38	no sample**	no sample**	**434**	5.75
7.5	**506**	2.36	**741**	8.14	**471**	45.83	**399**	18.43	no sample**	no sample**	**432**	7.11
8.5	**569**	4.39	**756**	10.61	**653**	27.29	**384**	15.91	no sample**	no sample**	**396**	5.90
9.5	**569**	4.20	**1,021**	22.94	**507**	4.58	**420**	21.45	no sample**	no sample**	**382**	5.53
10.5	**589**	4.60	**1,015**	35.05	**620**	16.54	**580**	18.75	no sample**	no sample**	**413**	13.11
11.5	**620**	4.68	**989**	30.22	**567**	19.29	**663**	23.00	no sample**	no sample**	**454**	9.66
12.5	**631**	4.74	**1,046**	28.07	**640**	16.04	**5**	2.06	no sample**	no sample**	no sample**	no sample**
13.5	**641**	7.86	**1,016**	25.30	**683**	63.59	no sample ***	no sample ***	no sample**	no sample**	**541**	14.73
14.5	**666**	9.62	**1,001**	26.17	**696**	42.31	no sample ***	no sample ***	no sample**	no sample**	**585**	17.86
15.5	**678**	6.43	**974**	35.57	**666**	48.40	no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	0.17	0.01	0.08	0.00	0.36	0.07	0.19	0.03	1.23	7.69	0.36	0.15
blank 2	<LoD		0.09	0.01	0.27	0.04	0.20	0.04	0.11	36.98	<LoD	
blank 3	0.10	0.01	0.10	0.01	0.36	0.08	0.19	0.08	0.11	55.99	<LoD	
blank 4	0.14	0.02	0.10	0.01	0.33	0.09	<LoD		0.10	25.43	<LoD	
blank 5	0.17	0.02	0.13	0.01	0.36	0.06	0.24	0.04	0.11	53.30	<LoD	
correction value	0.12		0.10		0.33		0.16		0.49		0.07	
LoD	0.07		0.07		0.15		0.15		0.26		0.27	
LoQ	0.19		0.19		0.38		0.40		0.67		0.66	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 48: Nickel concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. Identified outliers are grayed out. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**2.49**	0.19	**2.25**	0.34	**7.08**	0.59	**3.37**	0.21	**9.93**	0.55	**2.25**	0.17
-4.5	**3.58**	0.24	**4.44**	0.34	**12.26**	0.19	**1.09**	0.10	**10.16**	0.93	**2.28**	0.21
-3.5	**2.84**	0.19	**5.45**	0.25	**11.58**	0.55	**1.72**	0.19	**10.66**	0.33	**2.57**	0.21
-2.5	**2.57**	0.14	**5.20**	0.23	**9.58**	0.10	**1.91**	0.17	**5.45**	0.34	**2.36**	0.12
-1.5	**4.82**	0.35	**6.47**	0.17	**12.37**	1.02	**1.79**	0.12	**4.37**	0.21	**2.66**	0.15
-0.5	**3.24**	0.27	**6.07**	0.38	**11.26**	0.78	**2.18**	0.22	**9.87**	0.94	**3.93**	0.28
0.5	**4.34**	0.13	**6.76**	0.31	**8.61**	0.69	**2.72**	0.23	**6.65**	0.36	**4.34**	0.25
1.5	**16.65**	0.44	**3.70**	0.28	**3.51**	1.09	**2.42**	0.16	**12.64**	0.80	**1.82**	0.09
2.5	**47.64**	0.35	**3.05**	0.05	**3.08**	0.19	**9.43**	0.52	**11.57**	0.81	**1.71**	0.20
3.5	**10.63**	1.13	**2.57**	0.17	**1.70**	0.35	**3.52**	0.17	**5.65**	0.34	**1.28**	0.11
4.5	**38.68**	1.98	**2.77**	0.16	**1.56**	0.09	**3.67**	0.15	**3.93**	0.40	**1.89**	0.16
5.5	**107.66**	3.40	**2.79**	0.34	**1.75**	0.16	**2.55**	0.12	**2.15**	0.18	**0.84**	0.07
6.5	**2.34**	0.29	**2.07**	0.14	**1.16**	0.34	**1.38**	0.08	**2.17**	0.16	**0.69**	0.04
7.5	**2.17**	0.06	**3.03**	0.04	**0.89**	0.21	**1.40**	0.09	**2.23**	0.31	**0.41**	0.03
8.5	**18.49**	3.85	**3.03**	0.30	**1.10**	0.13	**1.22**	0.12	**1.49**	0.12	**0.34**	0.04
9.5	**48.50**	2.26	**11.04**	0.99	**1.50**	0.22	**0.93**	0.07	**2.00**	0.19	**0.27**	0.04
10.5	**39.42**	2.55	**12.32**	2.57	**0.70**	0.23	**0.59**	0.15	**1.34**	0.19	**0.64**	0.07
11.5	**13.92**	1.18	**31.73**	0.75	**0.44**	0.07	**15.60**	0.37	**1.45**	0.10	**0.37**	0.05
12.5	**76.64**	2.28	**72.15**	5.64	**23.58**	1.99	**0.59**	0.16	**0.99**	0.08	**0.31**	0.04
13.5	**5.65**	0.47	**107.63**	1.04	**52.27**	3.88	**0.68**	0.06	**1.14**	0.11	**0.27**	0.02
14.5	**52.44**	0.76	**200.12**	4.77	**185.32**	5.86	**0.55**	0.08	**0.75**	0.08	**0.17**	0.03
15.5	**112.27**	3.69	**130.19**	3.16	**258.31**	5.51	**0.71**	0.06	**0.79**	0.14	**0.27**	0.04
blank 1	0.23	0.02	0.15	0.06	2.51	0.35	0.19	0.04	0.99	0.14	0.11	0.01
blank 2	0.12	0.03	<LoD		1.25	0.05	0.11	0.05	0.10	0.04	0.07	0.00
blank 3	2.64	0.22	0.83	0.10	1.33	0.07	0.17	0.04	0.25	0.05	0.39	0.02
blank 4	0.85	0.06	0.18	0.03	0.97	0.13	0.15	0.03	0.07	0.02	0.17	0.02
blank 5	0.23	0.05	0.07	0.03	1.79	0.09	0.72	0.10	0.67	0.06	0.08	0.00
correction value	0.82		0.24		1.57		0.27		0.41		0.16	
LoD	0.04		0.04		0.04		0.02		0.02		0.01	
LoQ	0.10		0.10		0.10		0.06		0.06		0.03	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**15.85**	0.38	**18.18**	0.26	**24.21**	1.51	**47.95**	1.81	**58.97**	2.51	**43.75**	1.77
-4.5	**16.40**	0.41	**18.23**	0.57	**25.43**	1.19	**59.76**	1.76	**68.28**	1.72	**39.52**	1.17
-3.5	**13.88**	0.29	**17.53**	0.44	**26.40**	0.84	**64.79**	2.01	**79.67**	2.75	**970.43**	41.94
-2.5	**11.98**	0.37	**16.84**	0.44	**32.33**	2.01	**40.70**	3.52	**91.57**	1.96	**79.35**	0.94
-1.5	**12.12**	0.21	**16.93**	0.44	**23.05**	1.31	**51.90**	1.71	**91.43**	5.63	**56.50**	1.96
-0.5	**12.72**	0.23	**16.75**	0.53	**24.51**	1.70	**50.94**	1.08	**98.37**	5.10	**40.38**	1.52
0.5	**14.43**	0.18	**14.91**	0.36	**8.36**	0.82	**12.96**	0.74	**55.93**	1.49	**24.02**	0.56
1.5	**7.85**	0.08	**4.35**	0.10	**0.32**	0.05	<LoD		**5.61**	0.31	**12.70**	0.70
2.5	**3.94**	0.03	**0.79**	0.02	0.09	0.04	<LoD		**0.53**	0.09	**15.00**	0.56
3.5	**3.11**	0.02	**0.38**	0.02	**0.21**	0.09	<LoD		<LoD		**5.89**	0.35
4.5	**1.96**	0.03	0.31	0.01	0.19	0.09	<LoD		0.20	0.04	**0.68**	0.11
5.5	**1.40**	0.02	0.31	0.01	**0.26**	0.08	<LoD		0.13	0.05	**0.37**	0.04
6.5	**1.19**	0.03	**0.40**	0.02	no sample *	no sample *	<LoD		0.15	0.06	**0.33**	0.07
7.5	**1.05**	0.01	0.27	0.01	no sample *	no sample *	<LoD		<LoD		**0.40**	0.05
8.5	**0.99**	0.03	0.27	0.01	no sample *	no sample *	<LoD		<LoD		**0.66**	0.12
9.5	**0.84**	0.03	0.29	0.02	<LoD		**0.96**	0.28	<LoD		**0.49**	0.03
10.5	**0.73**	0.03	0.22	0.01	0.10	0.08	<LoD		<LoD		**0.37**	0.07
11.5	**0.65**	0.01	0.31	0.02	0.19	0.02	<LoD		**0.57**	0.02	**0.44**	0.03
12.5	**0.60**	0.02	**0.34**	0.02	0.07	0.07	<LoD		0.12	0.05	**0.34**	0.07
13.5	**0.75**	0.01	**0.37**	0.03	<LoD		<LoD		0.18	0.03	**0.35**	0.08
14.5	**0.55**	0.02	**0.36**	0.02	<LoD		<LoD		0.12	0.06	no sample **	no sample **
15.5	**0.59**	0.01	0.20	0.02	<LoD		<LoD		<LoD		0.25	0.09
blank 1	<LoD		<LoD		0.45	0.04	1.01	0.11	0.27	0.07	<LoD	
blank 2	<LoD		<LoD		0.72	0.06	0.53	0.08	0.48	0.10	<LoD	
blank 3	<LoD		<LoD		0.46	0.04	1.79	0.15	1.36	0.04	0.30	0.07
blank 4	<LoD		<LoD		0.78	0.02	2.42	0.20	0.13	0.03	<LoD	
blank 5	<LoD		<LoD		0.63	0.05	4.14	0.27	0.12	0.03	0.16	0.05
correction value	0.00		0.00		0.61		1.98		0.47		0.09	
LoD	0.14		0.14		0.07		0.09		0.09		0.13	
LoQ	0.33		0.33		0.20		0.21		0.21		0.32	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 49: Nickel concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**4.37**	0.21	**7.63**	0.28	**19.05**	0.71	**4.02**	0.61	**7.59**	0.18	**5.13**	0.11
-4.5	**4.14**	0.37	**6.29**	0.36	**17.27**	0.55	**1.69**	0.11	**14.68**	0.56	**8.18**	0.11
-3.5	**4.86**	0.30	**5.88**	0.26	**15.70**	1.25	**2.11**	0.18	**13.75**	0.92	**8.34**	0.19
-2.5	**5.66**	0.31	**6.53**	0.28	**14.94**	1.15	**2.34**	0.14	**13.19**	0.54	**9.01**	0.10
-1.5	**5.17**	0.34	**5.89**	0.32	**15.87**	1.10	**2.58**	0.03	**10.40**	0.60	**9.82**	0.22
-0.5	**4.74**	0.26	**8.53**	0.38	**12.69**	0.79	**2.78**	0.17	**7.29**	0.42	**10.83**	0.18
0.5	**13.33**	0.60	**53.08**	1.06	**32.83**	1.04	**1.58**	0.10	**11.70**	0.80	**16.54**	0.20
1.5	**118.40**	8.74	**125.50**	3.77	**64.03**	2.12	**4.41**	0.24	**33.30**	0.54	**6.05**	0.07
2.5	**204.13**	10.06	**164.95**	10.12	**45.51**	0.87	**22.76**	0.48	**53.25**	2.04	**7.01**	0.45
3.5	**168.27**	7.18	**134.35**	4.87	**46.27**	1.91	**96.75**	2.24	**37.81**	0.88	**4.61**	0.07
4.5	**204.50**	5.23	**32.44**	1.31	**25.29**	1.35	**91.64**	2.90	**18.22**	0.64	**4.12**	0.06
5.5	**224.48**	6.74	**13.53**	0.61	**8.95**	0.21	**23.53**	0.99	**9.97**	1.48	**2.34**	0.06
6.5	**118.17**	6.81	**9.66**	0.48	**8.50**	0.81	no sample ***	no sample ***	**7.91**	0.37	**2.24**	0.05
7.5	**62.33**	3.52	**7.15**	0.49	**7.21**	0.46	no sample ***	no sample ***	**4.36**	0.20	**1.90**	0.04
8.5	**143.97**	3.48	**17.98**	0.46	**6.29**	0.31	no sample ***	no sample ***	**3.29**	0.17	**1.12**	0.01
9.5	**227.39**	4.55	**95.02**	4.25	**24.99**	0.98	no sample ***	no sample ***	**3.02**	0.16	**1.04**	0.01
10.5	**262.42**	18.60	**273.28**	7.98	**39.16**	2.23	**3.48**	0.25	**10.67**	0.36	**1.17**	0.03
11.5	**304.69**	20.72	**423.24**	17.74	**67.76**	1.49	**3.64**	0.11	**8.80**	0.24	**0.76**	0.02
12.5	**315.55**	24.80	**405.99**	7.88	**271.43**	8.98	**3.40**	0.19	**4.36**	0.28	**0.71**	0.03
13.5	**381.78**	21.47	**349.85**	14.45	**396.42**	14.04	**2.70**	0.19	**6.57**	0.27	**0.59**	0.02
14.5	**384.04**	15.21	**290.85**	6.10	**337.30**	8.77	**2.61**	0.20	**2.93**	0.15	**0.65**	0.01
15.5	**400.59**	21.46	**322.87**	13.27	**326.86**	19.45	no sample ***	no sample ***	**2.62**	0.25	**0.60**	0.03
blank 1	1.35	0.08	0.92	0.04	1.79	0.08	0.35	0.08	0.08	0.03	0.11	0.01
blank 2	1.10	0.09	0.57	0.03	1.63	0.05	0.69	0.08	0.75	0.09	0.07	0.01
blank 3	1.22	0.11	0.69	0.06	1.20	0.10	0.12	0.05	<LoD		0.10	0.01
blank 4	1.24	0.04	0.52	0.05	1.71	0.07	0.08	0.04	<LoD		0.08	0.00
blank 5	1.74	0.11	0.33	0.02	1.16	0.08	0.09	0.03			0.20	0.01
correction value	1.33		0.61		1.50		0.26		0.17		0.11	
LoD	0.07		0.07		0.07		0.08		0.08		0.03	
LoQ	0.16		0.16		0.16		0.23		0.23		0.08	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**21.21**	0.36	**19.96**	0.20	**27.96**	0.93	**53.94**	3.60	**60.58**	1.68	**37.88**	1.56
-4.5	**18.82**	0.48	**18.90**	0.44	**20.01**	1.06	**51.90**	2.40	**63.20**	1.43	**34.73**	0.39
-3.5	**18.53**	0.34	**18.92**	0.10	**26.08**	1.25	**46.54**	1.41	**79.25**	4.31	**922.48**	21.89
-2.5	**20.18**	0.40	**18.62**	0.21	**21.44**	0.92	**47.78**	2.38	**86.56**	3.85	**78.94**	2.63
-1.5	**20.72**	0.46	**18.64**	0.20	**22.91**	0.66	**49.59**	1.84	**69.04**	2.99	**57.49**	2.32
-0.5	**16.83**	0.34	**18.35**	0.11	**20.96**	0.58	**41.64**	1.32	**64.01**	2.93	**40.12**	0.68
0.5	**18.74**	0.42	**16.46**	0.08	**7.25**	0.32	**13.05**	1.02	**54.96**	0.86	**23.42**	0.21
1.5	**13.83**	0.16	**4.91**	0.08	**0.53**	0.04	**0.37**	0.08	**5.42**	0.30	**13.16**	0.78
2.5	**5.75**	0.15	**0.54**	0.03	**0.24**	0.07	0.09	0.10	**0.79**	0.10	**16.12**	0.53
3.5	**4.04**	0.11	**0.29**	0.02	0.10	0.07	**0.26**	0.12	0.11	0.03	**6.86**	0.18
4.5	**3.49**	0.13	**0.25**	0.01	0.17	0.05	0.19	0.17	**0.38**	0.05	**1.00**	0.02
5.5	**2.26**	0.06	**0.23**	0.01	0.16	0.05	**0.28**	0.08	0.19	0.04	no sample **	no sample **
6.5	**1.69**	0.03	**0.39**	0.01	no sample *	no sample *	**0.33**	0.05	**0.54**	0.06	**0.42**	0.11
7.5	**1.21**	0.02	**0.29**	0.02	no sample *	no sample *	0.15	0.07	**0.24**	0.04	**0.43**	0.29
8.5	**1.81**	0.02	**0.26**	0.01	no sample *	no sample *	0.18	0.09	**0.29**	0.02	0.35	0.05
9.5	**1.59**	0.05	**0.23**	0.02	**0.18**	0.08	**0.22**	0.11	**0.21**	0.04	0.49	0.11
10.5	**1.00**	0.01	**0.27**	0.03	**0.29**	0.08	**0.43**	0.09	**0.48**	0.06	0.50	0.08
11.5	**0.95**	0.05	**0.24**	0.02	**0.21**	0.09	**0.35**	0.06	**0.52**	0.03	no sample **	no sample **
12.5	**0.85**	0.04	**0.19**	0.01	**0.19**	0.08	**0.27**	0.11	**0.25**	0.06	no sample **	no sample **
13.5	**0.92**	0.02	**0.18**	0.01	**0.19**	0.12	**0.27**	0.04	**0.27**	0.04	no sample **	no sample **
14.5	**0.72**	0.02	**0.19**	0.01	**1.13**	0.18	**0.44**	0.10	0.20	0.03	no sample **	no sample **
15.5	**0.80**	0.02	**0.38**	0.03	**1.37**	0.10	**0.22**	0.07	**0.33**	0.03	no sample **	no sample **
blank 1	0.08	0.01	0.07	0.00	0.37	0.04	0.16	0.06	0.25	0.04	<LoD	
blank 2	0.09	0.01	0.20	0.02	0.30	0.05	0.15	0.07	0.69	0.11	<LoD	
blank 3	0.09	0.01	0.11	0.01	0.38	0.03	0.08	0.02	0.27	0.07	0.30	0.07
blank 4	0.10	0.01	0.36	0.01	0.31	0.07	0.41	0.06	<LoD		<LoD	
blank 5	0.13	0.01	0.07	0.01	0.39	0.02	0.25	0.06			0.16	0.05
correction value	0.10		0.16		0.35		0.21		0.24		0.09	
LoD	0.03		0.01		0.07		0.07		0.09		0.13	
LoQ	0.08		0.03		0.18		0.20		0.21		0.32	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 50: Nickel concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**6.59**	0.45	**5.10**	0.18	**9.07**	1.33	**5.65**	0.60	**3.53**	0.15	**5.14**	0.10
-4.5	**5.62**	0.56	**6.21**	0.32	**13.53**	1.08	**5.64**	0.34	**4.75**	0.35	**5.85**	0.11
-3.5	**5.71**	0.23	**8.40**	0.33	**14.07**	1.21	**3.09**	0.21	**7.61**	0.44	**6.15**	0.11
-2.5	**5.35**	0.28	**9.30**	0.69	**12.34**	1.03	**4.67**	0.12	**4.73**	0.20	**7.66**	0.22
-1.5	**6.68**	0.61	**9.09**	0.22	**17.48**	0.60	**2.91**	0.12	**11.87**	0.27	**7.38**	0.20
-0.5	**7.37**	0.30	**8.76**	0.24	**10.93**	0.60	**3.68**	0.21	**9.06**	0.54	**10.20**	0.28
0.5	**6.58**	0.59	**3.60**	0.45	**7.34**	0.26	**2.73**	0.28	**9.45**	0.88	**7.81**	0.13
1.5	**11.47**	1.05	**2.85**	0.27	**5.69**	0.39	**2.98**	0.26	**7.05**	0.30	**3.42**	0.07
2.5	**94.20**	3.25	**2.92**	0.10	**3.96**	0.10	**4.87**	0.39	**13.83**	0.48	**1.91**	0.07
3.5	**37.51**	1.95	**2.36**	0.07	**4.03**	0.05	**5.08**	0.40	**24.16**	0.45	**2.23**	0.08
4.5	**70.41**	4.50	**1.94**	0.24	**3.33**	0.04	**2.20**	0.16	**43.45**	2.80	**0.46**	0.01
5.5	**171.31**	15.34	**1.84**	0.19	**3.13**	0.18	**1.39**	0.06	**72.38**	0.94	**2.26**	0.06
6.5	**21.57**	0.27	**2.06**	0.13	**3.41**	0.48	**1.31**	0.05	**113.74**	6.93	**0.60**	0.03
7.5	**5.36**	0.38	**1.77**	0.15	**4.31**	0.22	**1.31**	0.08	**93.14**	5.71	**1.60**	0.04
8.5	**22.64**	2.64	**2.65**	0.31	**2.94**	0.15	**2.46**	0.22	**90.21**	3.92	**0.42**	0.02
9.5	**108.51**	4.26	**1.88**	0.40	**2.55**	0.07	**1.55**	0.13	**127.64**	3.89	**1.41**	0.04
10.5	**65.79**	8.32	**2.65**	0.35	**1.97**	0.27	**1.69**	0.06	**2.60**	0.25	**1.05**	0.02
11.5	**56.73**	0.73	**16.05**	0.31	**2.08**	0.25	**1.79**	0.20	**2.44**	0.16	**0.90**	0.05
12.5	**109.08**	7.56	**76.23**	1.59	**2.68**	0.07	**1.38**	0.12	**1.82**	0.18	**0.84**	0.03
13.5	**10.77**	0.48	**131.59**	3.79	**31.11**	3.10	**1.37**	0.12	**1.54**	0.11	**0.71**	0.03
14.5	**52.09**	1.84	**196.56**	13.98	**97.89**	5.00	**2.24**	0.13	**2.45**	0.22	**0.64**	0.02
15.5	**154.71**	14.97	**106.27**	2.93	**170.57**	9.31	**3.36**	0.10	**1.76**	0.13	**0.68**	0.02
blank 1	0.05	0.02	0.07	0.01	0.08	0.03	0.11	0.03	0.16	0.05	0.11	0.08
blank 2	0.15	0.02	<LoD		0.10	0.03	0.15	0.05	0.31	0.07	<LoD	
blank 3	0.16	0.05	0.06	0.03	0.31	0.04	0.45	0.05	0.40	0.05	0.14	0.06
blank 4	0.23	0.06	<LoD		<LoD		0.14	0.02	0.43	0.05	0.16	0.04
blank 5	0.40	0.05	0.28	0.04	0.05	0.02	0.25	0.04	0.17	0.06	<LoD	
correction value	0.20		0.08		0.11		0.22		0.30		0.08	
LoD	0.04		0.04		0.04		0.02		0.02		0.07	
LoQ	0.10		0.10		0.10		0.06		0.06		0.18	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**5.68**	0.11	**7.67**	0.08	**3.34**	0.27	**2.70**	0.15	**26.41**	1.72	**2.09**	0.17
-4.5	**4.83**	0.05	**6.03**	0.09	**4.02**	0.16	**4.44**	0.26	**13.65**	0.84	**2.60**	0.24
-3.5	**4.53**	0.07	**5.55**	0.04	**3.38**	0.19	**5.21**	0.29	**6.51**	0.27	**2.52**	0.20
-2.5	**3.80**	0.09	**5.02**	0.08	**3.70**	0.30	**5.93**	0.29	**4.95**	0.21	**2.72**	0.26
-1.5	**3.93**	0.08	**4.56**	0.13	**3.17**	0.33	**6.04**	0.24	**4.42**	0.40	**3.00**	0.18
-0.5	**4.04**	0.04	**3.57**	0.09	**3.23**	0.40	**4.96**	0.25	**3.98**	0.14	**4.48**	0.34
0.5	**5.45**	0.12	**1.10**	0.03	**2.03**	0.09	**3.40**	0.31	**4.60**	0.43	**2.37**	0.28
1.5	**3.92**	0.05	**0.52**	0.02	**1.02**	0.16	**2.00**	0.05	**3.80**	0.19	**1.21**	0.13
2.5	**2.36**	0.06	**0.37**	0.02	**0.72**	0.09	**1.85**	0.14	**1.72**	0.17	**0.98**	0.10
3.5	**1.80**	0.05	**0.34**	0.01	**0.58**	0.11	**1.16**	0.09	**1.55**	0.12	**0.77**	0.07
4.5	**1.44**	0.04	0.33	0.01	**0.74**	0.11	**2.30**	0.12	**1.12**	0.11	**0.61**	0.05
5.5	**1.35**	0.02	0.30	0.01	**0.50**	0.10	**0.87**	0.07	**0.87**	0.07	**0.71**	0.10
6.5	**1.16**	0.01	0.30	0.01	**0.42**	0.14	**1.23**	0.09	**0.78**	0.08	**0.67**	0.08
7.5	**0.98**	0.02	0.32	0.02	**0.56**	0.08	**4.01**	0.15	**0.46**	0.06	**0.42**	0.03
8.5	**0.92**	0.04	**0.33**	0.02	**0.54**	0.13	**2.55**	0.24	**0.52**	0.07	**0.40**	0.08
9.5	**1.02**	0.04	0.32	0.02	**0.49**	0.10	**0.79**	0.07	**0.39**	0.03	**0.55**	0.12
10.5	no sample**	no sample**	0.30	0.01	**0.42**	0.06	**1.12**	0.08	**0.37**	0.05	**0.48**	0.05
11.5	**0.69**	0.02	0.31	0.01	**0.31**	0.14	**0.40**	0.03	**0.27**	0.08	**0.41**	0.05
12.5	no sample**	no sample**	0.30	0.01	**0.42**	0.07	**0.39**	0.03	**0.51**	0.06	**0.45**	0.06
13.5	**0.61**	0.02	**12.37**	0.30	**0.43**	0.13	**0.39**	0.04	<LoD		0.20	0.07
14.5	no sample**	no sample**	**2.79**	0.03	0.17	0.10	**0.40**	0.17	**0.48**	0.07	0.26	0.05
15.5	**0.60**	0.01	0.37	0.03	no sample**	no sample**	**0.34**	0.09	**0.29**	0.05	**0.32**	0.05
blank 1	<LoD		<LoD		1.07	0.16	0.12	0.02	0.31	0.04	0.19	0.02
blank 2	<LoD		<LoD		0.77	0.03	0.10	0.04	0.13	0.03	0.09	0.03
blank 3	<LoD		<LoD		0.47	0.03	<LoD		0.10	0.03	0.14	0.03
blank 4	<LoD		<LoD		0.43	0.10	<LoD		0.15	0.03	0.15	0.04
blank 5	<LoD		<LoD		0.37	0.11	<LoD		0.52	0.11	0.13	0.02
correction value	0.00		0.00		0.51		0.04		0.32		0.14	
LoD	0.14		0.14		0.07		0.09		0.09		0.13	
LoQ	0.33		0.33		0.20		0.21		0.21		0.32	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 51: Nickel concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**7.50**	0.38	**4.86**	0.27	**11.75**	0.57	**8.25**	0.68	**21.32**	1.74	**4.77**	0.10
-4.5	**10.18**	0.29	**13.47**	0.82	**20.25**	1.09	**5.62**	0.46	**14.83**	0.95	**3.69**	0.05
-3.5	**8.57**	0.30	**14.65**	0.62	**14.59**	1.00	**8.34**	0.74	**24.24**	0.98	**6.14**	0.19
-2.5	**9.02**	0.48	**15.69**	0.66	**14.36**	0.36	**7.61**	0.19	**25.78**	1.13	**7.52**	0.22
-1.5	**8.79**	0.31	**13.77**	0.55	**16.08**	0.56	**5.48**	0.14	**24.84**	1.59	**6.86**	0.13
-0.5	**9.34**	0.23	**14.70**	0.54	**17.49**	1.00	**5.46**	0.14	**21.77**	1.14	**7.88**	0.17
0.5	**17.47**	0.49	**35.42**	1.43	**30.96**	1.22	**6.12**	0.42	**35.38**	1.21	**9.27**	0.21
1.5	**118.78**	5.18	**34.47**	0.80	**35.49**	1.04	**9.88**	0.18	**34.41**	0.68	**4.17**	0.04
2.5	**218.19**	10.04	**18.15**	1.23	**13.37**	0.70	no sample ***	no sample ***	**44.98**	1.71	**3.11**	0.15
3.5	**288.67**	8.99	**6.86**	0.21	**7.35**	0.18	no sample ***	no sample ***	**68.86**	1.43	**2.83**	0.07
4.5	**401.38**	25.10	**4.31**	0.19	**5.45**	0.36	**18.93**	0.62	**125.02**	3.61	**2.94**	0.04
5.5	**354.79**	17.29	**2.93**	0.10	**4.61**	0.37	**5.14**	0.08	**172.63**	6.95	**2.12**	0.03
6.5	**348.96**	28.82	**16.01**	0.65	**5.22**	0.19	**6.82**	0.17	**168.09**	5.21	**1.61**	0.06
7.5	**364.96**	27.77	**4.72**	0.41	**4.33**	0.23	**10.11**	0.19	**149.20**	4.28	**1.25**	0.06
8.5	**350.94**	8.88	**3.64**	0.29	**3.50**	0.28	**71.52**	1.35	**183.42**	6.96	**1.21**	0.05
9.5	**360.34**	19.02	**4.11**	0.36	**14.24**	0.46	**72.73**	1.67	**175.99**	4.95	**1.10**	0.05
10.5	**441.19**	24.60	**8.74**	0.54	**14.19**	0.82	**86.63**	2.69	**142.25**	4.83	**0.87**	0.03
11.5	**454.21**	27.86	**27.73**	1.14	**37.46**	2.62	**85.30**	4.39	**138.39**	14.05	**0.93**	0.06
12.5	**367.63**	28.12	**92.92**	3.87	**124.72**	6.41	no sample ***	no sample ***	**179.04**	3.94	**0.87**	0.06
13.5	**486.97**	30.30	**183.41**	6.35	**223.07**	9.30	**49.75**	1.02	**194.07**	5.02	**0.79**	0.06
14.5	**457.64**	13.53	**221.10**	10.03	**230.98**	18.82	no sample ***	no sample ***	**215.75**	5.64	**0.56**	0.02
15.5	**372.54**	16.89	**248.09**	13.24	**320.25**	20.29	no sample ***	no sample ***	**220.10**	7.66	**0.67**	0.03
blank 1	2.14	0.14	0.17	0.03	0.38	0.06	0.16	0.05	0.20	0.06	0.06	0.00
blank 2	1.00	0.04	0.33	0.07	0.14	0.03	0.22	0.03	0.27	0.08	0.08	0.01
blank 3	0.96	0.06	0.68	0.07	0.13	0.04	0.28	0.07	0.35	0.09	0.14	0.02
blank 4	0.91	0.05	0.95	0.10	0.17	0.02	0.47	0.06	0.33	0.07	0.08	0.01
blank 5	0.95	0.06	1.49	0.10	0.09	0.01					0.08	0.01
correction value	1.19		0.72		0.18		0.23		0.23		0.09	
LoD	0.07		0.07		0.07		0.08		0.08		0.03	
LoQ	0.16		0.16		0.16		0.23		0.23		0.08	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**4.04**	0.09	**8.14**	0.16	**2.16**	0.19	**1.58**	0.12	**26.73**	1.09	**1.76**	0.11
-4.5	**5.25**	0.10	**6.82**	0.08	**3.12**	0.15	**1.94**	0.09	**9.36**	0.89	**2.60**	0.05
-3.5	**5.05**	0.10	**6.16**	0.04	**3.19**	0.20	**2.54**	0.25	**5.68**	0.49	**2.47**	0.21
-2.5	**4.11**	0.09	**5.61**	0.05	**2.38**	0.17	**2.80**	0.15	**4.03**	0.15	**2.58**	0.09
-1.5	**4.20**	0.09	**4.96**	0.14	**2.97**	0.07	**3.42**	0.17	**2.85**	0.18	**2.82**	0.18
-0.5	**4.36**	0.04	**4.05**	0.05	**3.32**	0.19	**3.37**	0.27	**2.78**	0.15	**3.21**	0.12
0.5	**6.22**	0.06	**1.12**	0.03	**2.93**	0.18	**1.49**	0.17	**3.58**	0.21	**2.42**	0.10
1.5	**4.66**	0.07	**0.54**	0.02	**0.87**	0.21	**1.36**	0.18	**3.01**	0.06	**1.30**	0.14
2.5	**3.27**	0.02	**0.42**	0.01	**0.68**	0.10	**0.80**	0.09	**2.37**	0.20	**0.80**	0.09
3.5	**2.36**	0.08	**0.42**	0.01	**0.32**	0.06	**0.62**	0.13	**2.08**	0.16	**1.57**	0.18
4.5	**1.69**	0.04	**0.41**	0.03	**0.35**	0.13	**0.50**	0.07	**1.60**	0.13	**0.62**	0.02
5.5	**1.41**	0.06	**0.36**	0.01	**0.38**	0.10	**0.41**	0.08	**1.00**	0.06	**1.14**	0.06
6.5	**1.34**	0.05	**0.39**	0.02	**0.42**	0.12	**0.47**	0.03	no sample**	no sample**	**0.37**	0.05
7.5	**1.53**	0.03	**0.44**	0.01	**0.22**	0.07	**0.43**	0.08	no sample**	no sample**	**0.58**	0.17
8.5	**1.08**	0.03	**0.34**	0.02	**0.47**	0.09	**0.33**	0.09	no sample**	no sample**	**0.53**	0.09
9.5	**0.83**	0.04	**0.39**	0.02	0.16	0.12	**0.35**	0.07	no sample**	no sample**	**0.64**	0.06
10.5	**0.83**	0.04	**0.39**	0.01	**0.35**	0.08	**1.12**	0.12	no sample**	no sample**	**0.59**	0.13
11.5	**0.68**	0.03	**0.40**	0.03	0.11	0.05	**0.42**	0.11	no sample**	no sample**	**0.45**	0.13
12.5	**0.70**	0.01	**0.35**	0.02	**0.31**	0.10	<LoD		no sample**	no sample**	no sample**	no sample**
13.5	**0.66**	0.02	**0.34**	0.01	**0.28**	0.05	no sample ***	no sample ***	no sample**	no sample**	**0.42**	0.08
14.5	**0.61**	0.03	**0.35**	0.02	0.14	0.08	no sample ***	no sample ***	no sample**	no sample**	**0.61**	0.08
15.5	**0.80**	0.02	**0.37**	0.01	**0.19**	0.09	no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	0.17	0.01	0.10	0.01	0.36	0.03	0.09	0.03	0.11	21.28	0.32	0.03
blank 2	0.11	0.01	0.02	0.00	0.21	0.07	0.12	0.10	0.09	47.53	<LoD	
blank 3	0.17	0.01	0.26	0.01	0.42	0.04	0.10	0.03	0.07	41.00	0.21	0.01
blank 4	0.16	0.00	0.05	0.01	0.44	0.05	0.11	0.04	0.04	30.85	0.15	0.05
blank 5	0.14	0.01	0.04	0.00	0.58	0.14	0.10	0.02	0.06	19.39	0.21	0.03
correction value	0.15		0.09		0.40		0.11		0.09		0.18	
LoD	0.01		0.01		0.07		0.07		0.09		0.13	
LoQ	0.03		0.03		0.18		0.20		0.21		0.32	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 52: Lead concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.094**	0.015	**0.047**	0.009	**0.172**	0.016	<LoD		**0.505**	0.009	**0.146**	0.015
-4.5	**0.102**	0.007	**0.029**	0.004	**0.194**	0.004	<LoD		**0.442**	0.020	0.118	0.007
-3.5	**0.080**	0.003	**0.030**	0.005	**0.149**	0.009	<LoD		**0.426**	0.018	0.098	0.007
-2.5	**0.059**	0.008	**0.025**	0.002	**0.119**	0.001	<LoD		**0.213**	0.011	0.076	0.006
-1.5	**0.069**	0.008	**0.049**	0.003	**0.156**	0.009	<LoD		**0.172**	0.012	0.101	0.010
-0.5	**0.064**	0.005	**0.040**	0.003	**0.070**	0.003	<LoD		**0.312**	0.021	0.118	0.006
0.5	**0.011**	0.003	**0.009**	0.000	<LoD		<LoD		0.038	0.008	0.081	0.007
1.5	<LoD		<LoD		**0.020**	0.014	<LoD		<LoD		<LoD	
2.5	<LoD		0.003	0.003	**0.032**	0.007	<LoD		<LoD		<LoD	
3.5	<LoD		**0.015**	0.006	<LoD		<LoD		<LoD		<LoD	
4.5	<LoD		**0.033**	0.010	<LoD		<LoD		<LoD		<LoD	
5.5	<LoD		**0.047**	0.008	**0.009**	0.002	<LoD		<LoD		0.020	0.005
6.5	<LoD		<LoD		**0.055**	0.013	<LoD		0.056	0.001	<LoD	
7.5	**0.024**	0.006	**0.143**	0.008	**0.024**	0.008	<LoD		<LoD		<LoD	
8.5	**0.010**	0.007	**0.096**	0.004	<LoD		<LoD		<LoD		<LoD	
9.5	**0.002**	0.005	<LoD		<LoD		<LoD		<LoD		<LoD	
10.5	**0.004**	0.000	0.003	0.007	<LoD		<LoD		<LoD		<LoD	
11.5	<LoD		<LoD		<LoD		<LoD		0.032	0.005	<LoD	
12.5	<LoD		**0.025**	0.007	<LoD		<LoD		<LoD		<LoD	
13.5	0.003	0.003	<LoD		<LoD		<LoD		<LoD		<LoD	
14.5	**0.052**	0.006	<LoD		<LoD		<LoD		<LoD		<LoD	
15.5	<LoD		**0.004**	0.001	<LoD		<LoD		**0.444**	0.017	<LoD	
blank 1	0.022	0.001	0.029	0.004	0.042	0.006	<LoD		0.066	0.007	0.228	0.008
blank 2	0.013	0.001	0.018	0.003	0.041	0.005	<LoD		<LoD		<LoD	
blank 3	0.022	0.001	0.033	0.003	0.071	0.004	<LoD		<LoD		<LoD	
blank 4	0.016	0.003	0.019	0.002	0.043	0.004	0.068	0.005	<LoD		<LoD	
blank 5	0.051	0.004	0.028	0.004	0.058	0.006	0.672	0.108	0.109	0.005	<LoD	
correction value	0.025		0.025		0.051		0.148		0.035		0.046	
LoD	0.001		0.001		0.001		0.060		0.060		0.044	
LoQ	0.003		0.003		0.003		0.166		0.166		0.127	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.054**	0.004	**0.283**	0.013	**8.094**	0.197	**13.066**	0.349	**23.786**	0.708	**71.383**	1.994
-4.5	0.019	0.002	**1.026**	0.023	**6.591**	0.114	**12.703**	0.369	**24.100**	0.746	**66.181**	0.428
-3.5	0.001	0.002	**1.713**	0.018	**12.942**	0.351	**13.014**	0.295	**23.048**	0.639	**45.319**	1.012
-2.5	<LoD		**1.986**	0.048	**15.329**	0.346	**8.372**	0.849	**28.834**	0.543	**37.398**	0.752
-1.5	<LoD		**1.861**	0.171	**5.754**	0.229	**11.347**	0.207	**24.287**	0.318	**34.814**	0.295
-0.5	0.010	0.003	**1.980**	0.028	**10.665**	0.149	**10.509**	0.289	**25.503**	0.491	**34.335**	0.427
0.5	<LoD		**0.344**	0.081	<LoD		**0.178**	0.010	**22.492**	0.625	**16.627**	0.248
1.5	0.002	0.001	<LoD		<LoD		0.045	0.004	0.049	0.024	0.045	0.011
2.5	<LoD		**0.281**	0.006	<LoD		0.035	0.006	0.060	0.007	0.023	0.007
3.5	<LoD		<LoD		<LoD		<LoD		<LoD		0.045	0.008
4.5	**0.034**	0.004	<LoD		<LoD		0.030	0.005	0.011	0.007	0.068	0.011
5.5	<LoD		<LoD		<LoD		0.031	0.006	0.027	0.004	0.035	0.006
6.5	**0.076**	0.004	<LoD		no sample *	no sample *	0.024	0.005	<LoD		0.034	0.006
7.5	<LoD		<LoD		no sample *	no sample *	<LoD		<LoD		0.024	0.005
8.5	**0.022**	0.003	<LoD		no sample *	no sample *	0.023	0.006	0.010	0.004	0.041	0.008
9.5	**0.028**	0.001	<LoD		<LoD		<LoD		<LoD		0.074	0.010
10.5	<LoD		<LoD		**0.172**	0.039	0.028	0.004	<LoD		0.053	0.008
11.5	<LoD		<LoD		<LoD		0.034	0.002	0.050	0.005	0.047	0.010
12.5	0.003	0.001	<LoD		<LoD		<LoD		0.003	0.004	0.026	0.012
13.5	0.020	0.002	<LoD		<LoD		0.040	0.008	<LoD		0.085	0.007
14.5	<LoD		<LoD		<LoD		<LoD		0.018	0.003	no sample **	no sample **
15.5	0.004	0.000	<LoD		<LoD		<LoD		<LoD		0.021	0.010
blank 1	0.030	0.001	0.087	0.003	0.570	0.034	<LoD		<LoD		0.045	0.006
blank 2	0.019	0.000	2.187	0.037	0.680	0.049	<LoD		0.033	0.005	<LoD	
blank 3	0.041	0.001	0.095	0.002	0.561	0.012	<LoD		0.126	0.010	0.058	0.003
blank 4	0.033	0.001	0.271	0.006	0.632	0.038	0.041	0.003	<LoD		<LoD	
blank 5	0.054	0.001	0.057	0.001	0.487	0.037	<LoD		<LoD		0.073	0.003
correction value	0.035		0.539		0.586		0.008		0.032		0.035	
LoD	0.007		0.007		0.020		0.029		0.029		0.032	
LoQ	0.020		0.020		0.054		0.079		0.079		0.095	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 53: Lead concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.150**	0.008	**0.109**	0.004	**0.235**	0.010	0.109	0.014	**0.622**	0.023	**0.822**	0.004
-4.5	**0.132**	0.004	<LoD		**0.307**	0.014	0.067	0.011	**0.942**	0.027	**0.585**	0.012
-3.5	**0.148**	0.006	<LoD		**0.194**	0.009	0.176	0.013	**0.673**	0.029	**0.218**	0.008
-2.5	**0.176**	0.005	<LoD		**0.196**	0.007	0.188	0.018	**0.622**	0.038	**0.198**	0.004
-1.5	**0.185**	0.006	<LoD		**0.194**	0.005	1.363	0.028	**0.464**	0.026	**0.036**	0.002
-0.5	**0.118**	0.007	<LoD		**0.091**	0.011	0.213	0.010	**0.307**	0.011	**0.126**	0.006
0.5	**0.089**	0.007	0.050	0.005	<LoD		<LoD		**0.300**	0.019	**0.140**	0.004
1.5	0.026	0.006	<LoD		<LoD		0.148	0.010	<LoD		**0.092**	0.005
2.5	<LoD		0.029	0.005	<LoD		0.085	0.011	<LoD		**0.080**	0.008
3.5	0.063	0.006	<LoD		<LoD		0.241	0.015	<LoD		**0.079**	0.002
4.5	<LoD		<LoD		<LoD		0.249	0.017	<LoD		<LoD	
5.5	<LoD		<LoD		<LoD		**3.478**	0.078	<LoD		<LoD	
6.5	<LoD		<LoD		**0.076**	0.008	no sample ***	no sample ***	<LoD		<LoD	
7.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
8.5	<LoD		**0.154**	0.012	<LoD		no sample ***	no sample ***	<LoD		**0.036**	0.003
9.5	**0.193**	0.014	<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
10.5	<LoD		0.056	0.004	<LoD		0.195	0.029	<LoD		<LoD	
11.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
12.5	<LoD		<LoD		<LoD		0.217	0.012	<LoD		<LoD	
13.5	<LoD	21.474	<LoD		<LoD		<LoD		<LoD		<LoD	
14.5	<LoD		**0.109**	0.007	<LoD		<LoD		<LoD		<LoD	
15.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
blank 1	0.053	0.006	0.039	0.004	0.045	0.003	0.420	0.042	<LoD		0.056	0.002
blank 2	0.037	0.004	0.036	0.003	0.040	0.003	<LoD		<LoD		0.021	0.002
blank 3	0.039	0.003	0.039	0.002	0.039	0.002	<LoD		<LoD		0.032	0.001
blank 4	0.040	0.003	0.047	0.002	0.046	0.004	<LoD		<LoD		0.052	0.001
blank 5	0.054	0.003	0.063	0.005	0.063	0.002	<LoD				0.052	0.003
correction value	0.045		0.045		0.046		0.084		0.000		0.043	
LoD	0.024		0.024		0.024		0.103		0.103		0.015	
LoQ	0.072		0.072		0.072		0.296		0.296		0.023	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.166**	0.005	**0.626**	0.028	**9.149**	0.353	**13.949**	0.479	**23.564**	0.283	**57.657**	0.805
-4.5	**0.163**	0.005	**1.364**	0.041	**5.576**	0.343	**11.475**	0.361	**21.632**	0.473	**58.183**	0.822
-3.5	<LoD		**2.053**	0.024	**6.631**	0.196	**9.847**	0.157	**25.359**	0.678	**42.841**	0.863
-2.5	<LoD		**2.250**	0.029	**5.334**	0.153	**9.525**	0.246	**24.607**	0.320	**36.332**	0.585
-1.5	<LoD		**2.164**	0.025	**5.668**	0.189	**10.138**	0.254	**18.388**	0.271	**35.026**	0.851
-0.5	<LoD		**2.272**	0.042	**4.987**	0.091	**8.805**	0.269	**16.537**	0.117	**33.862**	0.700
0.5	<LoD		**1.658**	0.028	**0.976**	0.041	**1.458**	0.044	**21.413**	0.177	**16.979**	0.263
1.5	<LoD		<LoD		<LoD		<LoD		**0.365**	0.021	**0.201**	0.015
2.5	<LoD		<LoD		<LoD		<LoD		**0.499**	0.009	**0.149**	0.004
3.5	<LoD		**0.403**	0.009	<LoD		**0.273**	0.016	<LoD		**0.227**	0.006
4.5	<LoD		<LoD		<LoD		<LoD		<LoD		**0.097**	0.008
5.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
6.5	<LoD		<LoD		no sample *	no sample *	<LoD		<LoD		0.066	0.012
7.5	<LoD		<LoD		no sample *	no sample *	<LoD		<LoD		0.031	0.037
8.5	<LoD		<LoD		no sample *	no sample *	<LoD		<LoD		0.039	0.004
9.5	<LoD		<LoD		<LoD		<LoD		<LoD		0.061	0.010
10.5	<LoD		<LoD		<LoD		<LoD		<LoD		**0.149**	0.010
11.5	<LoD		**0.404**	0.008	<LoD		<LoD		<LoD		no sample **	no sample **
12.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
13.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
14.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
15.5	<LoD		<LoD		<LoD		<LoD		<LoD		no sample **	no sample **
blank 1	<LoD		0.382	0.025	0.270	0.024	0.138	0.009	0.078	0.005	0.045	0.006
blank 2	<LoD		0.063	0.004	0.252	0.007	0.054	0.006	0.060	0.003	<LoD	
blank 3	<LoD		0.214	0.010	0.231	0.005	0.044	0.004	0.040	0.004	0.058	0.003
blank 4	0.091	0.001	0.201	0.009	0.185	0.008	0.104	0.018	0.029	0.002	<LoD	
blank 5	0.109	0.003	<LoD		0.231	0.007	0.058	0.007			0.073	0.003
correction value	0.040		0.172		0.234		0.080		0.046		0.035	
LoD	0.015		0.044		0.017		0.020		0.029		0.032	
LoQ	0.023		0.127		0.047		0.054		0.079		0.095	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 54: Lead concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.126**	0.008	**0.201**	0.020	**0.276**	0.029	0.082	0.005	0.071	0.008	**0.347**	0.016
-4.5	**0.134**	0.013	**0.165**	0.011	**0.397**	0.043	0.164	0.015	0.088	0.007	**0.294**	0.010
-3.5	**0.152**	0.002	**0.157**	0.005	**0.277**	0.029	<LoD		0.103	0.006	**0.255**	0.011
-2.5	**0.113**	0.007	**0.225**	0.011	**0.173**	0.010	0.127	0.009	0.048	0.008	**0.302**	0.011
-1.5	**0.139**	0.016	**0.149**	0.013	**0.135**	0.013	<LoD		0.166	0.015	**0.284**	0.013
-0.5	**0.175**	0.006	**0.059**	0.006	**0.021**	0.004	<LoD		0.122	0.007	**0.356**	0.017
0.5	**0.043**	0.009	**0.050**	0.008	**0.022**	0.003	<LoD		0.115	0.009	**0.153**	0.008
1.5	**0.022**	0.003	**0.023**	0.003	**0.037**	0.003	<LoD		<LoD		<LoD	
2.5	0.003	0.002	**0.018**	0.002	**0.016**	0.004	<LoD		0.042	0.008	<LoD	
3.5	<LoD		**0.015**	0.002	**0.016**	0.002	<LoD		0.150	0.013	<LoD	
4.5	<LoD		**0.020**	0.002	**0.016**	0.004	<LoD		0.050	0.005	<LoD	
5.5	**0.011**	0.006	**0.016**	0.006	**0.015**	0.005	<LoD		0.046	0.006	<LoD	
6.5	<LoD		**0.011**	0.001	**0.023**	0.007	<LoD		<LoD		<LoD	
7.5	<LoD		**0.012**	0.001	**0.043**	0.005	<LoD		0.031	0.004	0.022	0.003
8.5	<LoD		**0.033**	0.004	**0.086**	0.003	<LoD		**0.167**	0.010	<LoD	
9.5	**0.018**	0.005	**0.035**	0.011	**0.004**	0.001	<LoD		<LoD		<LoD	
10.5	<LoD		**0.015**	0.003	**0.041**	0.004	<LoD		0.063	0.010	<LoD	
11.5	<LoD		**0.020**	0.001	**0.016**	0.004	<LoD		0.037	0.004	<LoD	
12.5	**0.013**	0.002	**0.014**	0.003	**0.146**	0.011	<LoD		<LoD		<LoD	
13.5	<LoD		**0.042**	0.001	**0.011**	0.002	<LoD		0.042	0.005	<LoD	
14.5	**0.011**	0.005	**0.012**	0.001	<LoD		<LoD		<LoD		<LoD	
15.5	**0.004**	0.004	<LoD		<LoD		<LoD		0.040	0.003	<LoD	
blank 1	0.012	0.002	0.005	0.001	0.024	0.002	<LoD		<LoD		0.230	0.005
blank 2	0.028	0.002	0.006	0.001	0.016	0.001	<LoD		<LoD		<LoD	
blank 3	0.016	0.004	0.008	0.002	0.011	0.002	<LoD		0.060	0.005	<LoD	
blank 4	0.018	0.000	0.005	0.000	0.004	0.001	<LoD		0.093	0.006	0.020	0.002
blank 5	0.021	0.003	0.010	0.001	0.012	0.003	<LoD		<LoD		0.018	0.002
correction value	0.019		0.007		0.014		0.000		0.031		0.054	
LoD	0.001		0.001		0.001		0.060		0.060		0.017	
LoQ	0.003		0.003		0.003		0.166		0.166		0.047	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.143**	0.005	**0.668**	0.010	<LoD		0.067	0.006	0.093	0.008	**4.178**	0.061
-4.5	**0.048**	0.002	<LoD		<LoD		0.020	0.005	**0.163**	0.006	0.001	0.005
-3.5	**0.010**	0.002	<LoD		<LoD		**0.167**	0.013	0.079	0.006	0.012	0.006
-2.5	**0.196**	0.008	<LoD		<LoD		0.032	0.005	**0.434**	0.016	<LoD	
-1.5	**0.229**	0.006	0.006	0.001	<LoD		0.033	0.012	0.002	0.004	<LoD	
-0.5	<LoD		<LoD		<LoD		0.045	0.005	<LoD		<LoD	
0.5	<LoD		<LoD		<LoD		0.011	0.008	0.032	0.008	<LoD	
1.5	<LoD		**0.061**	0.004	<LoD		0.023	0.004	<LoD		<LoD	
2.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
3.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
4.5	**0.027**	0.002	0.015	0.002	<LoD		<LoD		0.045	0.009	<LoD	
5.5	0.003	0.003	0.013	0.003	<LoD		0.001	0.004	<LoD		0.013	0.015
6.5	0.004	0.003	0.011	0.003	<LoD		0.010	0.004	0.002	0.008	**0.106**	0.016
7.5	**0.144**	0.004	**0.159**	0.003	<LoD		0.036	0.007	<LoD		0.008	0.008
8.5	**0.063**	0.004	**0.025**	0.002	**0.060**	0.027	0.017	0.006	**0.247**	0.020	**0.123**	0.004
9.5	**0.038**	0.003	**0.301**	0.010	<LoD		0.045	0.005	**0.540**	0.014	**0.115**	0.009
10.5	no sample**	no sample**	**0.109**	0.002	<LoD		<LoD		**0.281**	0.014	0.039	0.012
11.5	**0.571**	0.005	<LoD		<LoD		0.016	0.005	0.007	0.001	**0.141**	0.013
12.5	no sample**	no sample**	<LoD		<LoD		0.048	0.010	**0.116**	0.005	**0.108**	0.006
13.5	**0.674**	0.042	**0.235**	0.003	<LoD		<LoD		<LoD		**0.157**	0.021
14.5	no sample**	no sample**	**0.141**	0.006	<LoD		<LoD		0.014	0.005	**0.103**	0.014
15.5	**0.027**	0.001	**0.139**	0.004	no sample**	no sample**	0.007	0.007	<LoD		0.057	0.009
blank 1	0.076	0.003	0.067	0.001	0.755	0.032	0.092	0.005	0.036	0.004	0.040	0.009
blank 2	0.050	0.002	0.015	0.000	0.725	0.036	<LoD		0.442	0.016	0.028	0.007
blank 3	0.032	0.001	0.073	0.001	0.351	0.024	0.106	0.006	0.049	0.003	0.130	0.008
blank 4	0.028	0.001	0.117	0.008	0.598	0.016	0.031	0.004	0.119	0.005	0.063	0.001
blank 5	0.069	0.002	0.567	0.006	0.251	0.007	0.073	0.010	0.180	0.014	0.079	0.005
correction value	0.051		0.068		0.536		0.049		0.036		0.068	
LoD	0.007		0.007		0.020		0.029		0.029		0.032	
LoQ	0.020		0.020		0.054		0.079		0.079		0.095	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 55: Lead concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.253**	0.009	**0.238**	0.009	**0.426**	0.009	0.212	0.022	**1.606**	0.102	**1.570**	0.045
-4.5	**0.374**	0.013	**0.372**	0.006	**0.567**	0.003	0.261	0.018	**1.072**	0.059	**0.989**	0.017
-3.5	**0.331**	0.014	**0.383**	0.014	**0.384**	0.009	0.265	0.022	**1.736**	0.044	**1.305**	0.017
-2.5	**0.338**	0.010	**0.448**	0.007	**0.355**	0.008	0.254	0.010	**1.677**	0.075	**1.437**	0.032
-1.5	**0.326**	0.008	**0.334**	0.009	**0.244**	0.006	0.235	0.007	**1.604**	0.090	**1.157**	0.015
-0.5	**0.378**	0.008	**0.103**	0.005	**0.087**	0.004	0.256	0.013	**1.321**	0.029	**1.365**	0.038
0.5	**0.339**	0.010	**0.081**	0.003	0.065	0.004	0.256	0.007	**1.012**	0.051	**1.139**	0.022
1.5	0.052	0.004	0.038	0.004	0.069	0.006	0.220	0.012	0.164	0.007	**0.090**	0.005
2.5	<LoD		<LoD		0.045	0.003	no sample ***	no sample ***	<LoD		**0.080**	0.006
3.5	<LoD		<LoD		0.037	0.002	no sample ***	no sample ***	<LoD		**0.031**	0.002
4.5	<LoD		<LoD		0.028	0.003	<LoD		<LoD		**0.042**	0.001
5.5	0.035	0.004	<LoD		**0.083**	0.108	<LoD		<LoD		**0.037**	0.002
6.5	<LoD		0.028	0.003	0.035	0.002	<LoD		<LoD		**0.107**	0.003
7.5	0.027	0.004	<LoD		0.032	0.003	<LoD		<LoD		**0.054**	0.005
8.5	**0.086**	0.002	<LoD		<LoD		<LoD		<LoD		**0.033**	0.003
9.5	0.054	0.003	<LoD		0.033	0.003	<LoD		<LoD		**0.034**	0.005
10.5	<LoD		<LoD		<LoD		<LoD		<LoD		**0.031**	0.001
11.5	<LoD		<LoD		0.025	0.001	<LoD		<LoD		**0.154**	0.012
12.5	<LoD		<LoD		0.027	0.002	no sample ***	no sample ***	<LoD		<LoD	
13.5	0.042	0.005	<LoD		<LoD		<LoD		<LoD		**0.086**	0.009
14.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
15.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		<LoD	
blank 1	0.057	0.003	<LoD		<LoD		<LoD		<LoD		0.015	0.003
blank 2	0.030	0.003	<LoD		<LoD		<LoD		<LoD		0.028	0.001
blank 3	0.026	0.003	0.066	0.002	<LoD		<LoD		<LoD		0.049	0.004
blank 4	0.034	0.004	0.050	0.004	<LoD		<LoD		<LoD		0.020	0.002
blank 5	<LoD		0.082	0.003	<LoD						<LoD	
correction value	0.029		0.040		0.000		0.000		0.000		0.023	
LoD	0.024		0.024		0.024		0.103		0.103		0.015	
LoQ	0.072		0.072		0.072		0.296		0.296		0.023	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.263**	0.010	**0.820**	0.028	<LoD		<LoD		**0.288**	0.017	0.025	0.009
-4.5	0.095	0.005	0.071	0.006	**0.131**	0.023	0.036	0.009	0.067	0.007	<LoD	
-3.5	0.030	0.005	<LoD		<LoD		**0.073**	0.012	0.041	0.004	<LoD	
-2.5	<LoD		0.046	0.005	<LoD		0.027	0.012	<LoD		<LoD	
-1.5	<LoD		**0.241**	0.011	<LoD		0.031	0.015	<LoD		<LoD	
-0.5	<LoD		0.038	0.003	<LoD		0.052	0.014	<LoD		<LoD	
0.5	0.040	0.004	<LoD		0.047	0.020	<LoD		<LoD		<LoD	
1.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
2.5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
3.5	<LoD		<LoD		<LoD		<LoD		**0.120**	0.019	<LoD	
4.5	<LoD		0.124	0.004	<LoD		<LoD		<LoD		<LoD	
5.5	<LoD		<LoD		<LoD		<LoD		**0.115**	0.006	**0.961**	0.052
6.5	0.045	0.004	0.042	0.004	<LoD		<LoD		no sample**	no sample**	<LoD	
7.5	<LoD		**0.335**	0.010	<LoD		0.054	0.008	no sample**	no sample**	<LoD	
8.5	<LoD		0.028	0.003	**0.223**	0.030	<LoD		no sample**	no sample**	0.028	0.010
9.5	<LoD		0.087	0.003	<LoD		<LoD		no sample**	no sample**	0.058	0.006
10.5	<LoD		0.100	0.007	<LoD		<LoD		no sample**	no sample**	0.050	0.002
11.5	<LoD		**0.275**	0.006	**1.643**	0.054	<LoD		no sample**	no sample**	<LoD	
12.5	<LoD		**0.193**	0.008	<LoD		<LoD		no sample**	no sample**	no sample**	no sample**
13.5	0.051	0.002	**0.286**	0.007	<LoD		no sample ***	no sample ***	no sample**	no sample**	0.065	0.016
14.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	no sample**	no sample**	**0.103**	0.005
15.5	<LoD		**1.242**	0.029	<LoD		no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	0.054	0.001	3.758	0.197	0.279	0.016	0.050	0.003	<LoD		0.121	0.004
blank 2	0.073	0.003	<LoD		0.186	0.008	0.099	0.004	<LoD		0.059	0.003
blank 3	0.066	0.004	0.222	0.011	0.270	0.016	0.205	0.017	<LoD		0.191	0.010
blank 4	0.056	0.002	0.048	0.003	0.295	0.011	0.078	0.011	<LoD		0.074	0.001
blank 5	0.102	0.004	0.083	0.003	0.278	0.016	0.293	0.022	<LoD		0.063	0.004
correction value	0.070		0.088		0.261		0.076		0.000		0.066	
LoD	0.044		0.044		0.017		0.020		0.029		0.032	
LoQ	0.127		0.127		0.047		0.054		0.079		0.095	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 56: Antimony concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.145**	0.021	**0.318**	0.021	**0.551**	0.045	**0.411**	0.037	**0.643**	0.025	**0.374**	0.078
-4.5	**0.183**	0.026	**0.307**	0.023	**0.529**	0.035	**0.527**	0.033	**0.649**	0.042	**0.365**	0.032
-3.5	**0.209**	0.009	**0.360**	0.031	**0.461**	0.056	**0.573**	0.019	**0.633**	0.029	**0.347**	0.033
-2.5	**0.196**	0.004	**0.280**	0.006	**0.465**	0.035	**0.481**	0.022	**0.321**	0.011	**0.333**	0.045
-1.5	**0.177**	0.025	**0.369**	0.024	**0.471**	0.055	**0.435**	0.040	**0.317**	0.018	**0.349**	0.072
-0.5	**0.217**	0.037	**0.274**	0.032	**0.491**	0.066	**0.453**	0.028	**0.554**	0.064	**0.286**	0.034
0.5	**0.201**	0.008	**0.123**	0.030	**0.116**	0.032	**0.582**	0.020	**0.574**	0.039	**0.338**	0.043
1.5	**0.068**	0.009	**0.064**	0.006	**0.067**	0.007	**0.302**	0.016	**0.230**	0.034	**0.079**	0.011
2.5	**0.044**	0.013	**0.053**	0.005	**0.065**	0.011	**0.082**	0.011	**0.112**	0.018	**0.081**	0.019
3.5	**0.047**	0.006	**0.061**	0.009	**0.051**	0.003	**0.048**	0.014	**0.059**	0.005	**0.050**	0.009
4.5	**0.047**	0.006	**0.062**	0.013	**0.062**	0.023	**0.037**	0.009	**0.060**	0.009	**0.069**	0.010
5.5	**0.047**	0.006	**0.067**	0.019	**0.047**	0.010	**0.030**	0.006	**0.047**	0.004	0.043	0.008
6.5	**0.034**	0.002	**0.043**	0.014	**0.049**	0.004	**0.026**	0.006	**0.055**	0.005	0.041	0.005
7.5	**0.046**	0.001	**0.050**	0.011	**0.048**	0.005	**0.029**	0.005	**0.081**	0.003	**0.044**	0.006
8.5	**0.055**	0.001	**0.040**	0.006	**0.047**	0.003	**0.028**	0.008	**0.048**	0.005	**0.050**	0.013
9.5	**0.021**	0.004	**0.038**	0.005	**0.055**	0.005	**0.031**	0.007	**0.055**	0.008	**0.047**	0.010
10.5	**0.043**	0.003	**0.047**	0.004	**0.049**	0.008	**0.024**	0.006	**0.058**	0.008	**0.066**	0.009
11.5	**0.034**	0.004	**0.039**	0.005	**0.033**	0.005	**0.022**	0.008	**0.056**	0.005	**0.064**	0.011
12.5	**0.035**	0.011	**0.041**	0.005	**0.029**	0.003	**0.025**	0.004	**0.052**	0.011	**0.052**	0.007
13.5	**0.028**	0.003	**0.037**	0.005	**0.040**	0.008	**0.025**	0.006	**0.053**	0.013	**0.067**	0.012
14.5	**0.038**	0.007	**0.054**	0.005	**0.035**	0.006	**0.023**	0.007	**0.055**	0.012	**0.044**	0.010
15.5	**0.030**	0.001	**0.041**	0.005	**0.034**	0.005	**0.019**	0.006	**0.046**	0.006	**0.048**	0.011
blank 1	0.009	0.006	0.005	0.002	0.008	0.004	0.008	0.002	0.016	0.005	<LoD	
blank 2	0.004	0.001	0.006	0.003	0.009	0.002	0.008	0.003	<LoD		<LoD	
blank 3	0.010	0.002	0.003	0.001	0.012	0.005	0.009	0.004	0.010	0.004	<LoD	
blank 4	0.006	0.006	0.003	0.001	0.010	0.003	0.008	0.003	0.007	0.002	<LoD	
blank 5	0.004	0.003	0.007	0.002	0.009	0.002	0.019	0.003	0.010	0.003	<LoD	
correction value	0.007		0.005		0.010		0.010		0.009		0.000	
LoD	0.001		0.001		0.001		0.006		0.006		0.020	
LoQ	0.002		0.002		0.002		0.016		0.016		0.044	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.842**	0.062	**0.063**	0.002	0.032	0.016	**0.080**	0.020	**0.161**	0.029	**0.071**	0.020
-4.5	**0.731**	0.038	**0.044**	0.003	0.023	0.013	**0.062**	0.012	**0.063**	0.013	**0.087**	0.005
-3.5	**0.651**	0.028	**0.059**	0.004	0.023	0.009	**0.046**	0.008	**0.048**	0.010	**0.098**	0.006
-2.5	**0.546**	0.020	**0.078**	0.005	0.035	0.013	0.019	0.006	**0.070**	0.018	**0.064**	0.016
-1.5	**0.517**	0.014	**0.064**	0.004	0.031	0.018	0.032	0.009	**0.050**	0.015	**0.043**	0.011
-0.5	**0.518**	0.012	**0.039**	0.001	0.022	0.011	0.034	0.004	0.038	0.005	**0.039**	0.007
0.5	**0.417**	0.013	**0.039**	0.004	**0.083**	0.013	**0.075**	0.004	0.034	0.010	**0.031**	0.014
1.5	**0.163**	0.002	**0.090**	0.005	**0.126**	0.032	**0.099**	0.008	**0.061**	0.015	**0.084**	0.005
2.5	**0.093**	0.004	**0.102**	0.009	**0.108**	0.016	**0.108**	0.012	**0.080**	0.014	**0.074**	0.011
3.5	**0.082**	0.004	**0.092**	0.003	**0.112**	0.024	**0.099**	0.026	**0.078**	0.008	**0.064**	0.014
4.5	**0.059**	0.004	**0.082**	0.002	**0.081**	0.020	**0.103**	0.011	**0.071**	0.006	**0.057**	0.011
5.5	**0.059**	0.002	**0.078**	0.003	**0.077**	0.029	**0.084**	0.007	**0.061**	0.010	**0.046**	0.012
6.5	**0.069**	0.003	**0.086**	0.006	no sample *	no sample *	**0.086**	0.014	**0.078**	0.016	**0.059**	0.009
7.5	**0.063**	0.001	**0.076**	0.006	no sample *	no sample *	**0.078**	0.018	**0.056**	0.022	**0.053**	0.002
8.5	**0.064**	0.005	**0.082**	0.006	no sample *	no sample *	**0.093**	0.012	**0.060**	0.017	**0.061**	0.003
9.5	**0.058**	0.006	**0.080**	0.004	0.038	0.004	**0.086**	0.010	**0.056**	0.009	**0.076**	0.008
10.5	**0.057**	0.004	**0.086**	0.003	**0.081**	0.020	**0.076**	0.021	**0.050**	0.008	**0.066**	0.008
11.5	**0.056**	0.004	**0.082**	0.008	0.047	0.012	**0.063**	0.014	**0.052**	0.010	**0.067**	0.008
12.5	**0.060**	0.002	**0.079**	0.007	0.052	0.013	**0.065**	0.022	**0.060**	0.014	**0.055**	0.006
13.5	**0.060**	0.003	**0.082**	0.007	**0.070**	0.016	**0.056**	0.009	**0.059**	0.009	**0.051**	0.007
14.5	**0.059**	0.004	**0.077**	0.005	0.036	0.013	**0.065**	0.017	**0.063**	0.016	no sample **	no sample **
15.5	**0.060**	0.002	**0.073**	0.006	0.052	0.016	**0.071**	0.016	**0.065**	0.009	**0.058**	0.005
blank 1	<LoD		<LoD		0.025	0.009	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.025	0.011	<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		0.020	0.009	<LoD		<LoD		<LoD	
blank 5	<LoD		0.017	0.002	<LoD		<LoD		<LoD		<LoD	
orrection valu	0.000		0.003		0.014		0.000		0.000		0.000	
LoD	0.015		0.015		0.020		0.014		0.014		0.006	
LoQ	0.044		0.044		0.054		0.040		0.040		0.013	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 57: Antimony concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.202**	0.015	**0.358**	0.021	**0.403**	0.021	**0.575**	0.044	**0.668**	0.026	**0.683**	0.051
-4.5	**0.201**	0.017	**0.313**	0.027	**0.529**	0.036	**0.427**	0.011	**1.224**	0.022	**0.740**	0.054
-3.5	**0.225**	0.015	**0.288**	0.008	**0.510**	0.044	**0.337**	0.019	**1.086**	0.060	**0.629**	0.046
-2.5	**0.254**	0.015	**0.326**	0.038	**0.502**	0.039	**0.356**	0.014	**1.125**	0.041	**0.660**	0.031
-1.5	**0.253**	0.009	**0.288**	0.021	**0.522**	0.038	**0.382**	0.021	**0.860**	0.024	**0.638**	0.041
-0.5	**0.244**	0.013	**0.320**	0.030	**0.414**	0.030	**0.312**	0.021	**0.636**	0.027	**0.612**	0.041
0.5	**0.313**	0.015	**0.087**	0.007	**0.147**	0.016	**0.354**	0.016	**0.757**	0.066	**0.106**	0.008
1.5	**0.110**	0.010	**0.068**	0.010	**0.085**	0.012	**0.249**	0.014	**0.216**	0.021	**0.157**	0.006
2.5	**0.074**	0.010	**0.069**	0.009	**0.038**	0.004	**0.067**	0.012	**0.104**	0.013	**0.111**	0.010
3.5	**0.068**	0.009	**0.068**	0.007	**0.053**	0.010	0.046	0.006	**0.066**	0.009	**0.075**	0.006
4.5	**0.051**	0.008	**0.060**	0.007	**0.063**	0.008	**0.052**	0.009	**0.067**	0.010	**0.065**	0.005
5.5	**0.045**	0.006	**0.066**	0.007	**0.044**	0.006	**0.050**	0.007	**0.063**	0.017	**0.056**	0.006
6.5	**0.044**	0.001	**0.058**	0.006	**0.058**	0.010	no sample ***	no sample ***	**0.059**	0.012	**0.051**	0.004
7.5	**0.041**	0.005	**0.052**	0.011	**0.049**	0.008	no sample ***	no sample ***	**0.061**	0.005	**0.047**	0.004
8.5	**0.044**	0.003	**0.053**	0.008	**0.037**	0.010	no sample ***	no sample ***	**0.052**	0.007	**0.046**	0.003
9.5	**0.047**	0.007	**0.045**	0.007	**0.032**	0.005	no sample ***	no sample ***	0.048	0.008	**0.044**	0.001
10.5	**0.045**	0.004	**0.038**	0.009	**0.032**	0.004	0.039	0.008	**0.061**	0.003	**0.047**	0.002
11.5	**0.048**	0.008	**0.039**	0.006	**0.029**	0.004	0.031	0.004	**0.064**	0.009	**0.042**	0.004
12.5	**0.038**	0.008	**0.038**	0.011	**0.041**	0.010	0.036	0.013	**0.055**	0.009	**0.043**	0.003
13.5	**0.059**	21.474	**0.037**	0.003	**0.045**	0.003	0.036	0.006	**0.053**	0.011	**0.042**	0.002
14.5	**0.041**	0.006	**0.030**	0.004	**0.030**	0.007	0.039	0.003	**0.053**	0.008	**0.041**	0.001
15.5	**0.049**	0.008	**0.049**	0.008	**0.039**	0.007	no sample ***	no sample ***	**0.055**	0.011	**0.042**	0.005
blank 1	0.007	0.002	0.004	0.001	0.007	0.001	<LoD		<LoD		<LoD	
blank 2	0.005	0.002	0.005	0.001	0.009	0.002	<LoD		<LoD		<LoD	
blank 3	0.004	0.001	0.010	0.002	0.006	0.003	<LoD		<LoD		<LoD	
blank 4	0.003	0.002	0.003	0.002	0.010	0.002	<LoD		<LoD		<LoD	
blank 5	0.004	0.003	0.002	0.001	0.007	0.002	<LoD				<LoD	
correction value	0.005		0.005		0.008		0.000		0.000		0.000	
LoD	0.002		0.002		0.002		0.016		0.016		0.013	
LoQ	0.004		0.004		0.004		0.048		0.048		0.034	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**1.113**	0.049	0.038	0.003	**0.045**	0.011	0.035	0.015	**0.156**	0.022	**0.065**	0.011
-4.5	**0.868**	0.035	0.028	0.003	0.023	0.014	0.024	0.008	**0.058**	0.007	**0.080**	0.008
-3.5	**0.847**	0.047	0.033	0.002	0.026	0.007	<LoD		**0.053**	0.011	**0.086**	0.014
-2.5	**0.888**	0.046	0.028	0.001	0.019	0.003	<LoD		**0.050**	0.008	**0.067**	0.021
-1.5	**0.845**	0.015	0.028	0.004	0.022	0.010	<LoD		0.029	0.010	**0.048**	0.010
-0.5	**0.670**	0.010	<LoD		0.018	0.012	<LoD		0.024	0.008	**0.034**	0.010
0.5	**0.528**	0.009	**0.049**	0.005	**0.083**	0.018	0.053	0.010	0.035	0.011	**0.041**	0.011
1.5	**0.167**	0.016	**0.074**	0.006	**0.096**	0.013	**0.098**	0.029	**0.055**	0.009	**0.093**	0.011
2.5	**0.106**	0.007	**0.091**	0.007	**0.088**	0.026	**0.079**	0.026	**0.084**	0.008	**0.079**	0.013
3.5	**0.072**	0.006	**0.076**	0.006	**0.082**	0.017	**0.084**	0.020	**0.059**	0.011	**0.065**	0.013
4.5	**0.105**	0.007	**0.075**	0.003	**0.064**	0.014	0.049	0.008	**0.063**	0.008	**0.053**	0.009
5.5	**0.083**	0.006	**0.072**	0.007	**0.062**	0.017	**0.063**	0.011	**0.051**	0.015	no sample **	no sample **
6.5	**0.077**	0.007	**0.073**	0.006	no sample *	no sample *	**0.077**	0.005	**0.069**	0.015	**0.055**	0.003
7.5	**0.065**	0.004	**0.072**	0.006	no sample *	no sample *	**0.059**	0.013	**0.073**	0.026	**0.050**	0.005
8.5	**0.101**	0.005	**0.069**	0.004	no sample *	no sample *	0.051	0.013	**0.058**	0.013	**0.062**	0.012
9.5	**0.100**	0.006	**0.065**	0.003	**0.042**	0.013	0.056	0.021	**0.052**	0.007	**0.063**	0.017
10.5	**0.086**	0.005	**0.065**	0.005	**0.062**	0.010	**0.062**	0.020	**0.054**	0.012	**0.060**	0.012
11.5	**0.083**	0.003	**0.067**	0.004	**0.042**	0.017	0.056	0.006	**0.059**	0.007	no sample **	no sample **
12.5	**0.077**	0.007	**0.061**	0.006	**0.042**	0.016	**0.066**	0.016	**0.045**	0.007	no sample **	no sample **
13.5	**0.086**	0.004	**0.064**	0.005	**0.043**	0.014	**0.070**	0.013	**0.053**	0.007	no sample **	no sample **
14.5	**0.082**	0.003	**0.063**	0.004	**0.044**	0.015	**0.067**	0.008	**0.043**	0.007	no sample **	no sample **
15.5	**0.087**	0.005	**0.060**	0.005	**0.040**	0.008	**0.062**	0.012	**0.053**	0.010	no sample **	no sample **
blank 1	<LoD		<LoD		0.028	0.012	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.030	0.011	<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		0.023	0.007	<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		0.014	0.007	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		0.020	0.009	<LoD				<LoD	
correction value	0.000		0.000		0.023		0.000		0.000		0.000	
LoD	0.013		0.020		0.010		0.020		0.014		0.006	
LoQ	0.034		0.044		0.028		0.054		0.040		0.013	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 58: Antimony concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.350**	0.043	**0.653**	0.025	**0.832**	0.128	**0.439**	0.024	**0.598**	0.019	**0.583**	0.021
-4.5	**0.369**	0.045	**0.534**	0.039	**0.894**	0.064	**0.460**	0.039	**0.615**	0.014	**0.602**	0.018
-3.5	**0.326**	0.034	**0.588**	0.046	**0.826**	0.067	**0.256**	0.025	**0.932**	0.019	**0.571**	0.026
-2.5	**0.337**	0.014	**0.642**	0.056	**0.776**	0.036	**0.397**	0.041	**0.590**	0.017	**0.654**	0.033
-1.5	**0.438**	0.068	**0.590**	0.080	**0.660**	0.022	**0.239**	0.018	**1.391**	0.062	**0.610**	0.018
-0.5	**0.532**	0.039	**0.144**	0.009	**0.162**	0.009	**0.330**	0.021	**0.998**	0.032	**0.711**	0.018
0.5	**0.329**	0.028	**0.060**	0.001	**0.096**	0.028	**0.291**	0.027	**0.406**	0.045	**0.367**	0.017
1.5	**0.135**	0.009	**0.070**	0.003	**0.087**	0.011	**0.175**	0.008	**0.071**	0.009	**0.091**	0.005
2.5	**0.079**	0.009	**0.069**	0.008	**0.065**	0.013	**0.039**	0.008	**0.072**	0.006	**0.041**	0.002
3.5	**0.050**	0.014	**0.056**	0.003	**0.087**	0.010	**0.026**	0.004	**0.034**	0.006	**0.041**	0.005
4.5	**0.070**	0.015	**0.052**	0.009	**0.063**	0.009	**0.032**	0.009	**0.050**	0.010	0.027	0.003
5.5	**0.072**	0.003	**0.048**	0.008	**0.059**	0.008	**0.032**	0.004	**0.061**	0.007	**0.054**	0.005
6.5	**0.058**	0.006	**0.051**	0.011	**0.053**	0.010	**0.020**	0.005	**0.055**	0.009	**0.038**	0.005
7.5	**0.046**	0.003	**0.051**	0.008	**0.079**	0.003	**0.022**	0.008	**0.050**	0.007	**0.041**	0.005
8.5	**0.051**	0.015	**0.094**	0.009	**0.064**	0.012	**0.024**	0.008	**0.041**	0.008	0.024	0.002
9.5	**0.071**	0.017	**0.039**	0.002	**0.038**	0.001	**0.019**	0.008	**0.066**	0.010	**0.044**	0.003
10.5	**0.045**	0.012	**0.051**	0.007	**0.047**	0.015	**0.019**	0.011	**0.056**	0.006	**0.037**	0.004
11.5	**0.040**	0.002	**0.063**	0.007	**0.028**	0.008	**0.031**	0.009	**0.067**	0.005	**0.046**	0.005
12.5	**0.037**	0.006	**0.055**	0.006	**0.065**	0.010	**0.038**	0.004	**0.038**	0.011	**0.047**	0.003
13.5	**0.029**	0.007	**0.049**	0.008	**0.034**	0.005	**0.028**	0.006	**0.051**	0.011	**0.033**	0.004
14.5	**0.043**	0.001	**0.053**	0.011	**0.050**	0.013	**0.041**	0.009	**0.057**	0.014	**0.053**	0.004
15.5	**0.041**	0.011	**0.042**	0.011	**0.040**	0.007	**0.026**	0.006	**0.046**	0.010	**0.044**	0.001
blank 1	0.005	0.003	0.006	0.005	0.034	0.014	0.021	0.003	0.014	0.006	0.028	0.007
blank 2	0.007	0.004	0.002	0.001	0.005	0.002	0.012	0.003	0.011	0.005	0.020	0.004
blank 3	0.008	0.002	0.005	0.003	0.017	0.003	0.013	0.006	0.007	0.002	<LoD	
blank 4	0.002	0.002	0.002	0.000	0.007	0.002	0.017	0.005	0.012	0.003	0.012	0.006
blank 5	0.022	0.007	0.008	0.001	0.017	0.003	0.015	0.005	0.007	0.003	0.019	0.004
correction value	0.009		0.005		0.016		0.016		0.010		0.016	
LoD	0.001		0.001		0.001		0.006		0.006		0.010	
LoQ	0.002		0.002		0.002		0.016		0.016		0.028	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.465**	0.023	**0.139**	0.009	**0.280**	0.011	**0.113**	0.011	**0.171**	0.022	**0.118**	0.005
-4.5	**0.376**	0.023	**0.124**	0.005	**0.257**	0.045	**0.152**	0.026	**0.154**	0.026	**0.092**	0.010
-3.5	**0.348**	0.014	**0.108**	0.009	**0.248**	0.021	**0.168**	0.014	**0.200**	0.034	**0.088**	0.007
-2.5	**0.436**	0.015	**0.105**	0.007	**0.285**	0.039	**0.151**	0.024	**0.165**	0.024	**0.108**	0.007
-1.5	**0.288**	0.018	**0.110**	0.008	**0.214**	0.027	**0.157**	0.015	**0.179**	0.018	**0.114**	0.012
-0.5	**0.257**	0.014	**0.125**	0.007	**0.209**	0.015	**0.159**	0.022	**0.162**	0.022	**0.114**	0.014
0.5	**0.222**	0.012	**0.127**	0.010	**0.121**	0.010	**0.112**	0.015	**0.155**	0.021	**0.099**	0.013
1.5	**0.074**	0.007	**0.070**	0.003	**0.116**	0.015	**0.072**	0.012	**0.189**	0.022	**0.049**	0.001
2.5	**0.060**	0.004	**0.060**	0.004	**0.065**	0.018	**0.048**	0.012	**0.126**	0.017	**0.050**	0.004
3.5	**0.070**	0.007	**0.062**	0.005	**0.067**	0.021	0.037	0.008	**0.060**	0.016	**0.042**	0.012
4.5	**0.066**	0.007	**0.059**	0.007	**0.081**	0.015	0.039	0.004	**0.067**	0.009	**0.049**	0.003
5.5	**0.072**	0.006	**0.068**	0.001	**0.060**	0.013	**0.047**	0.012	**0.046**	0.006	**0.056**	0.006
6.5	**0.079**	0.005	**0.061**	0.003	**0.057**	0.005	**0.046**	0.008	**0.069**	0.009	**0.051**	0.010
7.5	**0.081**	0.008	**0.069**	0.004	0.045	0.013	**0.046**	0.006	**0.050**	0.006	**0.041**	0.011
8.5	**0.076**	0.007	**0.069**	0.005	0.051	0.016	**0.042**	0.011	**0.052**	0.006	**0.038**	0.006
9.5	**0.071**	0.006	**0.070**	0.002	**0.054**	0.004	**0.046**	0.007	**0.071**	0.020	**0.053**	0.013
10.5	no sample**	no sample**	**0.069**	0.004	**0.070**	0.015	**0.048**	0.013	**0.053**	0.012	**0.045**	0.010
11.5	**0.097**	0.008	**0.058**	0.001	0.042	0.016	0.038	0.011	**0.040**	0.006	**0.044**	0.022
12.5	no sample**	no sample**	**0.058**	0.004	0.049	0.021	**0.042**	0.015	**0.058**	0.009	**0.039**	0.009
13.5	**0.071**	0.006	**0.067**	0.003	**0.067**	0.010	0.038	0.007	**0.067**	0.017	**0.017**	0.004
14.5	no sample**	no sample**	**0.088**	0.002	0.042	0.008	**0.051**	0.015	**0.069**	0.003	**0.028**	0.007
15.5	**0.057**	0.006	**0.080**	0.006	no sample**	no sample**	**0.040**	0.014	**0.057**	0.009	**0.039**	0.008
blank 1	0.016	0.001	<LoD		<LoD		<LoD		<LoD		0.006	0.003
blank 2	0.017	0.002	<LoD		<LoD		<LoD		<LoD		0.003	0.005
blank 3	<LoD		<LoD		0.022	0.012	<LoD		<LoD		0.006	0.003
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		0.010	0.005
blank 5	<LoD		<LoD		0.022	0.007	<LoD		<LoD		0.001	0.003
correction value	0.007		0.000		0.009		0.000		0.000		0.005	
LoD	0.015		0.015		0.020		0.014		0.014		0.006	
LoQ	0.044		0.044		0.054		0.040		0.040		0.013	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 59: Antimony concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.379**	0.027	**0.471**	0.035	**0.647**	0.030	**0.375**	0.030	**0.544**	0.043	**0.525**	0.021
-4.5	**0.539**	0.026	**0.686**	0.029	**0.845**	0.056	**0.318**	0.015	**0.365**	0.027	**0.362**	0.008
-3.5	**0.460**	0.017	**0.762**	0.027	**0.697**	0.022	**0.435**	0.022	**0.820**	0.057	**0.525**	0.029
-2.5	**0.499**	0.024	**0.847**	0.048	**0.708**	0.040	**0.273**	0.011	**0.714**	0.051	**0.633**	0.034
-1.5	**0.502**	0.028	**0.648**	0.037	**0.519**	0.020	**0.277**	0.019	**0.675**	0.049	**0.551**	0.023
-0.5	**0.541**	0.025	**0.133**	0.009	**0.151**	0.012	**0.238**	0.022	**0.621**	0.018	**0.504**	0.019
0.5	**0.527**	0.027	**0.076**	0.011	**0.078**	0.008	**0.271**	0.015	**0.539**	0.053	**0.405**	0.026
1.5	**0.154**	0.021	**0.073**	0.004	**0.074**	0.014	**0.180**	0.012	**0.084**	0.007	**0.111**	0.007
2.5	**0.076**	0.012	**0.053**	0.003	**0.067**	0.012	no sample ***	no sample ***	**0.055**	0.007	**0.089**	0.007
3.5	**0.057**	0.011	**0.060**	0.007	**0.064**	0.011	no sample ***	no sample ***	**0.053**	0.009	**0.084**	0.005
4.5	**0.054**	0.014	**0.065**	0.006	**0.066**	0.008	**0.059**	0.008	**0.060**	0.010	**0.094**	0.003
5.5	**0.057**	0.008	**0.050**	0.005	**0.055**	0.008	0.030	0.005	**0.083**	0.014	**0.096**	0.004
6.5	**0.070**	0.008	**0.079**	0.008	**0.088**	0.017	0.030	0.002	**0.049**	0.005	**0.074**	0.007
7.5	**0.067**	0.009	**0.058**	0.008	**0.058**	0.010	0.032	0.005	**0.054**	0.013	**0.070**	0.004
8.5	**0.061**	0.007	**0.048**	0.010	**0.046**	0.003	0.034	0.008	**0.061**	0.008	**0.070**	0.005
9.5	**0.043**	0.001	**0.047**	0.003	**0.059**	0.008	0.035	0.010	**0.064**	0.010	**0.074**	0.004
10.5	**0.058**	0.012	**0.046**	0.007	**0.061**	0.006	0.034	0.007	**0.050**	0.010	**0.060**	0.003
11.5	**0.049**	0.008	**0.041**	0.005	**0.059**	0.008	0.038	0.006	**0.050**	0.013	**0.075**	0.001
12.5	**0.041**	0.006	**0.040**	0.006	**0.088**	0.012	no sample ***	no sample ***	**0.060**	0.013	**0.067**	0.002
13.5	**0.056**	0.010	**0.047**	0.003	**0.056**	0.009	0.041	0.013	**0.055**	0.008	**0.075**	0.007
14.5	**0.052**	0.007	**0.040**	0.009	**0.052**	0.012	no sample ***	no sample ***	**0.054**	0.009	**0.051**	0.003
15.5	**0.030**	0.006	**0.041**	0.009	**0.069**	0.017	no sample ***	no sample ***	**0.050**	0.010	**0.065**	0.005
blank 1	0.023	0.004	<LoD		0.006	0.002	<LoD		<LoD		<LoD	
blank 2	0.008	0.000	0.002	0.001	0.003	0.003	0.021	0.007	<LoD		<LoD	
blank 3	0.015	0.002	0.005	0.001	0.009	0.004	<LoD		<LoD		<LoD	
blank 4	0.010	0.004	0.009	0.001	<LoD		<LoD		<LoD		<LoD	
blank 5	0.007	0.003	0.016	0.004	0.002	0.001					<LoD	
correction value	0.013		0.006		0.004		0.004		0.000		0.000	
LoD	0.002		0.002		0.002		0.016		0.016		0.013	
LoQ	0.004		0.004		0.004		0.048		0.048		0.034	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.299**	0.018	**0.134**	0.006	**0.203**	0.035	**0.083**	0.013	**0.127**	0.011	**0.096**	0.010
-4.5	**0.395**	0.010	**0.104**	0.006	**0.215**	0.042	**0.070**	0.009	**0.130**	0.018	**0.109**	0.008
-3.5	**0.376**	0.011	**0.102**	0.009	**0.220**	0.021	**0.084**	0.013	**0.186**	0.019	**0.099**	0.006
-2.5	**0.303**	0.023	**0.089**	0.007	**0.193**	0.015	**0.094**	0.010	**0.116**	0.013	**0.090**	0.006
-1.5	**0.291**	0.011	**0.086**	0.004	**0.207**	0.028	**0.115**	0.015	**0.100**	0.010	**0.099**	0.009
-0.5	**0.273**	0.015	**0.111**	0.005	**0.193**	0.038	**0.100**	0.007	**0.109**	0.012	**0.104**	0.016
0.5	**0.229**	0.020	**0.114**	0.007	**0.162**	0.030	**0.063**	0.020	**0.106**	0.009	**0.104**	0.014
1.5	**0.069**	0.004	**0.056**	0.005	**0.054**	0.015	0.040	0.013	**0.118**	0.014	**0.061**	0.004
2.5	**0.065**	0.003	**0.056**	0.004	**0.061**	0.023	0.036	0.009	**0.110**	0.016	**0.054**	0.010
3.5	**0.060**	0.006	**0.056**	0.005	0.027	0.008	0.028	0.003	**0.074**	0.016	**0.049**	0.007
4.5	**0.084**	0.007	**0.060**	0.002	**0.032**	0.016	0.043	0.018	**0.048**	0.014	**0.058**	0.012
5.5	**0.053**	0.004	**0.055**	0.005	**0.032**	0.004	0.028	0.003	**0.058**	0.015	**0.054**	0.011
6.5	**0.060**	0.004	**0.054**	0.003	0.027	0.012	0.029	0.007	no sample**	no sample**	**0.043**	0.008
7.5	**0.060**	0.006	**0.052**	0.004	**0.039**	0.020	0.032	0.012	no sample**	no sample**	**0.054**	0.008
8.5	**0.047**	0.002	**0.049**	0.004	**0.056**	0.011	0.037	0.014	no sample**	no sample**	**0.086**	0.082
9.5	**0.054**	0.002	**0.054**	0.004	**0.031**	0.017	0.027	0.002	no sample**	no sample**	**0.051**	0.012
10.5	**0.048**	0.002	**0.058**	0.002	**0.029**	0.022	0.046	0.011	no sample**	no sample**	**0.052**	0.012
11.5	0.043	0.004	**0.056**	0.002	**0.032**	0.006	0.035	0.013	no sample**	no sample**	**0.047**	0.011
12.5	**0.052**	0.005	**0.047**	0.003	0.022	0.013	<LoD		no sample**	no sample**	no sample**	no sample**
13.5	**0.052**	0.003	**0.052**	0.003	**0.043**	0.012	no sample ***	no sample ***	no sample**	no sample**	**0.044**	0.007
14.5	**0.050**	0.004	**0.054**	0.004	**0.043**	0.012	no sample ***	no sample ***	no sample**	no sample**	**0.054**	0.009
15.5	**0.051**	0.003	**0.054**	0.004	**0.043**	0.018	no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	<LoD		<LoD		0.015	0.004	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.014	0.005	<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		0.041	0.012	<LoD		<LoD		<LoD	
blank 4	0.021	0.004	<LoD		0.023	0.008	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		0.042	0.010	<LoD		<LoD		<LoD	
correction value	0.004		0.000		0.027		0.000		0.000		0.000	
LoD	0.020		0.020		0.010		0.020		0.014		0.006	
LoQ	0.044		0.044		0.028		0.054		0.040		0.013	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 60: Thallium concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.119**	0.015	**0.072**	0.009	**0.223**	0.016	0.061	0.004	**0.540**	0.009	**0.191**	0.015
-4.5	**0.126**	0.007	**0.054**	0.004	**0.245**	0.004	0.078	0.005	**0.477**	0.020	**0.163**	0.007
-3.5	**0.105**	0.003	**0.055**	0.005	**0.200**	0.009	0.110	0.008	**0.461**	0.018	**0.144**	0.007
-2.5	**0.084**	0.008	**0.051**	0.002	**0.169**	0.001	0.127	0.006	**0.248**	0.011	**0.121**	0.006
-1.5	**0.094**	0.008	**0.074**	0.003	**0.207**	0.009	0.125	0.007	**0.207**	0.012	**0.147**	0.010
-0.5	**0.089**	0.005	**0.065**	0.003	**0.121**	0.003	0.105	0.005	**0.347**	0.021	**0.164**	0.006
0.5	**0.035**	0.003	**0.034**	0.000	**0.037**	0.004	0.115	0.008	0.073	0.008	**0.127**	0.007
1.5	**0.011**	0.003	**0.017**	0.001	**0.071**	0.014	0.068	0.005	<LoD		0.022	0.004
2.5	**0.017**	0.002	**0.028**	0.003	**0.083**	0.007	<LoD		<LoD		0.019	0.005
3.5	**0.016**	0.000	**0.040**	0.006	**0.031**	0.001	0.081	0.002	<LoD		<LoD	
4.5	**0.021**	0.000	**0.059**	0.010	**0.036**	0.004	<LoD		<LoD		0.026	0.002
5.5	**0.024**	0.001	**0.072**	0.008	**0.059**	0.002	<LoD		<LoD		0.066	0.005
6.5	**0.014**	0.003	**0.024**	0.004	**0.105**	0.013	<LoD		0.091	0.001	<LoD	
7.5	**0.049**	0.006	**0.169**	0.008	**0.074**	0.008	0.081	0.009	<LoD		<LoD	
8.5	**0.035**	0.007	**0.121**	0.004	**0.038**	0.001	<LoD		<LoD		0.027	0.002
9.5	**0.027**	0.005	**0.025**	0.001	**0.022**	0.002	<LoD		<LoD		<LoD	
10.5	**0.029**	0.000	**0.028**	0.007	**0.005**	0.001	<LoD		<LoD		<LoD	
11.5	**0.010**	0.001	**0.019**	0.002	**0.006**	0.001	<LoD		0.067	0.005	<LoD	
12.5	**0.009**	0.001	**0.050**	0.007	**0.009**	0.002	<LoD		<LoD		0.017	0.002
13.5	**0.027**	0.003	**0.025**	0.003	**0.006**	0.001	<LoD		<LoD		0.019	0.003
14.5	**0.076**	0.006	**0.025**	0.003	**0.022**	0.003	<LoD		<LoD		0.020	0.003
15.5	**0.010**	0.002	**0.029**	0.001	**0.008**	0.001	<LoD		**0.479**	0.017	<LoD	
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
correction value	0.000		0.000		0.000		0.000		0.000		0.000	
LoD	0.002		0.002		0.002		0.068		0.068		0.040	
LoQ	0.004		0.004		0.004		0.187		0.187		0.094	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.089**	0.004	**0.823**	0.013	**8.679**	0.197	**13.074**	0.349	**23.818**	0.708	**71.419**	1.994
-4.5	**0.054**	0.002	**1.566**	0.023	**7.176**	0.114	**12.711**	0.369	**24.131**	0.746	**66.216**	0.428
-3.5	0.036	0.002	**2.252**	0.018	**13.526**	0.351	**13.022**	0.295	**23.079**	0.639	**45.354**	1.012
-2.5	0.027	0.001	**2.525**	0.048	**15.914**	0.346	**8.380**	0.849	**28.865**	0.543	**37.434**	0.752
-1.5	0.030	0.001	**2.400**	0.171	**6.339**	0.229	**11.354**	0.207	**24.319**	0.318	**34.850**	0.295
-0.5	0.045	0.003	**2.519**	0.028	**11.250**	0.149	**10.517**	0.289	**25.534**	0.491	**34.370**	0.427
0.5	0.014	0.001	**0.883**	0.081	**0.465**	0.030	**0.186**	0.010	**22.524**	0.625	**16.662**	0.248
1.5	0.037	0.001	0.042	0.003	**0.434**	0.032	**0.053**	0.004	**0.080**	0.024	**0.080**	0.011
2.5	0.030	0.002	**0.821**	0.006	**0.247**	0.010	**0.042**	0.006	**0.092**	0.007	**0.058**	0.007
3.5	0.012	0.001	**0.082**	0.002	**0.482**	0.051	<LoD		<LoD		**0.080**	0.008
4.5	**0.069**	0.004	**0.054**	0.002	**0.425**	0.037	**0.038**	0.005	**0.042**	0.007	**0.103**	0.011
5.5	0.016	0.001	**0.156**	0.002	**0.240**	0.012	**0.039**	0.006	**0.059**	0.004	**0.070**	0.006
6.5	**0.111**	0.004	**0.225**	0.002	no sample *	no sample *	**0.032**	0.005	**0.029**	0.001	**0.069**	0.006
7.5	0.010	0.001	**0.062**	0.006	no sample *	no sample *	<LoD		<LoD		**0.060**	0.005
8.5	**0.057**	0.003	**0.086**	0.002	no sample *	no sample *	**0.031**	0.006	**0.041**	0.004	**0.076**	0.008
9.5	**0.063**	0.001	**0.086**	0.003	**0.370**	0.012	<LoD		<LoD		**0.109**	0.010
10.5	0.035	0.002	**0.093**	0.002	**0.757**	0.039	**0.035**	0.004	<LoD		**0.088**	0.008
11.5	0.032	0.002	**0.141**	0.003	**0.447**	0.020	**0.042**	0.002	**0.081**	0.005	**0.082**	0.010
12.5	0.038	0.001	**0.097**	0.001	**0.195**	0.010	<LoD		**0.034**	0.004	**0.061**	0.012
13.5	**0.056**	0.002	**0.087**	0.001	**0.407**	0.022	**0.047**	0.008	<LoD		**0.120**	0.007
14.5	0.032	0.002	**0.083**	0.002	**0.333**	0.022	<LoD		**0.049**	0.003	no sample **	no sample **
15.5	0.039	0.000	**0.066**	0.002	**0.194**	0.009	<LoD		**0.029**	0.003	**0.056**	0.010
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		0.002	0.001	<LoD		<LoD	
blank 3	<LoD		<LoD		0.003	0.001	<LoD		0.002	0.001	<LoD	
blank 4	<LoD		<LoD		0.004	0.001	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
correction value	0.000		0.000		0.001		0.000		0.000		0.000	
LoD	0.020		0.020		0.003		0.002		0.002		0.003	
LoQ	0.050		0.050		0.008		0.005		0.005		0.009	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 61: Thallium concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.195**	0.008	**0.154**	0.004	**0.281**	0.010	0.193	0.014	**0.622**	0.023	**0.865**	0.004
-4.5	**0.176**	0.004	**0.059**	0.004	**0.354**	0.014	0.151	0.011	**0.942**	0.027	**0.628**	0.012
-3.5	**0.193**	0.006	**0.051**	0.003	**0.241**	0.009	**0.260**	0.013	**0.673**	0.029	**0.261**	0.008
-2.5	**0.221**	0.005	**0.059**	0.002	**0.242**	0.007	**0.272**	0.018	**0.622**	0.038	**0.241**	0.004
-1.5	**0.230**	0.006	**0.054**	0.002	**0.241**	0.005	**1.447**	0.028	**0.464**	0.026	0.079	0.002
-0.5	**0.163**	0.007	**0.067**	0.003	**0.138**	0.011	**0.296**	0.010	**0.307**	0.011	**0.168**	0.006
0.5	**0.134**	0.007	**0.095**	0.005	**0.061**	0.005	<LoD		**0.300**	0.019	**0.182**	0.004
1.5	**0.070**	0.006	**0.052**	0.006	**0.042**	0.003	**0.232**	0.010	<LoD		**0.135**	0.005
2.5	**0.045**	0.005	**0.074**	0.005	0.027	0.002	0.169	0.011	<LoD		**0.123**	0.008
3.5	**0.108**	0.006	**0.036**	0.002	**0.042**	0.002	**0.325**	0.015	<LoD		**0.121**	0.002
4.5	0.028	0.004	0.029	0.003	0.030	0.003	**0.333**	0.017	<LoD		0.048	0.001
5.5	0.030	0.004	0.028	0.001	**0.040**	0.004	**3.562**	0.078	<LoD		0.024	0.001
6.5	0.028	0.004	0.032	0.004	**0.122**	0.008	no sample ***	no sample ***	<LoD		0.061	0.002
7.5	0.025	0.002	0.026	0.003	**0.043**	0.003	no sample ***	no sample ***	<LoD		0.064	0.002
8.5	0.035	0.002	**0.199**	0.012	0.027	0.004	no sample ***	no sample ***	<LoD		0.079	0.003
9.5	0.237	0.014	**0.059**	0.004	<LoD		no sample ***	no sample ***	<LoD		0.030	0.002
10.5	<LoD		**0.101**	0.004	<LoD		**0.279**	0.029	<LoD		0.042	0.001
11.5	<LoD		0.028	0.002	<LoD		<LoD		<LoD		0.022	0.001
12.5	0.026	0.004	<LoD		<LoD		**0.301**	0.012	<LoD		0.042	0.002
13.5	0.035	21.474	0.025	0.002	<LoD		<LoD		<LoD		<LoD	
14.5	<LoD		**0.154**	0.007	<LoD		<LoD		<LoD		0.018	0.002
15.5	<LoD		<LoD		<LoD		no sample ***	no sample ***	<LoD		0.047	0.004
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		<LoD				<LoD	
correction value	0.000		0.000		0.000		0.000		0.000		0.000	
LoD	0.016		0.016		0.016		0.069		0.069		0.047	
LoQ	0.036		0.036		0.036		0.195		0.195		0.101	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.206**	0.005	**0.798**	0.028	**9.375**	0.353	**14.029**	0.479	**23.610**	0.283	**57.693**	0.805
-4.5	**0.203**	0.005	**1.537**	0.041	**5.803**	0.343	**11.554**	0.361	**21.678**	0.473	**58.219**	0.822
-3.5	0.049	0.003	**2.226**	0.024	**6.857**	0.196	**9.927**	0.157	**25.405**	0.678	**42.876**	0.863
-2.5	0.049	0.002	**2.422**	0.029	**5.560**	0.153	**9.605**	0.246	**24.653**	0.320	**36.367**	0.585
-1.5	0.037	0.002	**2.336**	0.025	**5.894**	0.189	**10.218**	0.254	**18.434**	0.271	**35.061**	0.851
-0.5	<LoD		**2.444**	0.042	**5.213**	0.091	**8.885**	0.269	**16.583**	0.117	**33.897**	0.700
0.5	<LoD		**1.830**	0.028	**1.202**	0.041	**1.538**	0.044	**21.459**	0.177	**17.014**	0.263
1.5	0.032	0.003	0.053	0.003	**0.217**	0.022	**0.061**	0.004	**0.411**	0.021	**0.236**	0.015
2.5	<LoD		**0.097**	0.002	**0.176**	0.007	**0.029**	0.001	**0.545**	0.009	**0.184**	0.004
3.5	0.036	0.001	**0.575**	0.009	**0.182**	0.008	**0.353**	0.016	<LoD		**0.263**	0.006
4.5	<LoD		0.076	0.003	**0.151**	0.012	**0.025**	0.005	**0.032**	0.004	**0.132**	0.008
5.5	<LoD		0.076	0.002	**0.154**	0.012	**0.029**	0.007	<LoD		no sample **	no sample **
6.5	<LoD		**0.120**	0.004	no sample *	no sample *	**0.021**	0.004	<LoD		**0.101**	0.012
7.5	<LoD		**0.110**	0.002	no sample *	no sample *	**0.092**	0.007	**0.052**	0.010	**0.066**	0.037
8.5	<LoD		**0.165**	0.008	no sample *	no sample *	**0.030**	0.002	<LoD		**0.075**	0.004
9.5	0.021	0.002	0.050	0.002	**0.127**	0.007	<LoD		<LoD		**0.096**	0.010
10.5	0.027	0.002	0.092	0.002	**0.189**	0.008	**0.025**	0.004	**0.056**	0.005	**0.184**	0.010
11.5	0.019	0.002	**0.577**	0.008	**0.145**	0.007	<LoD		**0.054**	0.004	no sample **	no sample **
12.5	0.016	0.002	<LoD		**0.180**	0.010	<LoD		<LoD		no sample **	no sample **
13.5	0.061	0.003	**0.166**	0.003	**0.148**	0.009	<LoD		<LoD		no sample **	no sample **
14.5	<LoD		0.074	0.003	**0.174**	0.003	<LoD		**0.039**	0.003	no sample **	no sample **
15.5	<LoD		**0.175**	0.004	**0.165**	0.002	**0.033**	0.004	<LoD		no sample **	no sample **
blank 1	<LoD		<LoD		0.031	0.006	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.003	0.002	<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		0.002	0.002	<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		0.001	0.000	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		<LoD				<LoD	
correction value	0.000		0.000		0.008		0.000		0.000		0.000	
LoD	0.047		0.040		0.001		0.003		0.002		0.003	
LoQ	0.101		0.094		0.003		0.008		0.005		0.009	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 62: Thallium concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.145**	0.008	**0.208**	0.020	**0.289**	0.029	0.082	0.005	0.102	0.008	**0.398**	0.016
-4.5	**0.153**	0.013	**0.172**	0.011	**0.410**	0.043	0.164	0.015	0.119	0.007	**0.345**	0.010
-3.5	**0.171**	0.002	**0.164**	0.005	**0.290**	0.029	<LoD		0.134	0.006	**0.306**	0.011
-2.5	**0.132**	0.007	**0.232**	0.011	**0.186**	0.010	0.127	0.009	0.078	0.008	**0.353**	0.011
-1.5	**0.158**	0.016	**0.156**	0.013	**0.148**	0.013	<LoD		**0.196**	0.015	**0.335**	0.013
-0.5	**0.194**	0.006	**0.066**	0.006	**0.033**	0.004	<LoD		0.153	0.007	**0.407**	0.017
0.5	**0.062**	0.009	**0.056**	0.008	**0.035**	0.003	<LoD		0.146	0.009	**0.204**	0.008
1.5	**0.041**	0.003	**0.030**	0.003	**0.050**	0.003	<LoD		<LoD		<LoD	
2.5	**0.022**	0.002	**0.025**	0.002	**0.029**	0.004	<LoD		0.072	0.008	<LoD	
3.5	**0.010**	0.002	**0.022**	0.002	**0.029**	0.002	<LoD		0.180	0.013	<LoD	
4.5	**0.016**	0.002	**0.027**	0.002	**0.029**	0.004	<LoD		0.081	0.005	<LoD	
5.5	**0.031**	0.006	**0.023**	0.006	**0.028**	0.005	<LoD		0.077	0.006	<LoD	
6.5	**0.013**	0.002	**0.018**	0.001	**0.036**	0.007	<LoD		<LoD		<LoD	
7.5	**0.014**	0.000	**0.019**	0.001	**0.056**	0.005	<LoD		0.061	0.004	0.073	0.003
8.5	**0.020**	0.004	**0.039**	0.004	**0.099**	0.003	<LoD		**0.198**	0.010	<LoD	
9.5	**0.037**	0.005	**0.041**	0.011	**0.017**	0.001	<LoD		<LoD		<LoD	
10.5	**0.015**	0.002	**0.022**	0.003	**0.054**	0.004	<LoD		0.094	0.010	<LoD	
11.5	**0.009**	0.000	**0.027**	0.001	**0.029**	0.004	<LoD		0.067	0.004	<LoD	
12.5	**0.032**	0.002	**0.021**	0.003	**0.159**	0.011	<LoD		<LoD		<LoD	
13.5	**0.015**	0.002	**0.049**	0.001	**0.024**	0.002	<LoD		0.073	0.005	<LoD	
14.5	**0.030**	0.005	**0.019**	0.001	**0.010**	0.001	<LoD		<LoD		<LoD	
15.5	**0.023**	0.004	**0.008**	0.003	**0.005**	0.001	<LoD		0.071	0.003	<LoD	
blank 1	<LoD		<LoD		0.003	0.001	<LoD		<LoD		0.003	0.001
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		0.003	0.001
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		0.002	0.001
blank 5	<LoD		<LoD		<LoD		<LoD		<LoD		0.004	0.001
correction value	0.000		0.000		0.001		0.000		0.000		0.003	
LoD	0.002		0.002		0.002		0.068		0.068		0.001	
LoQ	0.004		0.004		0.004		0.187		0.187		0.003	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.194**	0.005	**0.736**	0.010	**0.305**	0.012	**0.115**	0.006	**0.128**	0.008	**4.246**	0.061
-4.5	**0.099**	0.002	**0.035**	0.002	**0.266**	0.004	**0.069**	0.005	**0.199**	0.006	**0.069**	0.005
-3.5	**0.061**	0.002	**0.057**	0.001	**0.264**	0.013	**0.216**	0.013	**0.114**	0.006	**0.080**	0.006
-2.5	**0.247**	0.008	0.045	0.003	**0.250**	0.013	**0.080**	0.005	**0.470**	0.016	**0.067**	0.011
-1.5	**0.280**	0.006	**0.074**	0.001	**0.193**	0.011	**0.082**	0.012	**0.037**	0.004	<LoD	
-0.5	0.037	0.001	**0.052**	0.002	**0.395**	0.024	**0.094**	0.005	<LoD		**0.035**	0.004
0.5	0.047	0.002	0.033	0.002	**0.215**	0.005	**0.060**	0.008	**0.067**	0.008	<LoD	
1.5	0.020	0.001	**0.129**	0.004	**0.459**	0.012	**0.072**	0.004	<LoD		**0.035**	0.003
2.5	0.018	0.001	0.041	0.001	**0.406**	0.015	**0.050**	0.005	<LoD		<LoD	
3.5	**0.050**	0.001	**0.068**	0.002	**0.256**	0.014	<LoD		<LoD		**0.041**	0.004
4.5	**0.077**	0.002	**0.083**	0.002	**0.340**	0.020	**0.038**	0.004	**0.080**	0.009	**0.045**	0.003
5.5	**0.054**	0.003	**0.081**	0.003	**0.466**	0.025	**0.050**	0.004	**0.034**	0.007	**0.081**	0.015
6.5	**0.055**	0.003	**0.079**	0.003	**0.509**	0.016	**0.059**	0.004	**0.037**	0.008	**0.174**	0.016
7.5	**0.195**	0.004	0.227	0.003	**0.468**	0.016	**0.085**	0.007	#WERT!	#WERT!	**0.076**	0.008
8.5	**0.114**	0.004	**0.093**	0.002	**0.592**	0.027	**0.066**	0.006	**0.283**	0.020	**0.191**	0.004
9.5	**0.089**	0.003	0.369	0.010	**0.264**	0.017	**0.094**	0.005	**0.576**	0.014	**0.183**	0.009
10.5	no sample**	no sample**	**0.178**	0.002	**0.299**	0.010	<LoD		**0.317**	0.014	**0.107**	0.012
11.5	**0.622**	0.005	0.037	0.001	**0.288**	0.014	**0.065**	0.005	**0.043**	0.001	**0.209**	0.013
12.5	no sample**	no sample**	**0.063**	0.002	**0.309**	0.004	**0.097**	0.010	**0.151**	0.005	**0.176**	0.006
13.5	**0.725**	0.042	**0.303**	0.003	**0.336**	0.016	**0.048**	0.005	#WERT!	#WERT!	**0.225**	0.021
14.5	no sample**	no sample**	**0.209**	0.006	**0.356**	0.020	**0.033**	0.007	**0.050**	0.005	**0.171**	0.014
15.5	**0.077**	0.001	**0.207**	0.004	no sample**	no sample**	**0.056**	0.007	#WERT!	#WERT!	**0.125**	0.009
blank 1	<LoD		<LoD		0.007	0.001	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.004	0.001	<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		0.004	0.001	<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		0.005	0.001	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		0.002	0.001	<LoD		<LoD	
correction value	0.000		0.000		0.004		0.000		0.000		0.000	
LoD	0.020		0.020		0.003		0.002		0.002		0.003	
LoQ	0.050		0.050		0.008		0.005		0.005		0.009	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 63: Thallium concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.283**	0.009	**0.277**	0.009	**0.426**	0.009	**0.212**	0.022	**1.606**	0.102	**1.593**	0.045
-4.5	**0.404**	0.013	**0.412**	0.006	**0.567**	0.003	**0.261**	0.018	**1.072**	0.059	**1.012**	0.017
-3.5	**0.360**	0.014	**0.422**	0.014	**0.384**	0.009	**0.265**	0.022	**1.736**	0.044	**1.328**	0.017
-2.5	**0.367**	0.010	**0.487**	0.007	**0.355**	0.008	**0.254**	0.010	**1.677**	0.075	**1.459**	0.032
-1.5	**0.355**	0.008	**0.374**	0.009	**0.244**	0.006	**0.235**	0.007	**1.604**	0.090	**1.180**	0.015
-0.5	**0.407**	0.008	**0.142**	0.005	**0.087**	0.004	**0.256**	0.013	**1.321**	0.029	**1.388**	0.038
0.5	**0.368**	0.010	**0.121**	0.003	**0.065**	0.004	**0.256**	0.007	**1.012**	0.051	**1.162**	0.022
1.5	**0.082**	0.004	**0.078**	0.004	**0.069**	0.006	**0.220**	0.012	0.164	0.007	**0.112**	0.005
2.5	**0.049**	0.002	**0.051**	0.003	**0.045**	0.003	no sample ***	no sample ***	<LoD		**0.103**	0.006
3.5	**0.047**	0.005	**0.045**	0.002	**0.037**	0.002	no sample ***	no sample ***	<LoD		0.053	0.002
4.5	**0.041**	0.003	**0.059**	0.004	0.028	0.003	<LoD		<LoD		0.065	0.001
5.5	**0.064**	0.004	0.031	0.004	**0.083**	0.108	<LoD		<LoD		0.059	0.002
6.5	**0.049**	0.002	**0.068**	0.003	0.035	0.002	<LoD		<LoD		**0.130**	0.003
7.5	**0.056**	0.004	**0.041**	0.004	0.032	0.003	<LoD		<LoD		0.076	0.005
8.5	**0.116**	0.002	0.036	0.003	<LoD		<LoD		<LoD		0.055	0.003
9.5	**0.083**	0.003	**0.038**	0.004	0.033	0.003	<LoD		<LoD		0.057	0.005
10.5	0.026	0.001	**0.057**	0.002	<LoD		<LoD		<LoD		0.054	0.001
11.5	0.029	0.005	0.028	0.003	0.025	0.001	<LoD		<LoD		**0.177**	0.012
12.5	**0.037**	0.002	**0.048**	0.004	0.027	0.002	no sample ***	no sample ***	<LoD		0.034	0.002
13.5	**0.071**	0.005	**0.039**	0.002	<LoD		<LoD		<LoD		**0.108**	0.009
14.5	<LoD		**0.048**	0.002	<LoD		no sample ***	no sample ***	<LoD		0.044	0.004
15.5	<LoD		0.027	0.002	<LoD		no sample ***	no sample ***	<LoD		0.036	0.002
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD						<LoD	
correction value	0.000		0.000		0.000		0.000		0.000		0.000	
LoD	0.016		0.016		0.016		0.069		0.069		0.047	
LoQ	0.036		0.036		0.036		0.195		0.195		0.101	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.333**	0.010	**0.908**	0.028	**0.180**	0.011	**0.054**	0.005	**0.315**	0.017	**0.091**	0.009
-4.5	**0.165**	0.005	**0.160**	0.006	**0.386**	0.023	**0.112**	0.009	**0.093**	0.007	<LoD	
-3.5	**0.101**	0.005	**0.112**	0.004	**0.217**	0.010	**0.149**	0.012	**0.067**	0.004	<LoD	
-2.5	0.076	0.002	**0.134**	0.005	**0.169**	0.012	**0.103**	0.012	**0.032**	0.004	**0.038**	0.002
-1.5	0.056	0.001	**0.329**	0.011	**0.177**	0.006	**0.106**	0.015	**0.041**	0.007	**0.039**	0.005
-0.5	<LoD		**0.126**	0.003	**0.200**	0.012	**0.128**	0.014	**0.031**	0.004	**0.042**	0.005
0.5	**0.110**	0.004	<LoD		**0.301**	0.020	**0.058**	0.007	**0.031**	0.006	**0.041**	0.006
1.5	<LoD		0.068	0.002	**0.199**	0.009	**0.085**	0.004	<LoD		**0.052**	0.005
2.5	0.068	0.002	0.061	0.003	**0.220**	0.014	**0.070**	0.008	**0.041**	0.007	<LoD	
3.5	<LoD		0.076	0.002	**0.206**	0.013	<LoD		**0.146**	0.019	<LoD	
4.5	<LoD		**0.212**	0.004	**0.221**	0.014	**0.057**	0.005	<LoD		**0.070**	0.010
5.5	<LoD		0.059	0.002	**0.196**	0.008	**0.065**	0.005	**0.141**	0.006	**1.026**	0.052
6.5	**0.115**	0.004	**0.130**	0.004	**0.199**	0.008	**0.097**	0.014	no sample**	no sample**	<LoD	
7.5	<LoD		**0.423**	0.010	**0.154**	0.012	**0.130**	0.008	no sample**	no sample**	**0.059**	0.011
8.5	<LoD		**0.116**	0.003	**0.478**	0.030	**0.047**	0.003	no sample**	no sample**	**0.093**	0.010
9.5	<LoD		**0.175**	0.003	**0.155**	0.012	**0.050**	0.002	no sample**	no sample**	**0.123**	0.006
10.5	<LoD		**0.188**	0.007	**0.205**	0.008	**0.099**	0.007	no sample**	no sample**	**0.116**	0.002
11.5	<LoD		**0.363**	0.006	**1.897**	0.054	**0.031**	0.007	no sample**	no sample**	**0.034**	0.006
12.5	0.045	0.000	**0.281**	0.008	**0.218**	0.021	<LoD		no sample**	no sample**	no sample**	no sample**
13.5	**0.121**	0.002	**0.374**	0.007	**0.217**	0.018	no sample ***	no sample ***	no sample**	no sample**	**0.131**	0.016
14.5	<LoD		**0.072**	0.002	**0.225**	0.017	no sample ***	no sample ***	no sample**	no sample**	**0.169**	0.005
15.5	<LoD		**1.331**	0.029	**0.190**	0.015	no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	<LoD		<LoD		0.008	0.003	<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		0.006	0.002	<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		0.009	0.001	<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		0.006	0.002	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		0.007	0.002	<LoD		<LoD		<LoD	
correction value	0.000		0.000		0.007		0.000		0.000		0.000	
LoD	0.040		0.040		0.001		0.003		0.002		0.003	
LoQ	0.094		0.094		0.003		0.008		0.005		0.009	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 64: Vanadium concentration across the SWI **(<0.45 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.131**	0.013	**0.150**	0.014	**0.274**	0.010	**0.204**	0.012	**0.392**	0.010	**0.173**	0.015
-4.5	**0.165**	0.008	**0.157**	0.013	**0.299**	0.005	**0.310**	0.013	**0.434**	0.031	**0.158**	0.011
-3.5	**0.173**	0.005	**0.205**	0.013	**0.280**	0.028	**0.382**	0.022	**0.445**	0.024	**0.177**	0.007
-2.5	**0.146**	0.011	**0.141**	0.007	**0.292**	0.031	**0.342**	0.019	**0.207**	0.012	**0.178**	0.008
-1.5	**0.147**	0.025	**0.187**	0.008	**0.302**	0.044	**0.339**	0.025	**0.196**	0.008	**0.169**	0.015
-0.5	**0.182**	0.042	**0.180**	0.006	**0.251**	0.009	**0.374**	0.021	**0.368**	0.023	**0.128**	0.008
0.5	**0.191**	0.002	**0.126**	0.013	**0.124**	0.015	**0.440**	0.020	**0.187**	0.002	**0.157**	0.020
1.5	**0.073**	0.008	**0.070**	0.008	**0.133**	0.004	**0.247**	0.006	**0.190**	0.010	**0.088**	0.004
2.5	**0.059**	0.010	**0.095**	0.003	**0.189**	0.010	**0.105**	0.007	**0.185**	0.009	**0.156**	0.012
3.5	**0.060**	0.007	**0.148**	0.009	**0.180**	0.011	**0.080**	0.009	**0.147**	0.013	**0.117**	0.010
4.5	**0.080**	0.014	**0.184**	0.004	**0.218**	0.026	**0.088**	0.011	**0.176**	0.007	**0.161**	0.008
5.5	**0.129**	0.011	**0.221**	0.020	**0.172**	0.020	**0.078**	0.006	**0.156**	0.002	**0.114**	0.007
6.5	**0.104**	0.011	**0.175**	0.022	**0.173**	0.020	**0.068**	0.004	**0.161**	0.007	**0.119**	0.011
7.5	**0.119**	0.013	**0.180**	0.030	**0.131**	0.006	**0.083**	0.004	**0.201**	0.016	**0.118**	0.011
8.5	**0.195**	0.022	**0.113**	0.011	**0.128**	0.014	**0.087**	0.007	**0.164**	0.011	**0.138**	0.005
9.5	**0.079**	0.004	**0.116**	0.004	**0.128**	0.024	**0.077**	0.005	**0.187**	0.015	**0.119**	0.012
10.5	**0.110**	0.009	**0.117**	0.006	**0.117**	0.005	**0.082**	0.003	**0.159**	0.005	**0.224**	0.015
11.5	**0.081**	0.005	**0.075**	0.005	**0.129**	0.003	**0.087**	0.004	**0.159**	0.003	**0.121**	0.007
12.5	**0.122**	0.011	**0.078**	0.008	**0.098**	0.008	**0.078**	0.005	**0.164**	0.009	**0.131**	0.004
13.5	**0.078**	0.004	**0.078**	0.004	**0.125**	0.015	**0.071**	0.003	**0.177**	0.008	**0.160**	0.015
14.5	**0.096**	0.019	**0.145**	0.021	**0.141**	0.010	**0.077**	0.003	**0.171**	0.007	**0.104**	0.009
15.5	**0.090**	0.010	**0.093**	0.009	**0.157**	0.012	**0.087**	0.006	**0.178**	0.014	**0.127**	0.004
blank 1	0.003	0.001	0.003	0.001	0.011	0.001	<LoD		<LoD		<LoD	
blank 2	0.004	0.001	0.002	0.000	0.008	0.001	<LoD		<LoD		0.003	0.000
blank 3	0.006	0.001	0.004	0.001	0.008	0.000	<LoD		<LoD		<LoD	
blank 4	0.005	0.001	0.010	0.001	0.007	0.002	<LoD		<LoD		<LoD	
blank 5	0.005	0.001	0.002	0.001	0.007	0.002	<LoD		<LoD		0.004	0.001
correction value	0.005		0.004		0.008		0.000		0.000		0.001	
LoD	0.002		0.002		0.002		0.021		0.021		0.003	
LoQ	0.004		0.004		0.004		0.057		0.057		0.009	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.102**	0.008	**0.016**	0.001	<LoD		**0.034**	0.005	**0.032**	0.001	**0.081**	0.005
-4.5	**0.086**	0.004	**0.015**	0.001	<LoD		0.019	0.003	0.017	0.002	0.057	0.006
-3.5	**0.068**	0.002	**0.011**	0.001	<LoD		0.021	0.002	0.017	0.003	**0.092**	0.006
-2.5	**0.051**	0.004	**0.012**	0.000	0.014	0.004	0.009	0.002	0.017	0.003	**0.093**	0.007
-1.5	**0.049**	0.002	**0.010**	0.000	<LoD		0.011	0.002	0.015	0.003	0.060	0.003
-0.5	**0.041**	0.002	**0.010**	0.001	<LoD		0.011	0.003	0.015	0.001	0.055	0.004
0.5	**0.034**	0.001	0.007	0.001	<LoD		0.015	0.001	0.012	0.002	<LoD	
1.5	**0.047**	0.001	**0.010**	0.001	<LoD		**0.025**	0.003	0.016	0.001	0.030	0.003
2.5	**0.082**	0.003	**0.034**	0.002	0.006	0.006	**0.023**	0.003	0.019	0.003	0.039	0.003
3.5	**0.140**	0.006	**0.077**	0.003	**0.066**	0.011	**0.027**	0.004	**0.027**	0.003	0.033	0.002
4.5	**0.127**	0.005	**0.122**	0.007	**0.096**	0.014	**0.068**	0.034	**0.052**	0.006	0.032	0.003
5.5	**0.131**	0.005	**0.161**	0.004	**0.106**	0.011	**0.085**	0.010	**0.089**	0.009	0.040	0.004
6.5	**0.139**	0.004	**0.178**	0.006	no sample *	no sample *	**0.141**	0.009	**0.122**	0.009	0.050	0.006
7.5	**0.131**	0.003	**0.179**	0.007	no sample *	no sample *	**0.157**	0.008	**0.120**	0.009	0.052	0.003
8.5	**0.136**	0.002	**0.186**	0.009	no sample *	no sample *	**0.207**	0.019	**0.128**	0.007	**0.080**	0.004
9.5	**0.134**	0.009	**0.195**	0.002	**0.063**	0.011	**0.197**	0.016	**0.124**	0.007	**0.111**	0.009
10.5	**0.125**	0.007	**0.195**	0.009	**0.124**	0.014	**0.132**	0.020	**0.144**	0.004	**0.127**	0.007
11.5	**0.123**	0.005	**0.200**	0.007	**0.099**	0.007	**0.135**	0.002	**0.146**	0.015	**0.124**	0.002
12.5	**0.118**	0.005	**0.190**	0.012	**0.142**	0.013	**0.136**	0.010	**0.114**	0.003	**0.122**	0.006
13.5	**0.116**	0.003	**0.189**	0.005	**0.158**	0.008	**0.170**	0.003	**0.117**	0.006	**0.103**	0.001
14.5	**0.122**	0.007	**0.178**	0.008	**0.107**	0.017	**0.174**	0.020	**0.145**	0.008	no sample **	no sample **
15.5	**0.125**	0.004	**0.171**	0.008	**0.160**	0.016	**0.209**	0.018	**0.188**	0.012	**0.099**	0.007
blank 1	0.005	0.001	0.003	0.001	0.104	0.008	<LoD		<LoD		<LoD	
blank 2	0.004	0.001	<LoD		0.131	0.006	<LoD		<LoD		<LoD	
blank 3	0.005	0.001	0.005	0.000	0.114	0.005	<LoD		<LoD		<LoD	
blank 4	0.004	0.000	<LoD		0.127	0.011	0.015	0.001	<LoD		<LoD	
blank 5	0.009	0.001	<LoD		0.128	0.013	<LoD		<LoD		<LoD	
correction val	0.006		0.002		0.121		0.003		0.000		0.000	
LoD	0.003		0.003		0.013		0.009		0.009		0.026	
LoQ	0.008		0.008		0.035		0.021		0.021		0.073	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 65: Vanadium concentration across the SWI **(<16 µm) of Experiment A** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.188**	0.006	**0.178**	0.007	**0.213**	0.009	**0.205**	0.016	**0.205**	0.010	**0.155**	0.012
-4.5	**0.172**	0.004	**0.160**	0.007	**0.291**	0.010	**0.193**	0.006	**0.397**	0.013	**0.175**	0.005
-3.5	**0.191**	0.006	**0.140**	0.006	**0.300**	0.011	**0.180**	0.008	**0.369**	0.019	**0.143**	0.013
-2.5	**0.219**	0.006	**0.169**	0.004	**0.293**	0.011	**0.215**	0.001	**0.376**	0.017	**0.135**	0.013
-1.5	**0.203**	0.009	**0.150**	0.008	**0.304**	0.009	**0.220**	0.013	**0.288**	0.015	**0.125**	0.009
-0.5	**0.199**	0.007	**0.184**	0.005	**0.207**	0.014	**0.201**	0.012	**0.204**	0.008	**0.112**	0.008
0.5	**0.337**	0.010	**0.127**	0.004	**0.161**	0.004	**0.206**	0.004	**0.226**	0.018	**0.030**	0.003
1.5	**0.213**	0.007	**0.136**	0.005	**0.181**	0.008	**0.155**	0.005	**0.167**	0.005	**0.045**	0.004
2.5	**0.173**	0.008	**0.176**	0.005	**0.134**	0.001	**0.064**	0.008	**0.162**	0.008	**0.099**	0.007
3.5	**0.146**	0.004	**0.209**	0.006	**0.178**	0.010	**0.101**	0.005	**0.128**	0.005	**0.116**	0.008
4.5	**0.141**	0.003	**0.213**	0.006	**0.216**	0.016	**0.118**	0.010	**0.135**	0.007	**0.116**	0.008
5.5	**0.187**	0.004	**0.247**	0.007	**0.175**	0.004	**0.064**	0.006	**0.151**	0.026	**0.114**	0.006
6.5	**0.152**	0.006	**0.230**	0.007	**0.175**	0.005	no sample ***	no sample ***	**0.141**	0.014	**0.109**	0.005
7.5	**0.148**	0.007	**0.183**	0.006	**0.158**	0.005	no sample ***	no sample ***	**0.142**	0.008	**0.126**	0.005
8.5	**0.159**	0.005	**0.163**	0.007	**0.113**	0.006	no sample ***	no sample ***	**0.144**	0.008	**0.118**	0.004
9.5	**0.195**	0.011	**0.165**	0.005	**0.087**	0.004	no sample ***	no sample ***	**0.145**	0.007	**0.123**	0.003
10.5	**0.193**	0.007	**0.172**	0.006	**0.107**	0.005	**0.083**	0.007	**0.179**	0.006	**0.130**	0.005
11.5	**0.210**	0.005	**0.200**	0.006	**0.107**	0.003	**0.061**	0.006	**0.178**	0.008	**0.134**	0.003
12.5	**0.209**	0.010	**0.188**	0.006	**0.174**	0.010	**0.052**	0.005	**0.172**	0.007	**0.140**	0.006
13.5	**0.243**	21.474	**0.182**	0.007	**0.212**	0.009	**0.056**	0.008	**0.172**	0.010	**0.146**	0.005
14.5	**0.221**	0.005	**0.170**	0.003	**0.195**	0.006	**0.069**	0.003	**0.176**	0.007	**0.150**	0.003
15.5	**0.242**	0.007	**0.196**	0.010	**0.183**	0.005	no sample ***	no sample ***	**0.196**	0.008	**0.162**	0.003
blank 1	<LoD		<LoD		<LoD		0.093	0.014	<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	0.016	0.002	<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		<LoD		<LoD				<LoD	
correction value	0.003		0.000		0.000		0.019		0.000		0.000	
LoD	0.008		0.008		0.008		0.016		0.016		0.011	
LoQ	0.022		0.022		0.022		0.043		0.043		0.031	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.161**	0.008	**0.010**	0.001	**0.041**	0.013	**0.096**	0.009	0.019	0.001	0.073	0.003
-4.5	**0.113**	0.003	<LoD		<LoD		0.015	0.003	0.012	0.004	0.047	0.005
-3.5	**0.094**	0.004	<LoD		<LoD		<LoD		0.010	0.002	**0.413**	0.032
-2.5	**0.095**	0.003	<LoD		<LoD		<LoD		<LoD	0.002	**0.112**	0.009
-1.5	**0.082**	0.002	<LoD		<LoD		<LoD		<LoD	0.001	0.072	0.004
-0.5	**0.056**	0.001	<LoD		<LoD		<LoD		<LoD	0.001	0.048	0.001
0.5	**0.047**	0.001	<LoD		<LoD		0.014	0.002	0.013	0.003	0.056	0.003
1.5	**0.037**	0.002	<LoD		0.013	0.014	0.025	0.004	**0.033**	0.004	0.055	0.004
2.5	**0.125**	0.004	**0.025**	0.002	**0.031**	0.010	0.019	0.002	**0.041**	0.002	0.054	0.003
3.5	**0.164**	0.004	**0.070**	0.005	**0.087**	0.006	**0.052**	0.006	**0.046**	0.002	**0.102**	0.006
4.5	**0.245**	0.020	**0.116**	0.007	**0.110**	0.007	**0.072**	0.006	**0.091**	0.002	0.054	0.001
5.5	**0.204**	0.004	**0.147**	0.010	**0.125**	0.009	**0.169**	0.013	**0.115**	0.006	no sample **	no sample **
6.5	**0.190**	0.007	**0.165**	0.008	no sample *	no sample *	**0.137**	0.008	**0.157**	0.015	0.058	0.003
7.5	**0.154**	0.002	**0.170**	0.008	no sample *	no sample *	**0.149**	0.016	**0.172**	0.022	**0.075**	0.005
8.5	**0.301**	0.010	**0.175**	0.009	no sample *	no sample *	**0.169**	0.010	**0.173**	0.012	**0.087**	0.004
9.5	**0.294**	0.004	**0.176**	0.010	**0.166**	0.017	**0.193**	0.013	**0.154**	0.009	**0.118**	0.011
10.5	**0.226**	0.010	**0.174**	0.009	**0.193**	0.019	**0.293**	0.009	**0.166**	0.011	**0.132**	0.008
11.5	**0.244**	0.005	**0.177**	0.007	**0.169**	0.008	**0.280**	0.003	**0.178**	0.008	no sample **	no sample **
12.5	**0.213**	0.003	**0.174**	0.005	**0.188**	0.026	**0.272**	0.018	**0.207**	0.020	no sample **	no sample **
13.5	**0.274**	0.009	**0.164**	0.008	**0.211**	0.013	**0.298**	0.036	**0.197**	0.006	no sample **	no sample **
14.5	**0.246**	0.005	**0.166**	0.007	**0.251**	0.020	**0.296**	0.004	**0.172**	0.011	no sample **	no sample **
15.5	**0.301**	0.004	**0.154**	0.009	**0.165**	0.020	**0.252**	0.011	**0.212**	0.006	no sample **	no sample **
blank 1	0.021	0.002	<LoD		0.113	0.006	<LoD		<LoD		<LoD	
blank 2	<LoD		0.011	0.001	0.108	0.007	<LoD		0.013	0.001	<LoD	
blank 3	<LoD		<LoD		0.114	0.013	<LoD		<LoD		<LoD	
blank 4	<LoD		0.004	0.001	0.084	0.005	<LoD		<LoD		<LoD	
blank 5	<LoD		<LoD		0.113	0.007	0.016	0.001			<LoD	
correction value	0.004		0.003		0.107		0.003		0.004		0.000	
LoD	0.011		0.003		0.010		0.013		0.009		0.026	
LoQ	0.031		0.009		0.025		0.035		0.021		0.073	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 66: Vanadium concentration across the SWI **(<0.45 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.268**	0.017	**0.179**	0.008	**0.335**	0.049	**0.202**	0.017	**0.206**	0.005	**0.340**	0.007
-4.5	**0.267**	0.024	**0.185**	0.006	**0.382**	0.016	**0.269**	0.020	**0.215**	0.005	**0.368**	0.017
-3.5	**0.218**	0.007	**0.223**	0.015	**0.348**	0.027	**0.166**	0.007	**0.321**	0.013	**0.345**	0.014
-2.5	**0.229**	0.013	**0.252**	0.026	**0.334**	0.017	**0.282**	0.012	**0.209**	0.006	**0.392**	0.014
-1.5	**0.273**	0.031	**0.315**	0.032	**0.245**	0.008	**0.182**	0.009	**0.512**	0.015	**0.361**	0.013
-0.5	**0.322**	0.032	**0.333**	0.039	**0.190**	0.007	**0.268**	0.016	**0.342**	0.019	**0.429**	0.012
0.5	**0.158**	0.013	**0.177**	0.001	**0.247**	0.055	**0.226**	0.015	**0.302**	0.025	**0.222**	0.007
1.5	**0.045**	0.004	**0.216**	0.016	**0.259**	0.010	**0.187**	0.013	**0.126**	0.009	**0.139**	0.004
2.5	**0.043**	0.003	**0.219**	0.025	**0.239**	0.015	**0.089**	0.008	**0.144**	0.004	**0.137**	0.006
3.5	**0.041**	0.006	**0.198**	0.004	**0.273**	0.011	**0.072**	0.007	**0.089**	0.003	**0.157**	0.006
4.5	**0.074**	0.008	**0.199**	0.013	**0.223**	0.003	**0.069**	0.003	**0.104**	0.006	**0.131**	0.003
5.5	**0.141**	0.010	**0.170**	0.019	**0.201**	0.015	**0.070**	0.006	**0.100**	0.008	**0.185**	0.002
6.5	**0.094**	0.007	**0.163**	0.032	**0.195**	0.020	**0.069**	0.006	**0.136**	0.010	**0.190**	0.017
7.5	**0.109**	0.010	**0.148**	0.007	**0.206**	0.015	**0.075**	0.004	**0.106**	0.007	**0.170**	0.003
8.5	**0.108**	0.005	**0.213**	0.013	**0.144**	0.015	**0.076**	0.004	**0.104**	0.010	**0.142**	0.004
9.5	**0.178**	0.032	**0.107**	0.009	**0.131**	0.013	**0.075**	0.005	**0.126**	0.003	**0.179**	0.004
10.5	**0.110**	0.016	**0.135**	0.012	**0.151**	0.011	**0.080**	0.005	**0.183**	0.006	**0.183**	0.007
11.5	**0.105**	0.009	**0.123**	0.006	**0.125**	0.006	**0.095**	0.007	**0.181**	0.015	**0.222**	0.003
12.5	**0.122**	0.013	**0.149**	0.011	**0.110**	0.007	**0.094**	0.008	**0.116**	0.004	**0.201**	0.006
13.5	**0.082**	0.004	**0.150**	0.005	**0.106**	0.011	**0.098**	0.006	**0.136**	0.009	**0.179**	0.004
14.5	**0.104**	0.013	**0.133**	0.011	**0.117**	0.012	**0.106**	0.003	**0.176**	0.009	**0.173**	0.005
15.5	**0.122**	0.009	**0.093**	0.004	**0.125**	0.010	**0.091**	0.004	**0.133**	0.009	**0.184**	0.005
blank 1	0.003	0.000	0.002	0.000	0.004	0.000	<LoD		<LoD		<LoD	
blank 2	0.003	0.000	0.003	0.000	0.004	0.000	<LoD		<LoD		<LoD	
blank 3	0.005	0.002	0.004	0.000	0.005	0.001	<LoD		<LoD		<LoD	
blank 4	0.003	0.001	0.003	0.001	<LoD		<LoD		0.026	0.002	<LoD	
blank 5	0.006	0.001	0.006	0.001	0.003	0.001	<LoD		<LoD		<LoD	
correction value	0.004		0.003		0.003		0.000		0.005		0.000	
LoD	0.002		0.002		0.002		0.021		0.021		0.010	
LoQ	0.004		0.004		0.004		0.057		0.057		0.025	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth (cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-5.5	**0.143**	0.007	**0.048**	0.001	**0.086**	0.008	**0.033**	0.003	**0.039**	0.006	**0.321**	0.013
-4.5	**0.103**	0.003	0.008	0.001	**0.055**	0.008	**0.039**	0.005	**0.029**	0.004	0.031	0.007
-3.5	**0.087**	0.002	0.007	0.001	**0.061**	0.014	**0.035**	0.003	**0.042**	0.006	<LoD	
-2.5	**0.066**	0.002	0.006	0.001	**0.050**	0.007	**0.035**	0.006	0.017	0.002	0.021	0.005
-1.5	**0.057**	0.004	0.007	0.001	0.004	0.010	**0.031**	0.007	0.014	0.005	0.023	0.003
-0.5	**0.054**	0.002	0.005	0.001	0.009	0.004	**0.033**	0.003	<LoD		<LoD	
0.5	**0.073**	0.004	**0.015**	0.002	<LoD		**0.059**	0.007	<LoD		0.021	0.002
1.5	**0.030**	0.002	**0.021**	0.001	**0.048**	0.009	**0.091**	0.007	<LoD		0.032	0.003
2.5	**0.071**	0.004	**0.027**	0.002	**0.081**	0.014	**0.072**	0.008	<LoD		0.063	0.006
3.5	**0.102**	0.006	**0.049**	0.005	**0.136**	0.015	**0.066**	0.006	0.009	0.004	**0.095**	0.006
4.5	**0.118**	0.005	**0.067**	0.002	**0.271**	0.030	**0.078**	0.007	**0.030**	0.002	**0.147**	0.006
5.5	**0.127**	0.004	**0.084**	0.002	**0.238**	0.039	**0.095**	0.007	**0.062**	0.007	**0.170**	0.011
6.5	**0.130**	0.006	**0.082**	0.003	**0.186**	0.022	**0.107**	0.007	**0.079**	0.006	**0.170**	0.009
7.5	**0.130**	0.004	**0.102**	0.001	**0.228**	0.014	**0.115**	0.006	**0.069**	0.007	**0.166**	0.012
8.5	**0.139**	0.005	**0.111**	0.002	**0.227**	0.017	**0.132**	0.005	**0.080**	0.004	**0.175**	0.004
9.5	**0.144**	0.006	**0.082**	0.004	**0.195**	0.014	**0.135**	0.011	**0.164**	0.008	**0.191**	0.010
10.5	no sample**	no sample**	**0.079**	0.004	**0.212**	0.014	**0.127**	0.008	**0.138**	0.010	**0.190**	0.008
11.5	**0.140**	0.003	**0.088**	0.002	**0.179**	0.024	**0.127**	0.013	**0.149**	0.008	**0.196**	0.006
12.5	no sample**	no sample**	**0.095**	0.004	**0.182**	0.010	**0.154**	0.007	**0.142**	0.009	**0.187**	0.007
13.5	**0.137**	0.006	**0.108**	0.002	**0.224**	0.024	**0.124**	0.009	**0.142**	0.012	**0.109**	0.008
14.5	no sample**	no sample**	**0.117**	0.006	**0.120**	0.013	**0.115**	0.010	**0.130**	0.009	**0.097**	0.006
15.5	**0.141**	0.007	**0.146**	0.005	no sample**	no sample**	**0.113**	0.005	**0.153**	0.007	**0.175**	0.011
blank 1	0.006	0.000	<LoD		0.133	0.008	<LoD		<LoD		0.007	0.002
blank 2	0.006	0.001	0.005	0.000	0.118	0.004	<LoD		0.076	0.009	0.005	0.001
blank 3	<LoD		0.005	0.000	0.126	0.003	<LoD		<LoD		0.004	0.001
blank 4	<LoD		0.004	0.000	0.102	0.002	<LoD		<LoD		0.005	0.000
blank 5	0.004	0.001	0.004	0.000	0.086	0.007	<LoD		0.013	0.001	0.006	0.001
correction value	0.003		0.004		0.113		0.000		0.030		0.005	
LoD	0.003		0.003		0.013		0.009		0.009		0.026	
LoQ	0.008		0.008		0.035		0.021		0.021		0.073	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

Table A2. 67: Vanadium concentration across the SWI **(<16 µm) of Experiment B** and detected blank values, LoDs and LoQs. Values <LoD were removed from the data set and values >LoQ are bold. All values in µg/L.

Day	-16		-9		-1		1		9		19	
Profile	1		2		3		4		5		6	
Depth												
-5.5	**0.314**	0.009	**0.137**	0.005	**0.273**	0.010	**0.173**	0.013	**0.379**	0.025	**0.337**	0.015
-4.5	**0.404**	0.011	**0.253**	0.011	**0.385**	0.008	**0.158**	0.007	**0.274**	0.015	**0.233**	0.004
-3.5	**0.349**	0.011	**0.299**	0.012	**0.284**	0.007	**0.233**	0.020	**0.475**	0.019	**0.338**	0.012
-2.5	**0.338**	0.006	**0.343**	0.004	**0.292**	0.008	**0.166**	0.009	**0.508**	0.021	**0.407**	0.019
-1.5	**0.341**	0.013	**0.354**	0.012	**0.198**	0.005	**0.175**	0.007	**0.484**	0.029	**0.348**	0.016
-0.5	**0.345**	0.012	**0.265**	0.003	**0.173**	0.003	**0.171**	0.008	**0.418**	0.019	**0.313**	0.011
0.5	**0.288**	0.008	**0.224**	0.007	**0.158**	0.004	**0.185**	0.006	**0.441**	0.019	**0.268**	0.011
1.5	**0.100**	0.003	**0.225**	0.012	**0.203**	0.009	**0.164**	0.005	**0.127**	0.004	**0.160**	0.007
2.5	**0.094**	0.004	**0.191**	0.010	**0.181**	0.006	no sample ***	no sample ***	**0.109**	0.005	**0.200**	0.007
3.5	**0.143**	0.005	**0.203**	0.012	**0.181**	0.010	no sample ***	no sample ***	**0.109**	0.007	**0.216**	0.002
4.5	**0.187**	0.004	**0.204**	0.009	**0.177**	0.008	**0.080**	0.004	**0.134**	0.007	**0.273**	0.007
5.5	**0.234**	0.010	**0.177**	0.005	**0.152**	0.007	**0.065**	0.003	**0.171**	0.007	**0.266**	0.009
6.5	**0.257**	0.013	**0.212**	0.010	**0.193**	0.008	**0.068**	0.008	**0.148**	0.006	**0.258**	0.010
7.5	**0.257**	0.004	**0.177**	0.009	**0.144**	0.006	**0.065**	0.002	**0.145**	0.004	**0.307**	0.006
8.5	**0.234**	0.007	**0.133**	0.004	**0.126**	0.008	**0.120**	0.004	**0.167**	0.011	**0.330**	0.013
9.5	**0.232**	0.012	**0.122**	0.006	**0.142**	0.003	**0.096**	0.003	**0.163**	0.009	**0.341**	0.013
10.5	**0.274**	0.011	**0.125**	0.006	**0.135**	0.005	**0.097**	0.004	**0.227**	0.008	**0.290**	0.007
11.5	**0.266**	0.014	**0.108**	0.006	**0.162**	0.007	**0.138**	0.007	**0.179**	0.026	**0.349**	0.019
12.5	**0.218**	0.006	**0.117**	0.004	**0.154**	0.008	no sample ***	no sample ***	**0.193**	0.008	**0.308**	0.012
13.5	**0.255**	0.009	**0.139**	0.002	**0.158**	0.004	**0.102**	0.004	**0.219**	0.012	**0.361**	0.009
14.5	**0.239**	0.009	**0.121**	0.004	**0.144**	0.006	no sample ***	no sample ***	**0.217**	0.011	**0.268**	0.008
15.5	**0.191**	0.004	**0.130**	0.003	**0.192**	0.002	no sample ***	no sample ***	**0.218**	0.012	**0.309**	0.007
blank 1	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 2	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 3	<LoD		<LoD		<LoD		<LoD		<LoD		<LoD	
blank 4	<LoD		0.021	0.002	<LoD		<LoD		<LoD		<LoD	
blank 5	<LoD		0.012	0.002	<LoD						<LoD	
correction value	0.000		0.007		0.000		0.000		0.000		0.000	
LoD	0.008		0.008		0.008		0.016		0.016		0.011	
LoQ	0.022		0.022		0.022		0.043		0.043		0.031	

Day	27		43		69		85		110		148	
Profile	7		8		9		10		11		12	
Depth												
-5.5	**0.094**	0.005	**0.095**	0.003	**0.050**	0.007	0.021	0.004	**0.261**	0.017	0.027	0.002
-4.5	**0.116**	0.005	**0.011**	0.001	**0.063**	0.015	0.013	0.001	**0.081**	0.007	0.030	0.002
-3.5	**0.117**	0.004	0.009	0.000	**0.059**	0.015	0.021	0.002	**0.064**	0.011	0.026	0.002
-2.5	**0.064**	0.004	<LoD		**0.027**	0.009	0.021	0.003	**0.036**	0.002	<LoD	
-1.5	**0.055**	0.002	<LoD		0.016	0.010	0.024	0.001	**0.023**	0.003	<LoD	
-0.5	**0.049**	0.004	0.009	0.001	**0.034**	0.008	0.025	0.002	0.019	0.002	<LoD	
0.5	**0.069**	0.004	**0.018**	0.001	**0.083**	0.016	**0.048**	0.002	**0.022**	0.004	0.050	0.004
1.5	**0.025**	0.003	**0.024**	0.001	**0.077**	0.009	**0.069**	0.005	**0.055**	0.007	0.046	0.002
2.5	**0.080**	0.005	**0.058**	0.002	**0.092**	0.017	**0.080**	0.004	**0.081**	0.004	0.071	0.004
3.5	**0.108**	0.004	**0.091**	0.002	**0.087**	0.008	**0.083**	0.006	**0.068**	0.002	**0.116**	0.006
4.5	**0.126**	0.004	**0.117**	0.004	**0.127**	0.014	**0.091**	0.005	**0.064**	0.003	**0.158**	0.010
5.5	**0.129**	0.006	**0.151**	0.005	**0.163**	0.020	**0.088**	0.006	**0.098**	0.008	**0.178**	0.012
6.5	**0.138**	0.004	**0.160**	0.003	**0.167**	0.014	**0.115**	0.007	no sample**	no sample**	**0.170**	0.015
7.5	**0.137**	0.004	**0.155**	0.004	**0.164**	0.015	**0.211**	0.007	no sample**	no sample**	**0.176**	0.005
8.5	**0.151**	0.006	**0.158**	0.006	**0.242**	0.023	**0.118**	0.005	no sample**	no sample**	**0.188**	0.007
9.5	**0.144**	0.001	**0.210**	0.008	**0.091**	0.018	**0.135**	0.013	no sample**	no sample**	**0.196**	0.008
10.5	**0.276**	0.012	**0.195**	0.005	**0.147**	0.022	**0.144**	0.011	no sample**	no sample**	**0.200**	0.013
11.5	**0.147**	0.006	**0.203**	0.005	**0.093**	0.019	**0.148**	0.007	no sample**	no sample**	**0.190**	0.010
12.5	**0.167**	0.008	**0.223**	0.004	**0.114**	0.012	<LoD		no sample**	no sample**	no sample**	no sample**
13.5	**0.170**	0.009	**0.203**	0.004	**0.178**	0.017	no sample ***	no sample ***	no sample**	no sample**	**0.194**	0.016
14.5	**0.167**	0.006	**0.195**	0.008	**0.155**	0.016	no sample ***	no sample ***	no sample**	no sample**	**0.187**	0.015
15.5	**0.178**	0.005	**0.179**	0.007	**0.150**	0.018	no sample ***	no sample ***	no sample**	no sample**	no sample**	no sample**
blank 1	0.007	0.001	<LoD		0.100	0.009	<LoD		0.002	104.980	<LoD	
blank 2	0.007	0.001	<LoD		0.081	0.005	<LoD		0.002	59.051	<LoD	
blank 3	0.007	0.000	<LoD		0.094	0.007	<LoD		0.003	24.510	<LoD	
blank 4	0.013	0.001	<LoD		0.094	0.007	<LoD		0.001	28.247	<LoD	
blank 5	0.009	0.001	<LoD		0.109	0.006	<LoD		0.002	39.203	<LoD	
correction value	0.009		0.000		0.096		0.000		0.002		0.000	
LoD	0.003		0.003		0.010		0.013		0.009		0.026	
LoQ	0.009		0.009		0.025		0.035		0.021		0.073	

* malfunction of the fraction collector; ** lost during sample preparation; *** limited sample volume available

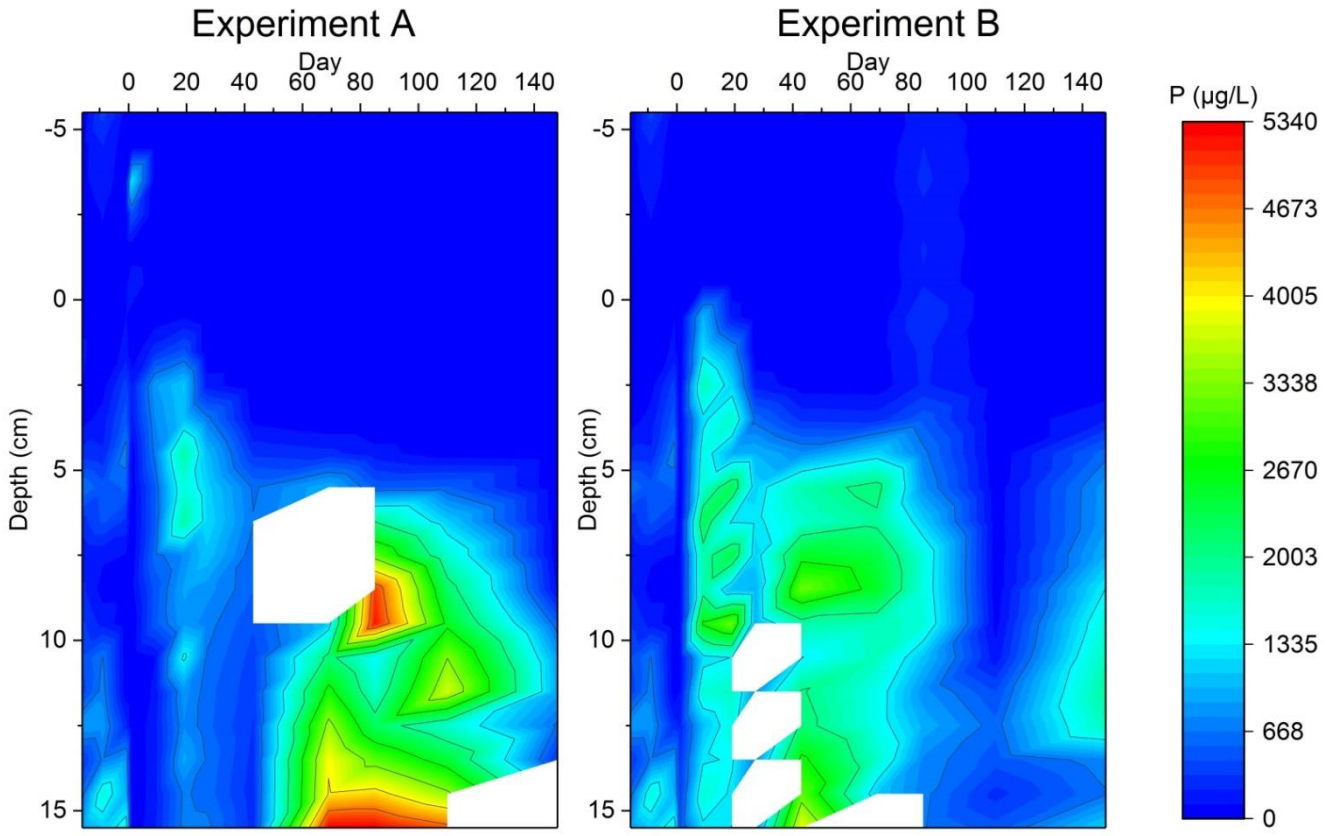


Figure A2. 3: Heatplot Phosphorous concentration in the dissolved fraction (<0.45 µm) across the SWI of Experiment A and Experiment B (values <LoD set to 0, missing samples and removed outliers displayed in white).

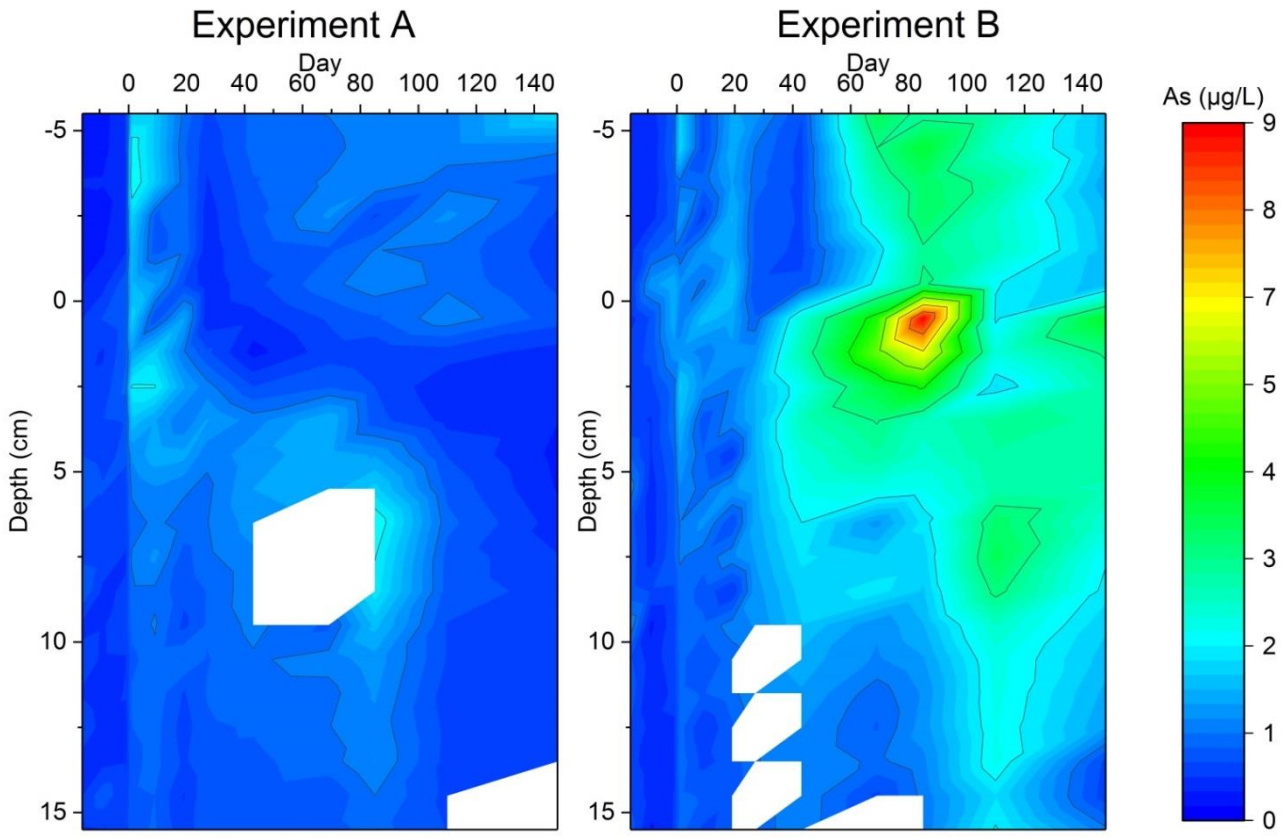


Figure A2. 4: Heatplot Arsenic concentration in the dissolved fraction (<0.45 µm) across the SWI of Experiment A and Experiment B (values <LoD set to 0, missing samples and removed outliers displayed in white).

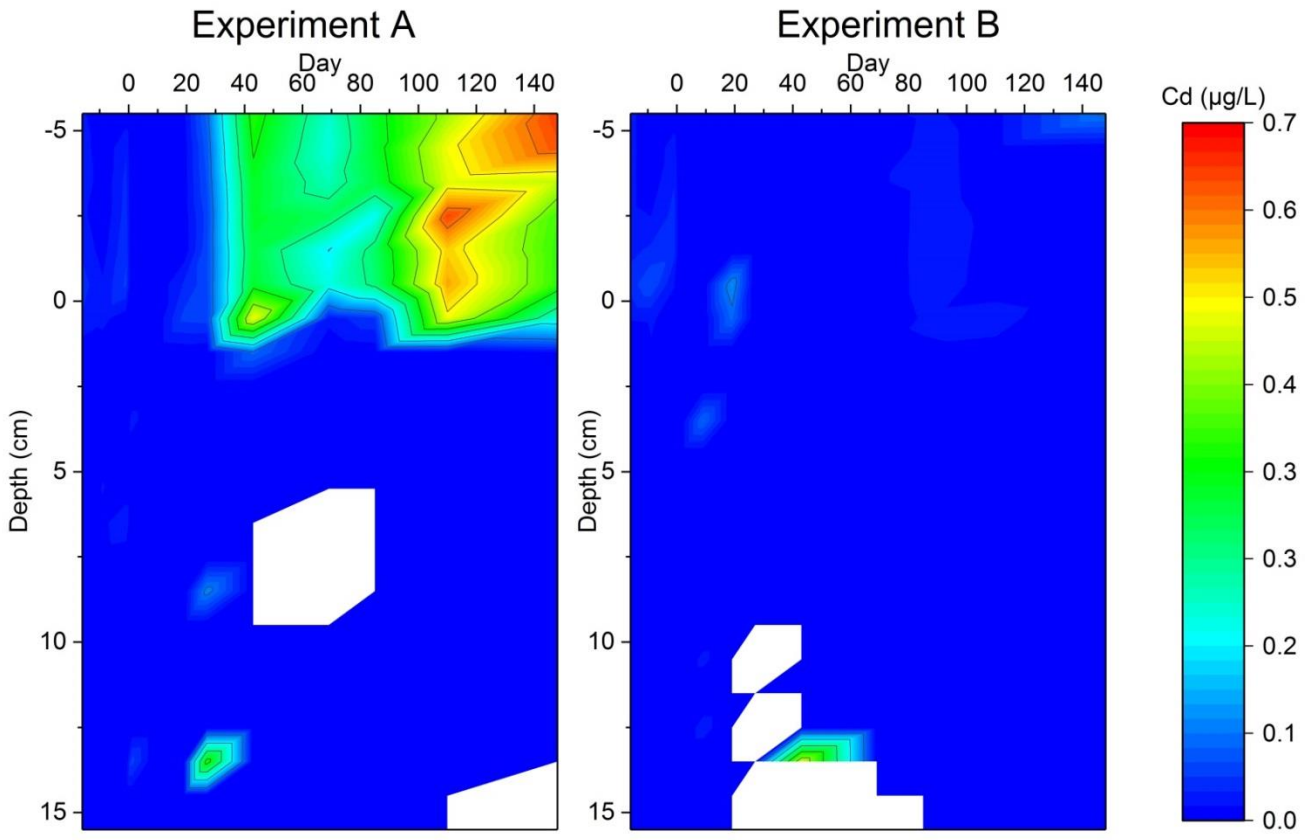


Figure A2. 5: Heatplot cadmium concentration in the dissolved fraction (<0.45 µm) across the SWI of Experiment A and Experiment B (values <LoD set to 0, missing samples and removed outliers displayed in white).

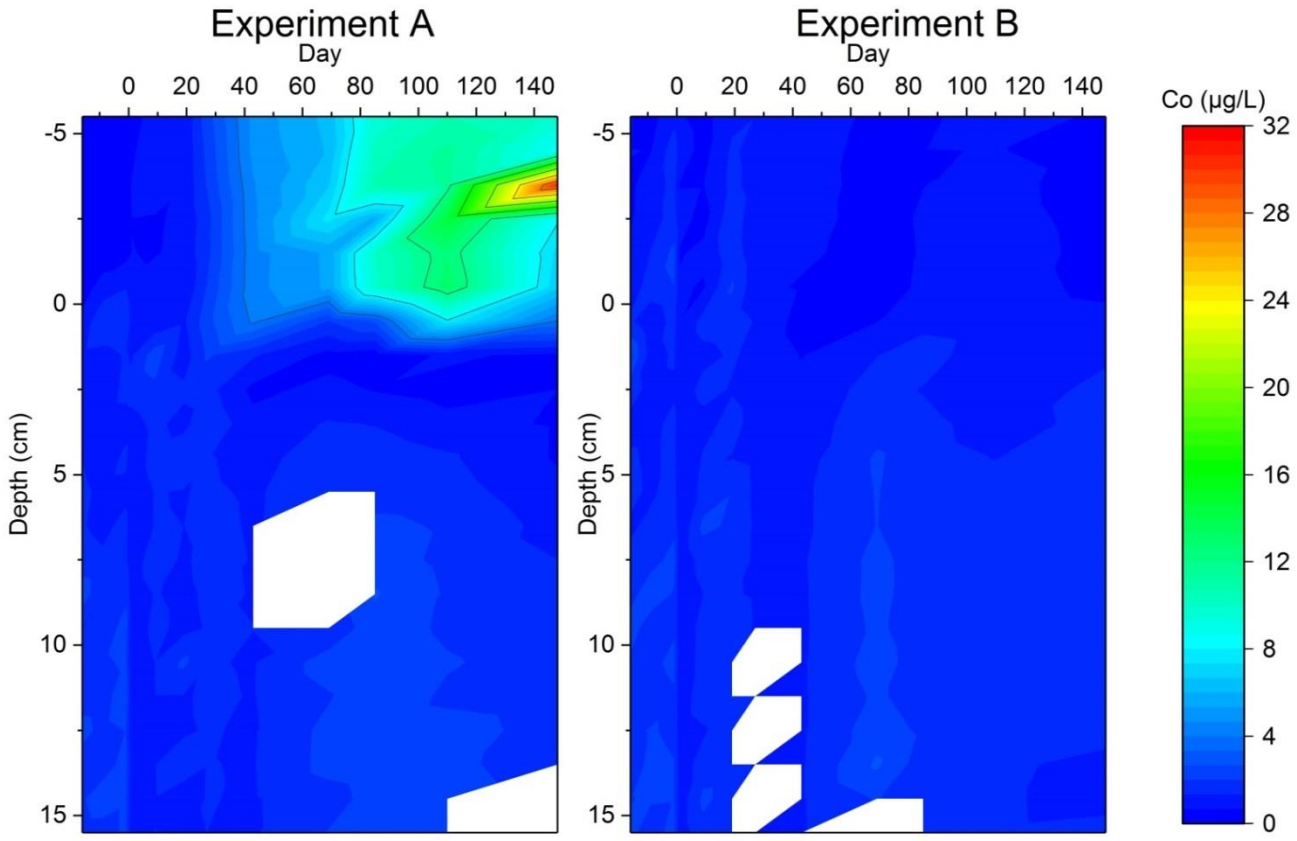


Figure A2. 6: Heatplot cobalt concentration in the dissolved fraction (<0.45 µm) across the SWI of Experiment A and Experiment B (values <LoD set to 0, missing samples and removed outliers displayed in white).

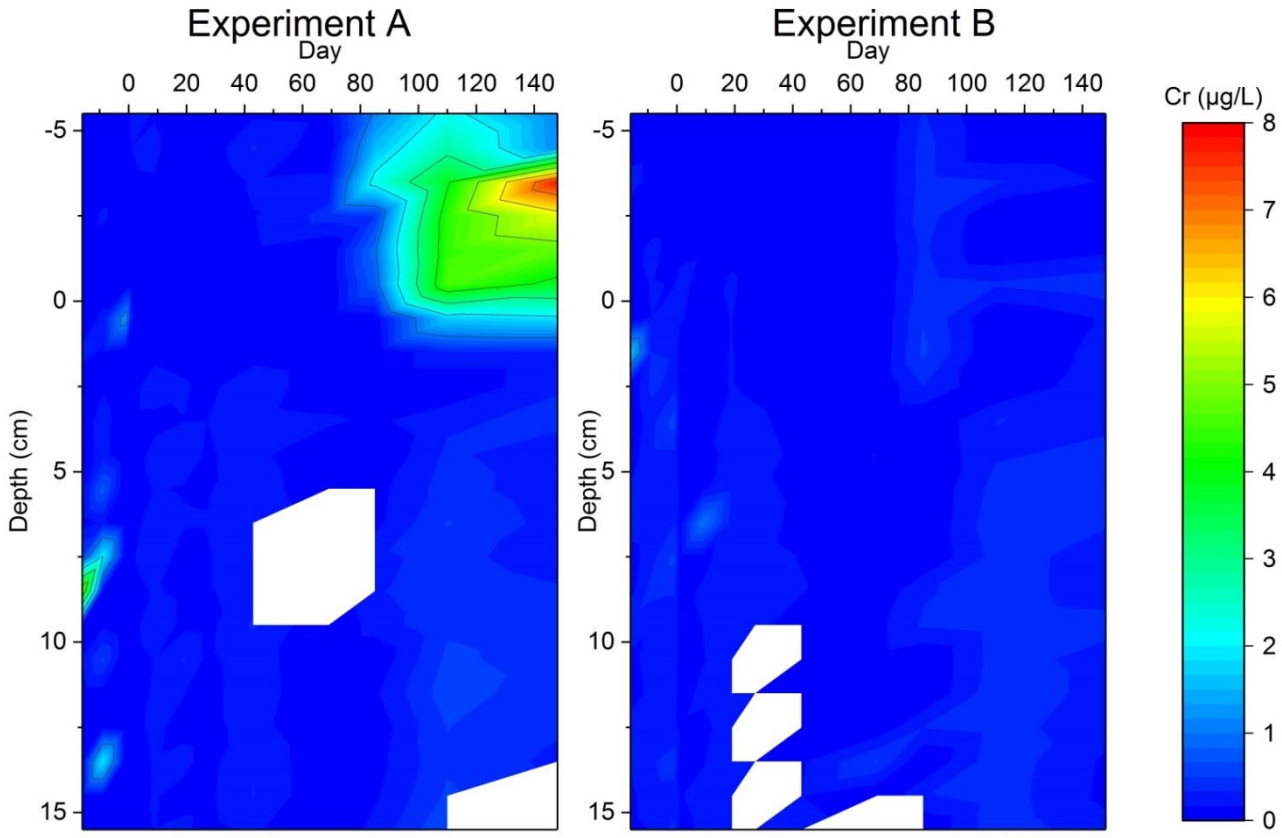


Figure A2. 7: Heatplot chromium concentration in the dissolved fraction (<0.45 µm) across the SWI of Experiment A and Experiment B (values <LoD set to 0, missing samples and removed outliers displayed in white).

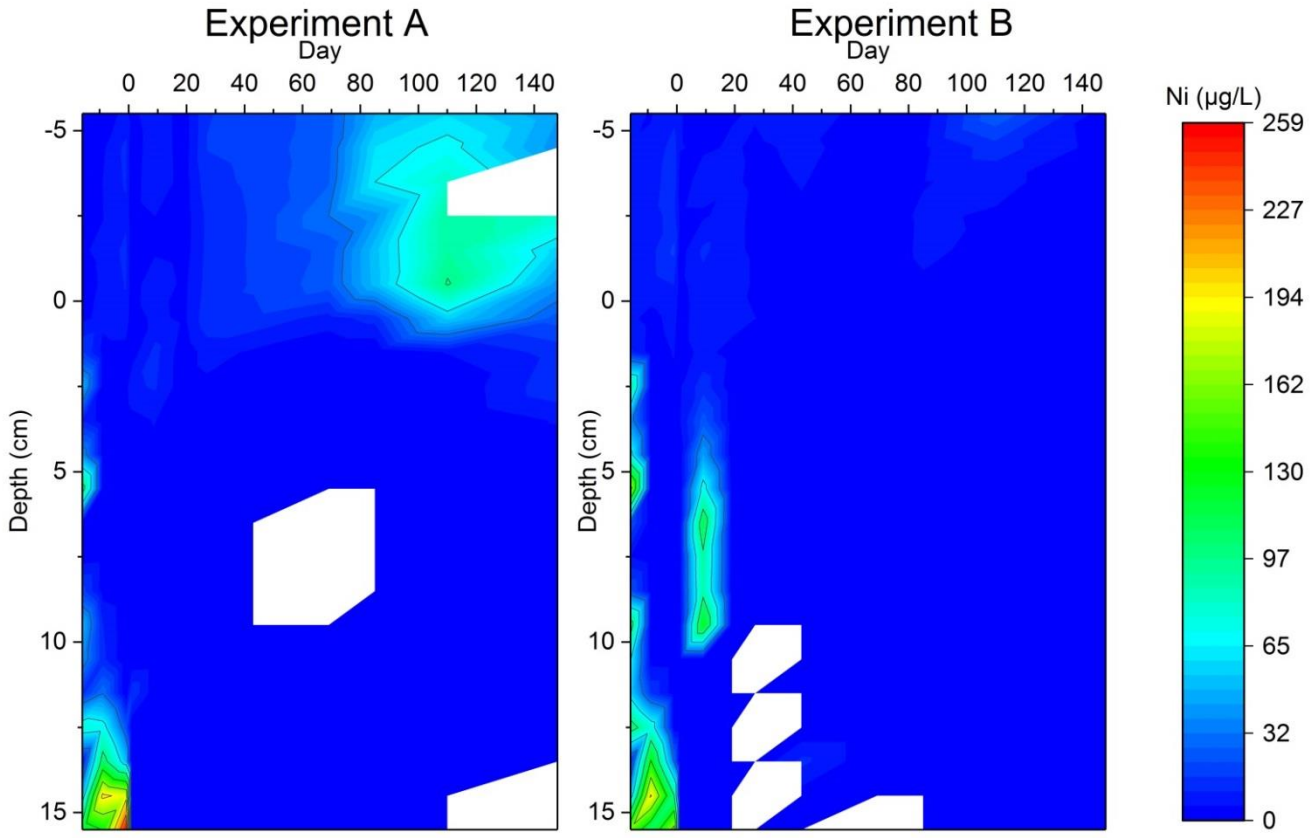


Figure A2. 8: Heatplot nickel concentration in the dissolved fraction (<0.45 µm) across the SWI of Experiment A and Experiment B (values <LoD set 0, missing samples and removed outliers displayed in white).

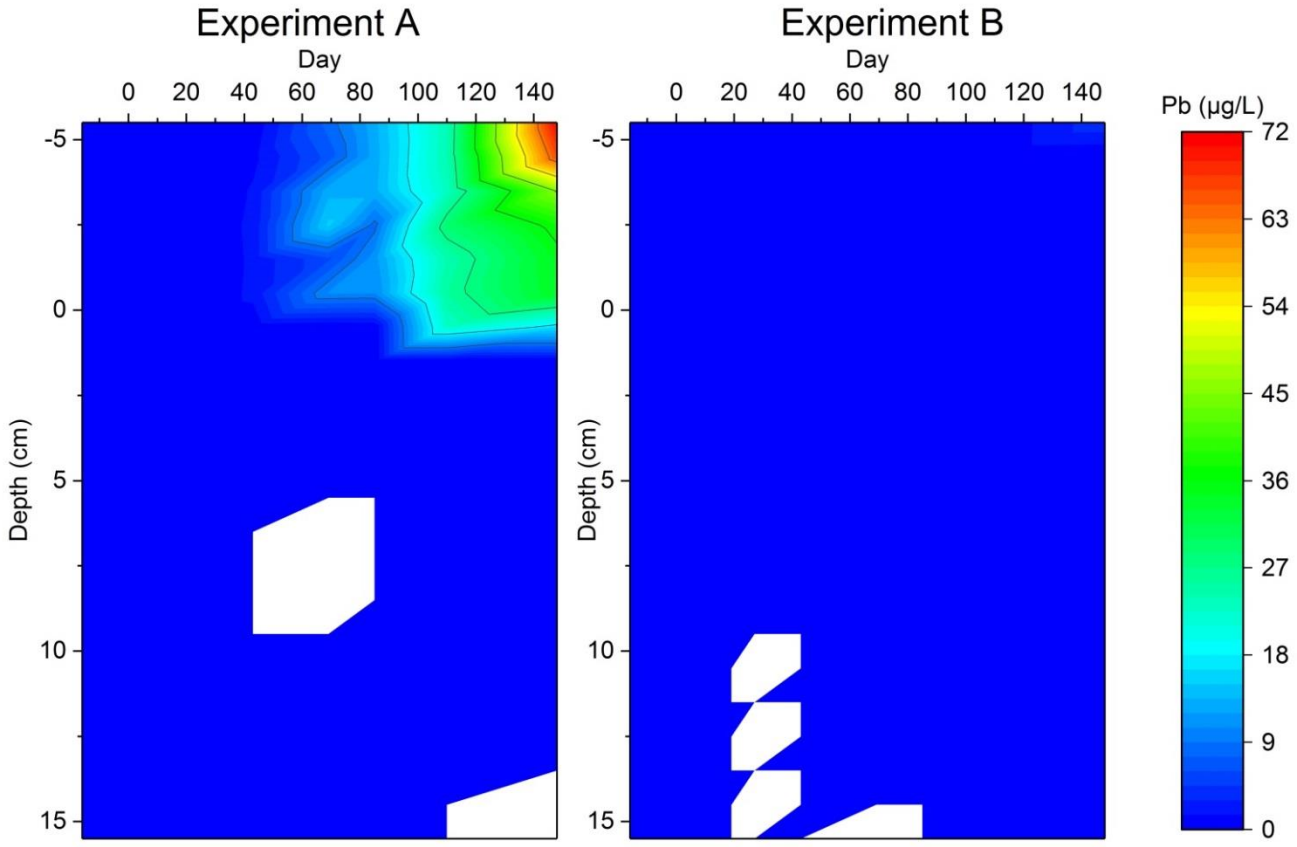


Figure A2. 9: Heatplot lead concentration in the dissolved fraction (<0.45 µm) across the SWI of Experiment A and Experiment B (values <LoD set to 0, missing samples and removed outliers displayed in white).

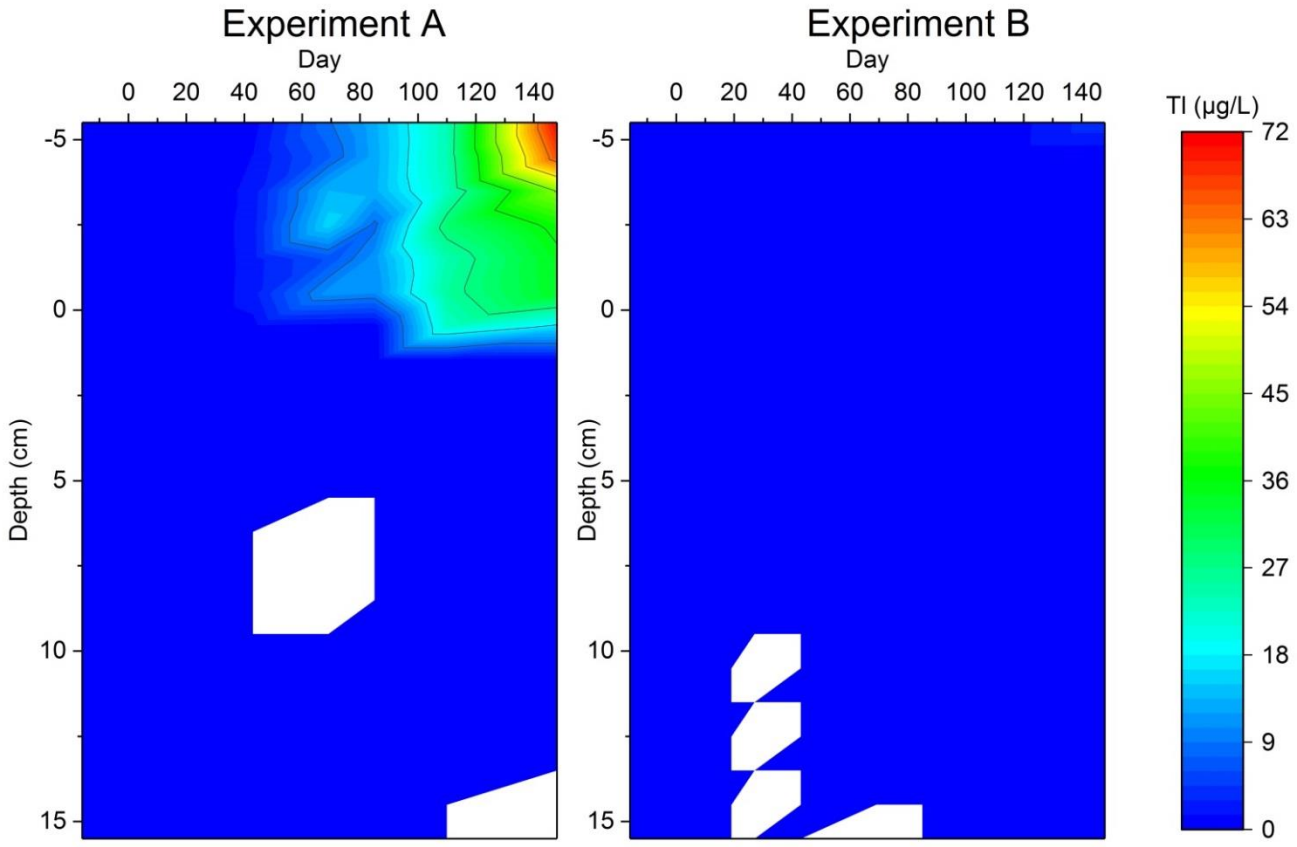


Figure A2. 10: Heatplot thallium concentration in the dissolved fraction (<0.45 µm) across the SWI of Experiment A and Experiment B (values <LoD set to 0, missing samples and removed outliers displayed in white).

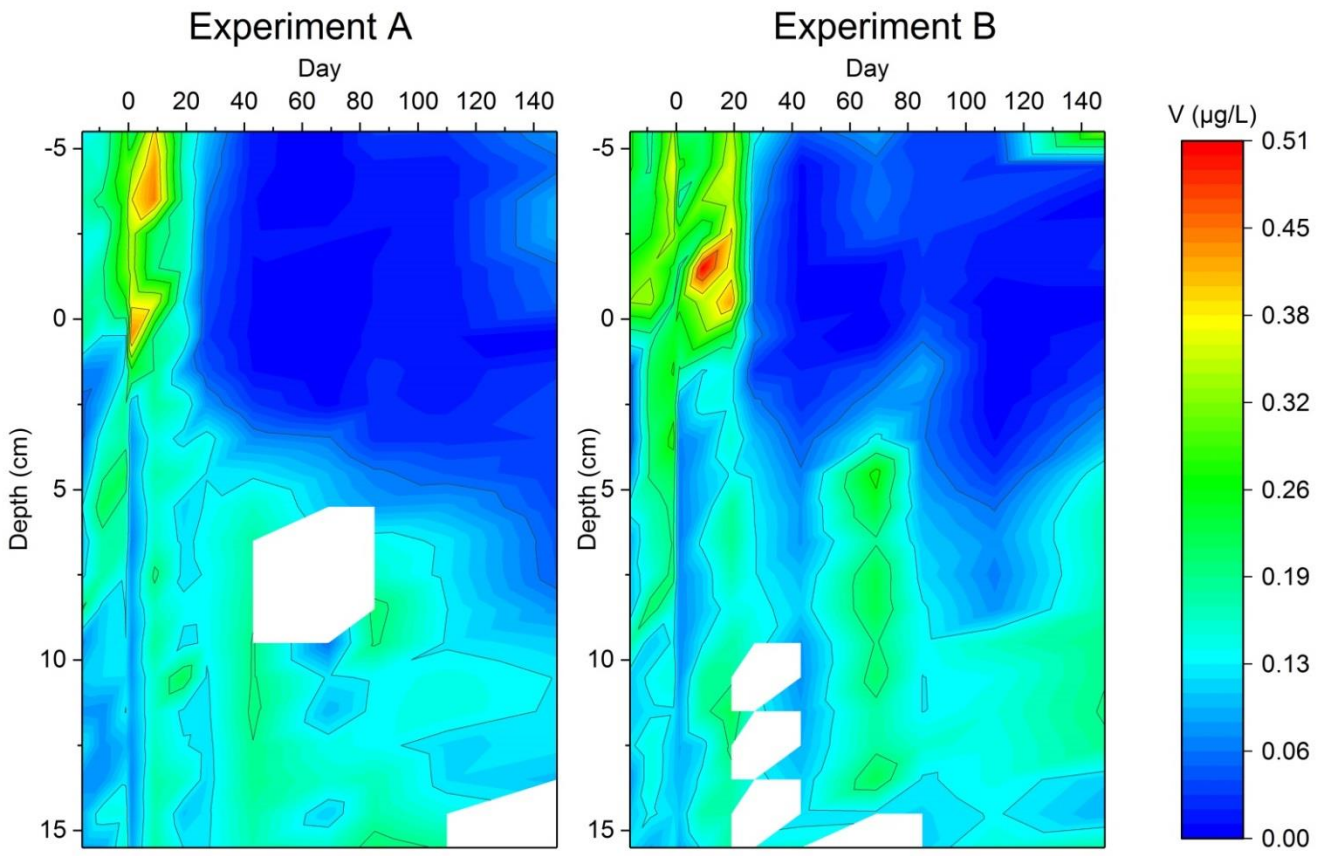


Figure A2. 11: Heatplot vanadium concentration in the dissolved fraction (<0.45 µm) across the SWI of Experiment A and Experiment B (values < LoD set to 0, missing samples and removed outliers displayed in white).

AII.IV Spearman based correlations

Table A2. 68: Spearman Correlations calculated for Experiment A

correlation factor	profiles 1-12	profiles 1-3	profiles 4-5	profiles 6-12
>0.9		C/Co	S/E_h, V/Sb	
>0.8	S/E_h	C/Sc, S/Sb, Sc/Cd, Cd/E_h, Sb/E_h	Sc/Tl	S/E_h, Ni/Cd, Cu/E_h
>0.7	Cu/E_h	C/Mn, S/Tl, S/E_h, Sc/Mn, , Mn/Co, Fe/Ni, Cd/Sb, Sb/Tl, Tl/E_h	C/Sc, S/Ni, S/Sb, P/Mn, V/Mo, Mn/As, Fe/Ni, Sb/E_h	C/P, P/V, Ni/Cu, Ni/Pb, Cd/Pb
>0.6	S/Cu, Mn/Fe, Mn/Co, Cd/Tl, Pb/E_h	S/Cd, Sc/Tl, , V/Cd, V/Sb, V/Tl, V/Pb, Mn/As, Cd/Tl, Cd/Pb, Sb/Pb, Tl/Pb, Pb/E_h	S/V, S/Pb, P/Cr, P/Co, Tl/Cr, V/Cu, V/Pb, Ni/E_h, Cu/Sb, Cu/Pb, As/Sb, Sb/Pb, Pb/E_h	C/V, S/Mn, S/Ni, S/Cu, Sc/Cd, Ni/E_h, Cu/Pb
>0.5	S/Pb, P/As, Cu/Pb	C/Tl, C/Fe, S/V, S/Pb, P/Mn, P/Fe, Tl/Mn, Tl/Cd, Mn/Fe, Fe/Co, Cu/Tl, Cu/E_h	C/Cr, C/Tl, S/Fe, S/Cu, S/As, P/Sc, P/As, Sc/Co, Tl/Co, V/Mn, V/As, V/E_h, Cr/Co, Mn/Sb, Fe/Sb, Ni/Sb, Cu/E_h, As/E_h	S/Pb, Mn/Fe, Mn/E_h, Co/Cd, Co/E_h, Cu/Cd, Pb/E_h
<-0.5	C/Ni, C/Cu, P/Ni	C/Cu, C/Pb, Sc/Cd, Sc/Pb, Tl/Eh, Mn/Pb, Fe/Cu, Fe/Cd, Co/Cd, Co/Tl, Co/Pb,		Sc/Fe, V/Cu
<-0.6	C/S, C/Pb, C/E_h	C/Cd, S/Mn, S/Fe, Sc/Cu, Sc/Sb, Sc/Tl, Mn/Cu, Mn/Sb, Mn/Tl, Fe/Sb, Co/Cu, Co/Sb, Cu/As		C/S, C/Pb, C/E_h, P/Ni, P/E_h, V/E_h
<-0.7		C/Sb, S/Sc, Mn/E_h		C/Cu, C/Cd, S/P, S/V
<-0.8		C/S, S/Co, Sc/E_h, Co/E_h		C/Ni
<-0.9		C/E_h		

Table A2. 69: Spearman Correlations calculated for Experiment B

correlation factor	profiles 1-12	profiles 1-3	profiles 4-5	profiles 6-12
>0.9		C/Sc	S/E_h, V/Sb	
>0.8	S/E_h	S/Sb, S/E_h, Fe/Ni	C/Sc, P/Co, Sc/Co, Mn/Co	S/Eh, Ni/E_h
>0.7		C/Mn, C/Co, S/Cd, S/Sb, Sc/Ti, Sc/Co, V/Cd, V/Sb, V/Pb, Cu/Sb, Cu/Pb, Cu/E_h, Cd/Sb, Cd/Pb, Sb/Pb, Sb/E_h	C/Mn, C/Co, S/Cu, P/Sc, P/Fe, Sc/Cr, V/Cu, Cu/Sb	S/Ni, V/Co, Ni/Sb, Cu/Pb, Sb/E_h
>0.6	C/Co, S/Sb, Cu/Pb, Sb/Eh	S/V, S/Cu, S/Pb, V/E_h, Mn/Co, Cu/Cd, Cu/Tl, Cd/E_h, Sb/Tl, Tl/Pb, Pb/E_h	C/P, C/Cr, S/Sb, SC/Mn, Cr/Co, Fe/Ni, Fe/Co, Cu/E_h, Sb/E_h	C/P, S/Sb, Sc/Tl, Cd/Sb, Cd/Tl
>0.5	V/Pb, Cd/Sb, Cd/Tl, Cd/E_h	S/Tl, Sc/Cr, V/Cu, Cr/Mn, Mn/Fe, Mo/E_h, Tl/E_h	S/V, P/Cr, P/Mn, Sc/Fe, V/Pb, V/E_h, Cr/Mn, Ni/Sb, Ni/Pb, Sb/Pb	C/Co, S/Mn, P/V, P/Co, Cd/E_h, Sb/Tl
<-0.5	S/Co, P/Ni	C/V, C/Tl, S/Ti, S/Mn, S/Co, Sc/Cd, Sc/Tl, CR/Cu, Mn/Cd, Mn/Sb, Mn/Tl, Mn/Pb, Co/Cu, Co/E_h		C/Ni, C/E_h, S/V, S/Co, P/Sb, Co/E_h
<-0.6	C/S, C/Eh, Co/E_h	C/Pb, Sc/Sb, Mn/E_h	S/P, S/Sc, S/Cr, S/Co, P/E_h, Sc/E_h, Cr/E_h, Co/E_h	P/Ni
<-0.7		C/Cu, C/Cd, C/Sb, C/Eh, S/Sc, Sc/Cu, Sc/E_h, Mn/Cu		S/P, P/E_h
<-0.8		C/S		
<-0.9				

AII.V Experimental setup

Table A2. 70: Experimental setup and timeline

profile / event	recorded parameters	depth interval	day
Sediment sampling			-86
Start *messy*-profile 1	pore water sampling, redox potential	cm -4 to 16	-23
Start *messy*-profile 2	pore water sampling, redox potential	cm -4 to 16	-16
Start *messy*-profile 3	pore water sampling, redox potential	cm -4 to 16	-9
microprofile (pH, redox, O_2)	pH, redox, O2	cm -4 to 4	-1
microprofile (pH, redox, O_2)	pH, redox, O2	cm -4 to 4	0
mechanical disturbance			0
Start *messy*-profile 4	pore water sampling, redox potential	cm -4 to 16	1
microprofile (pH, redox, O_2)	pH, redox, O2	cm -4 to 4	8
Start *messy*-profile 5	pore water sampling, redox potential	cm -4 to 16	9
microprofile (pH, redox, O_2)	pH, redox, O2	cm -4 to 4	18
Start *messy*-profile 6	pore water sampling, redox potential	cm -4 to 16	19
microprofile (pH, redox, O_2)	pH, redox, O2	cm -4 to 4	26
Start *messy*-profile 7	pore water sampling, redox potential	cm -4 to 16	27
Start *messy*-profile 8	pore water sampling, redox potential	cm -4 to 16	43
microprofile (pH, redox, O_2)	pH, redox, O2	cm -4 to 4	50
Start *messy*-profile 9	pore water sampling, redox potential, O_2	cm -4 to 16	69
microprofile (pH, redox, O_2)	pH, redox, O2	cm -4 to 4	76
Start *messy*-profile 10	pore water sampling, redox potential, O2	cm -4 to 16	85
microprofile (pH, redox, O_2)	pH, redox, O2	cm -4 to 4	92
Start *messy*-profile 11	pore water sampling, redox potential, O2	cm -4 to 16	110
microprofile (pH, redox, O_2)	pH, redox, O2	cm -4 to 4	117
Start *messy*-profile 12	pore water sampling, redox potential, O2	cm -4 to 16	148
microprofile (pH, redox, O_2)	pH, redox, O2	cm -4 to 4	155

Appendix III

Supporting Information Chapter 4:

Sediment water (interface) mobility of metal(loid)s and nutrients und undisturbed conditions and during resuspension

Henning Schroeder, Lars Duester, Anne-Lena Fabricius, Dennis Ecker, Vera Breitung and Thomas A. Ternes

AIII.I Sediment characteristics

AIII.I.I Grain size distribution of the investigated sediments

Grain size distributions of sub-samples from each sediment core were determined by laser diffraction particle size analyser (Beckman Coulter LS200, Beckman Coulter , Inc., USA).

Table A3. 1: Grain size distributions of the investigated sediments. All values in volume %.

	Sampling Site 1			Sampling Site 2			Sampling Site 3			Sampling Site 4		
size class	Core 1	Core 2	Core 3	Core 1	Core 2	Core 3	Core 1	Core 2	Core 3	Core 1	Core 2	Core 3
0.63-2 mm	1.482	2.21	1.259	0.11	0	0.36	0.265	0.737	0.457	0.205	0.298	0.298
0.2-0.63 mm	9.463	9.673	9.22	1.897	0.155	3.219	3.973	5.473	5.11	2.086	2.599	2.599
0.063-0.2 mm	38.73	33.26	27	36.07	20.59	19.24	31.31	32.83	31.92	30.28	27.76	27.76
0.02-0.063 mm	26.17	25.78	27.64	32.18	37.51	35.75	27.54	25.29	27.17	39.31	40.58	40.58
0.0063-0.02 mm	13.88	16.6	20.38	17.35	25.23	25.06	20.12	17.89	17.44	18.16	18.97	18.97
0.002-0.0063 mm	7.047	8.637	10.3	8.42	11.71	11.55	11.43	11.74	11.74	6.86	6.74	6.74
<0.002 mm	3.222	3.824	4.217	3.959	4.802	4.843	5.365	6.06	6.157	3.114	3.074	3.074

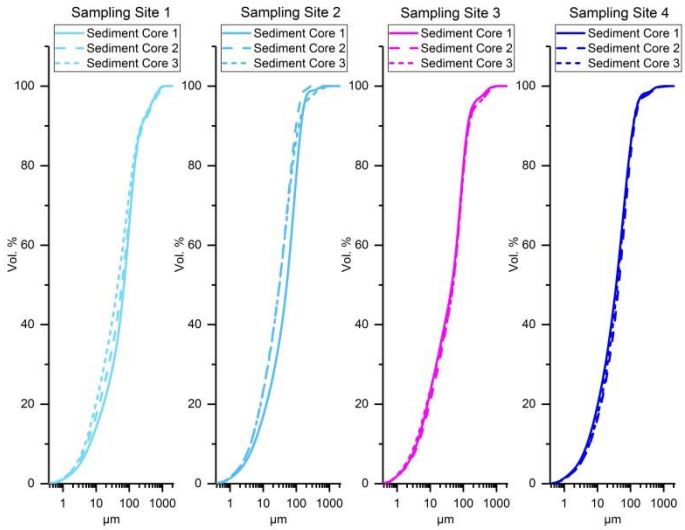


Figure A3. 1: Summation curves of the grain size distributions.

AIII.I.II Metal(loid) content of the investigated sediments

Subsequently to pore water sampling sub-cores were sampled from each sediment core in the laboratory, frozen and cut with a ceramic knife into 1 cm slices. Frieze dried sediment (Christ Gefriertrocknungsanlagen GmbH, Germany) samples were milled (planetary mill pulverisette, Fritsch, Germany) and digested by application of a microwave assisted procedure. Therefore, 1 g of the sediment was mixed with 10 mL of reverse *aqua regia* (2.5 mL 30% HCl + 7.5 mL 65% HNO_3) and digested in a five-step power-controlled program (refer to table A3. 2) using a Multiwave PRO (Anton Paar, Austria). After digestion, samples were diluted to 100 mL and analysed by means of ICP-OES (Optima 8300, Perkin Elmer).

Table A3. 2: Micro wave program.

Step	Program	Power	Time
		W	mm:ss
1	Power ramp	600	11:00
2	Power ramp	1500	3:00
3	Power hold	1500	13:00
4	Power ramp	860	9:30
5	Power hold	750	13:30

Table A3. 3: Metal(loid)s content of the investigated sediments. All values in mg/kg.

Sampling Site	Sediment Core	Al		As		Ca		Cd		Cr		Cu		Fe	
		wt%	SD	mg/kg	SD	wt%	SD	mg/kg	SD	mg/kg	SD	mg/kg	SD	wt%	SD
1	1	2.49	0.04	18.38	1.38	3.06	0.05	5.09	0.14	40.28	0.14	66.96	0.86	3.86	0.04
	2	2.73	0.03	18.75	1.08	2.36	0.02	5.31	0.09	40.35	0.38	70.60	0.94	3.84	0.03
	3	2.53	0.03	18.24	0.70	2.25	0.02	5.80	0.04	38.11	0.61	67.98	1.10	3.81	0.03
2	1	4.03	0.04	15.80	1.18	1.94	0.02	4.47	0.10	57.21	0.57	69.92	0.61	4.17	0.03
	2	4.07	0.08	14.16	0.82	1.72	0.03	3.25	0.07	56.04	0.44	64.95	0.29	3.97	0.06
	3	2.24	0.06	16.78	1.00	1.82	0.02	3.85	0.08	58.33	0.51	87.35	0.45	4.09	0.04
3	1	1.59	0.01	5.57	0.73	2.87	0.01	1.01	0.07	27.46	0.04	19.74	0.08	1.66	0.01
	2	1.86	0.01	6.86	0.27	3.08	0.01	1.22	0.06	30.19	0.09	22.83	0.18	1.87	0.01
	3	1.98	0.02	5.92	0.93	2.94	0.03	1.22	0.04	30.79	0.11	23.10	0.08	1.89	0.02
4	1	3.05	0.04	17.56	1.08	3.46	0.03	6.55	0.05	47.51	0.61	85.02	1.32	4.51	0.04
	2	3.33	0.02	17.49	0.45	3.46	0.02	6.16	0.10	50.02	0.45	81.37	0.94	4.50	0.03
	3	3.30	0.02	18.08	1.34	3.33	0.02	6.32	0.04	50.20	0.67	81.00	1.31	4.46	0.03

Sampling Site	Sediment Core	Li		Mg		Mn		Ni		P		Pb		Zn	
		mg/kg	SD	wt%	SD	mg/kg	SD	mg/kg	SD	mg/g	SD	mg/kg	SD	mg/kg	SD
1	1	19.45	0.18	0.84	0.01	634.13	6.73	20.94	0.13	1.59	0.02	254.24	2.48	760.21	3.22
	2	22.20	0.21	0.91	0.01	661.81	5.67	22.93	0.08	1.63	0.01	262.76	4.75	784.56	9.82
	3	20.95	0.26	0.87	0.01	625.60	4.80	22.03	0.09	1.50	0.02	270.09	3.97	828.38	5.08
2	1	33.88	0.78	1.27	0.02	399.32	6.01	32.33	0.11	0.99	0.01	281.36	3.38	1047.91	7.63
	2	34.21	0.39	1.31	0.02	343.46	4.84	31.06	0.09	1.09	0.01	220.39	3.67	796.36	4.73
	3	26.90	0.58	1.14	0.02	326.89	5.42	35.20	0.10	1.06	0.01	270.74	3.53	926.61	6.18
3	1	12.97	0.25	0.60	0.01	243.65	3.50	13.10	0.08	0.77	0.01	67.46	1.87	209.94	1.87
	2	14.93	0.29	0.65	0.01	264.57	4.05	14.48	0.08	0.81	0.01	73.97	1.46	237.78	2.36
	3	15.22	0.18	0.66	0.00	251.41	3.60	15.53	0.08	0.73	0.01	73.82	1.63	244.42	2.12
4	1	26.63	0.11	1.09	0.00	635.90	5.39	26.24	0.16	2.08	0.02	273.66	2.23	853.90	5.91
	2	27.80	0.28	1.05	0.01	601.12	5.93	27.07	0.14	1.93	0.01	262.79	2.66	783.39	3.38
	3	27.24	0.16	1.05	0.01	601.12	7.48	26.35	0.03	1.86	0.02	264.35	5.54	802.76	2.37

AIII.I.III Carbon, Nitrogen and Sulfur content of the investigated sediments

Total content of carbon, nitrogen and sulphur was determined in frieze dried and milled sub-samples from each sediment core by means of a total content analyser (Vario Macro, Elementar, Germany). For the analyses sulphur measurements, 120 mg of tungsten oxide (WO_3) were added to support the combustion process. Calibration was performed using sulphanilamide and verified by measurements of acetanilide. Two reference materials were included in the measurements (Leco 308, Leco 309).

Table A3. 4: Total CNS content of the investigated sediments.

Sampling Site	Sediment Core	TC	TOC	TIC	N	S
		weight %	weight %	weight %	weight %	weight %
1	1	6.23	5.27	0.96	0.48	1.87
	2	6.33	5.54	0.78	0.52	1.90
	3	5.72	5.03	0.68	0.54	1.83
2	1	6.07	5.42	0.65	0.67	2.38
	2	6.26	5.64	0.61	0.74	1.95
	3	5.98	5.35	0.62	0.65	2.18
3	1	2.76	1.73	1.03	0.25	0.54
	2	2.89	1.84	1.05	0.26	0.67
	3	2.87	1.91	0.96	0.26	0.64
4	1	7.56	6.38	1.18	0.69	2.31
	2	7.46	6.32	1.13	0.63	2.21
	3	7.38	6.31	1.08	0.61	2.31

AIII.II Details on analytical procedures

AIII.II.I ICP-QQQ-MS analyses

The information about the measurements of the metal(loid) and C, P, and S concentrations in the pore water samples and the samples from the mesocosm experiments are given in table A3. 8-A3. 27, A3. 31-A3. 50, A3. 54-A3. 73, A3. 77-A3. 96, A3. 100-A3. 119 and A3. 123-A3. 150. Elements were measured by application of a collision cell (He) with a He gas flow of 5 mL/min, or application of a collision cell (O_2) with 30% O_2 content. For validation purposes, four certified reference materials (CRMs) and three internal standards were included in the measurements (^{72}Ge, ^{103}Rh, ^{185}Re for He mode and ^{74}Ge, ^{103}Rh, ^{185}Re for O_2 mode). Additionally tartaric acid solution was used for the validation of carbon measurements. CRMs and tartaric acid were matrix adapted by addition of 10 Vol.% NaCl solution (15 g/L). The recoveries of at least two of the CRMs were in the range of ± 10% of the certified value, the maximum accepted variation of the internal standards was 20% from the initial value. Maximal accepted analytical instability of the measurements was 10% relative standard deviation (5 repetitions). Limits of detection (LoD, blank + 3 sigma) and limits of quantification (LoQ, blank + 10 sigma) are presented together with the results.

Table A3. 5: Information about ICP-QQQ-MS analyses. All concentrations in µg/L.

Isotope	Gas	Mode	CRM	TMRain*	TM26.4*	1640a*	SPS-SW1	tartaric acid
^{12}C	O_2	MS/MS	certified value x 10/11					200,000
^{31}P	O_2	MS/MS					90.91	
^{32}S	O_2	MS/MS					1.82	
^{55}Mn	He	SingleQuad		6.09	9.81	36.72	9.09	
^{56}Fe	He	SingleQuad		22.45	19.17	33.45	18.18	
^{60}Ni	He	SingleQuad		0.83	10.08	23.02	9.09	
^{63}Cu	He	SingleQuad		6.39	13.50	77.95	18.18	
^{66}Zn	He	SingleQuad		7.70	34.20	50.58	18.18	
^{51}V	O_2	MS/MS		0.62	11.34	13.68	9.09	
^{52}Cr	O_2	MS/MS		0.79	11.16	36.85	1.82	
^{59}Co	O_2	MS/MS		0.22	7.30	18.40	1.82	
^{75}As	O_2	MS/MS		1.04	7.83	7.34	9.09	
^{80}Se	O_2	MS/MS		0.76	4.86	18.30	1.82	
^{95}Mo	O_2	MS/MS		0.21	6.93	41.45	9.09	
^{109}Ag	O_2	MS/MS			6.17	7.35		
^{114}Cd	O_2	MS/MS		0.48	6.39	3.63	0.47	
^{120}Sn	O_2	MS/MS		0.67	5.20			
^{121}Sb	O_2	MS/MS		0.32	2.52	4.64		
^{208}Pb	He	SingleQuad		0.31	9.36	11.00	4.55	

*** Certified Reference Material for Trace Elements, Environment Canada matrix adapted by addition of 10 Vol.% NaCl solution (15 g/L)**

AIII.II.II IC measurements

Samples were, diluted 1:50 with a stock solution containing the analytes NO_2^-, NO_3^-, PO_4^{3-} SO_4^{2-} and NH_4^+ in concentrations of 0.1 mg/L by mixing 40 µL sample volume and 1960 µL stock solution. Two vials each were filled with 500 µL of the diluted sample to analyse the anions and NH_4^+ in parallel. The stock solution was included to the measurements for later correction of measured values.

2 certified reference materials (CRM) and 2 validation solutions prepared from calibration standards were included to the anion measurements for validation purposes. The recoveries of at least two of the CRMs/in house references were in the range of ± 10% of the certified/intended value. For validation of NH_4^+ measurements an in house reference was integrated twice to the measurements.

Table A3. 6: Information about IC analyses. All concentrations in mg/L.

Ion		SPS-WW1	STD 6		Validation solution 1	Validation solution 2	NH_4^+ solution 1
Cl^-	CRM*	5.00 ± 0.05	60.00	validation solution from callibration standards **	5.00	10.00	
NO_3^-		1.0 ± 0.01	15.00		0.10	0.20	
NO_2^-			0.10		0.10	0.20	
PO_4^{3-}		1.5 ± 0.02	0.30		0.10	0.20	
SO_4^{2-}		20.0 ± 0.2	60.00		5.00	5.00	
NH_4^+							0.10
* Certified Reference Material for Anions (Merck, Germany)							
** In house referencs for measurement validation were produced weekly from ultrapure water, Chloride-, Nitrate-, Nitrite-, Phosphate- and Sulfate-standards for aqueous matrices (Merck, Germany) or from ultrapure water and Ammonium-standard for aquoueus matrices (Merck, Germany)							

AIII.III Metal(loid) content in the different fractions of the sequential extraction

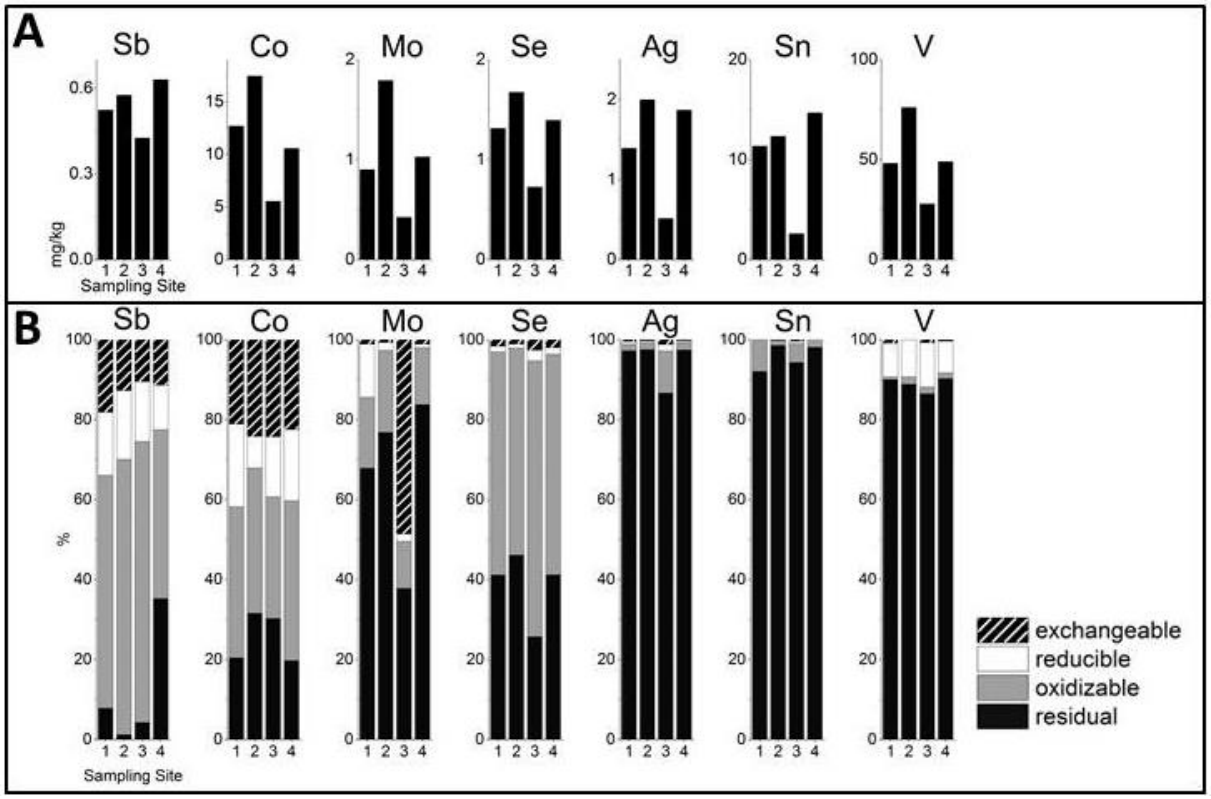


Figure A3. 2: Total content (A) and binding form (B) of Ag, Co, Mo, Sb, Se, Sn and V in the sediments of sampling site 1 to 4. Data is presented as average value of the sediments of a sampling site.

The results of individual measurements are given in Table A3. 10, section 9.

AIII.IV Laboratory conditions during *messy*

AIII.IV.I O_2-saturation across the SWI during suction-based pore water sampling

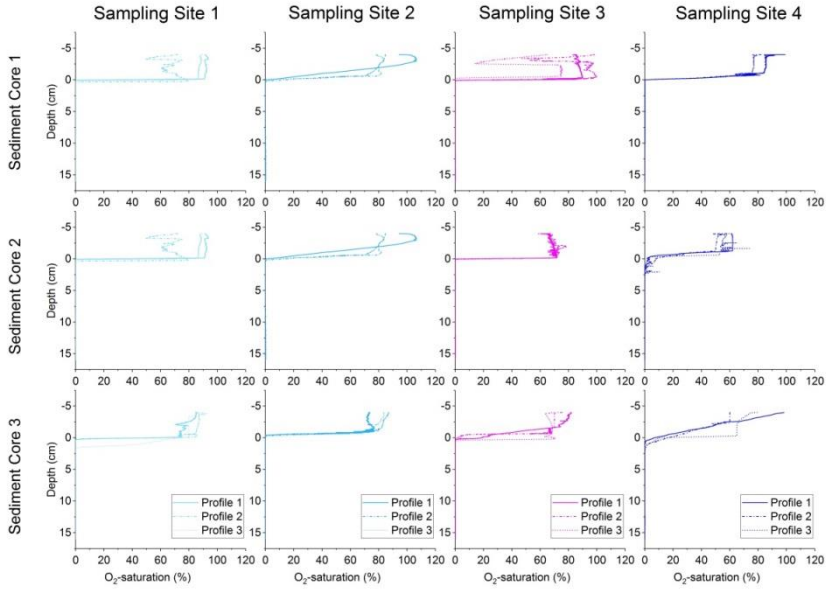


Figure A3. 3: Profiles of the O_2-saturation across the SWI of the sediment cores measured during suction-based pore water sampling in the lab.

AIII.IV.II Redox-potential across the SWI during suction-based pore water sampling

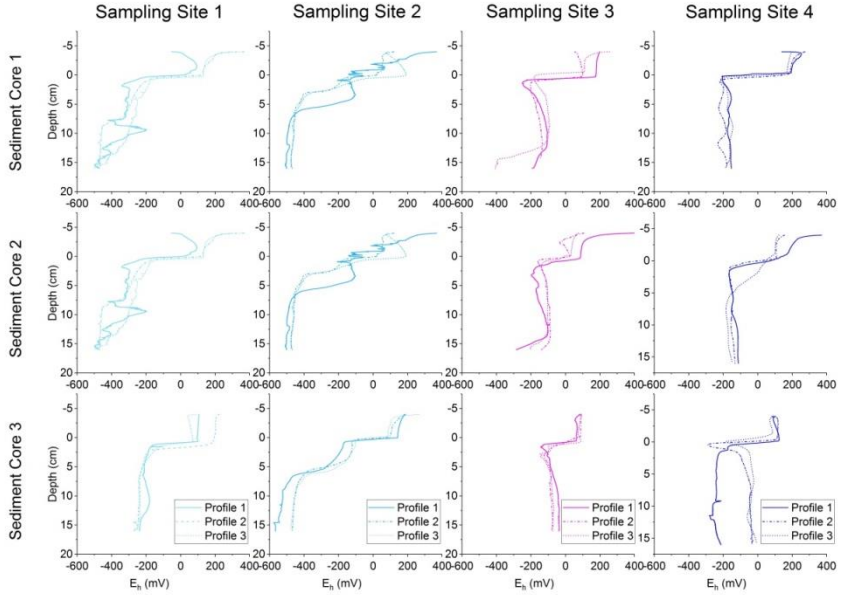


Figure A3. 4: Profiles of the redox potential across the SWI of the sediment cores measured during suction-based pore water sampling in the lab.

AIII.V Pore water depth profiles

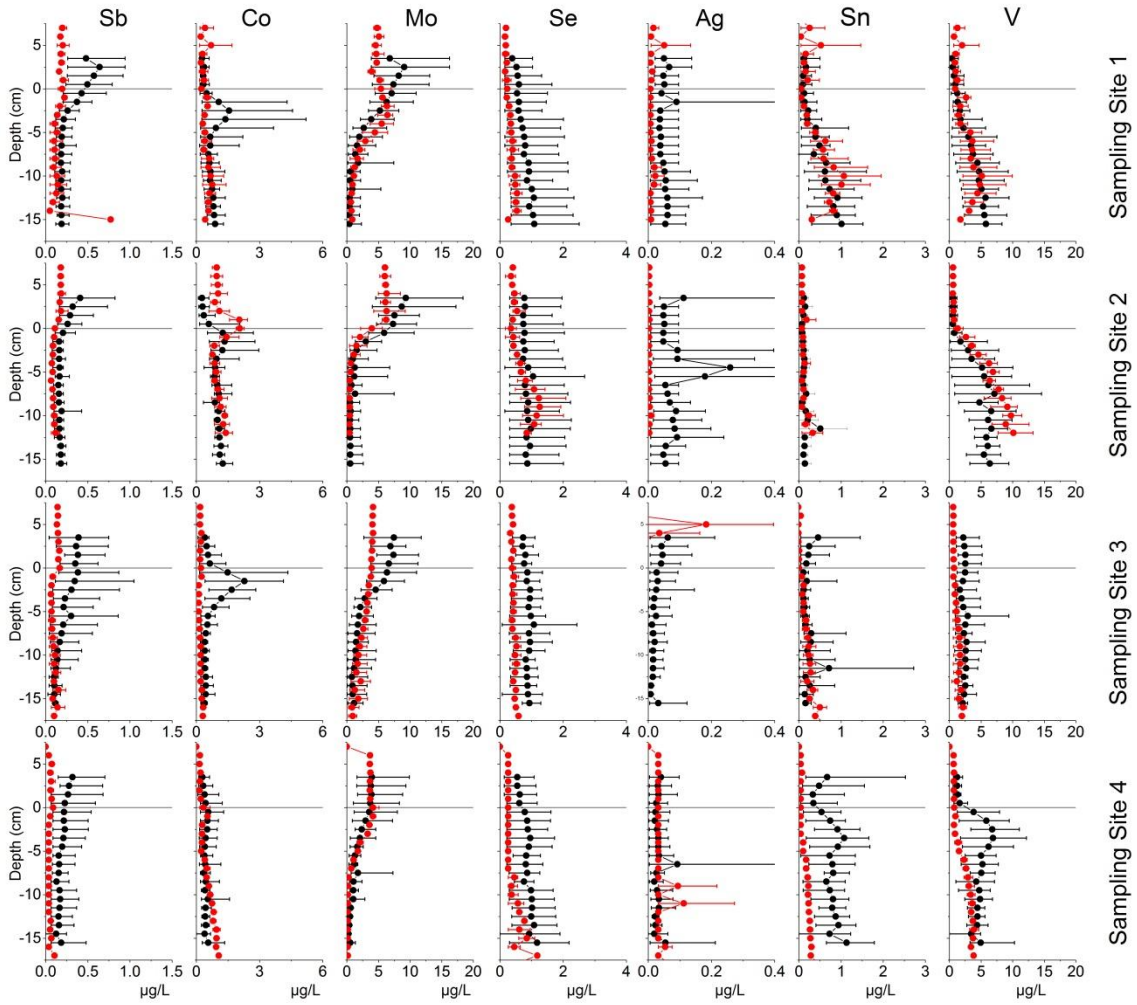


Figure A3. 5: Laterally averaged dissolved concentrations of Sb, Co, Mo, Se, Ag, Sn and V in suction based (n=9, black) and dialyses based (n=3, red) pore water samples of the 4 sampling sites. Error bars represent the minimum and maximum concentration measured at the respective depth. Grey lines represent the SWI.

The results of individual measurements are given in Table A3. 11-A3. 125, section 9.

AIII.VI Mesocosm Experiments

AIII.VI.I Course of pH and E_h during the resuspension experiments

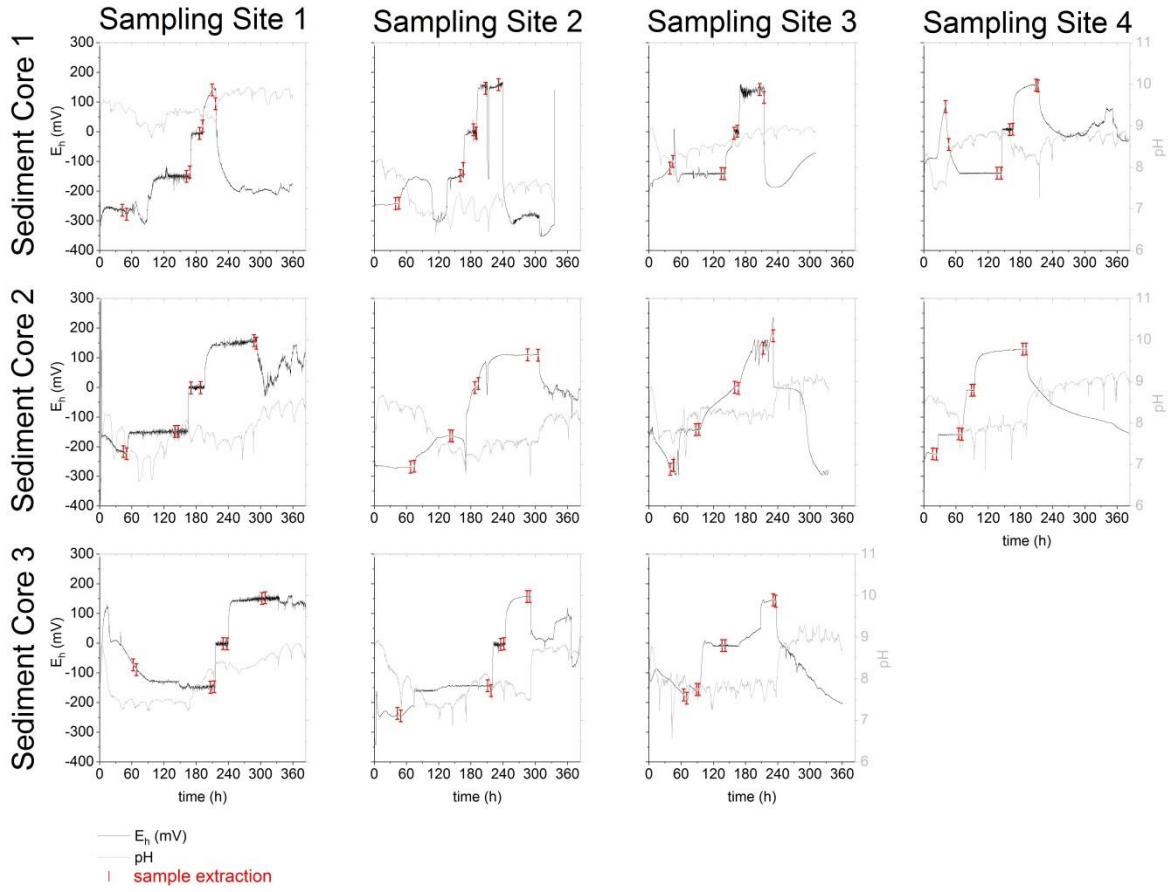


Figure A3. 6: Course of Eh and pH during the individual resuspension experiments and timing of sampling. Sediment core 3 of sampling site 4 is missing due to handling error.

AIII.VI.II Measured concentrations in mesocosm samples

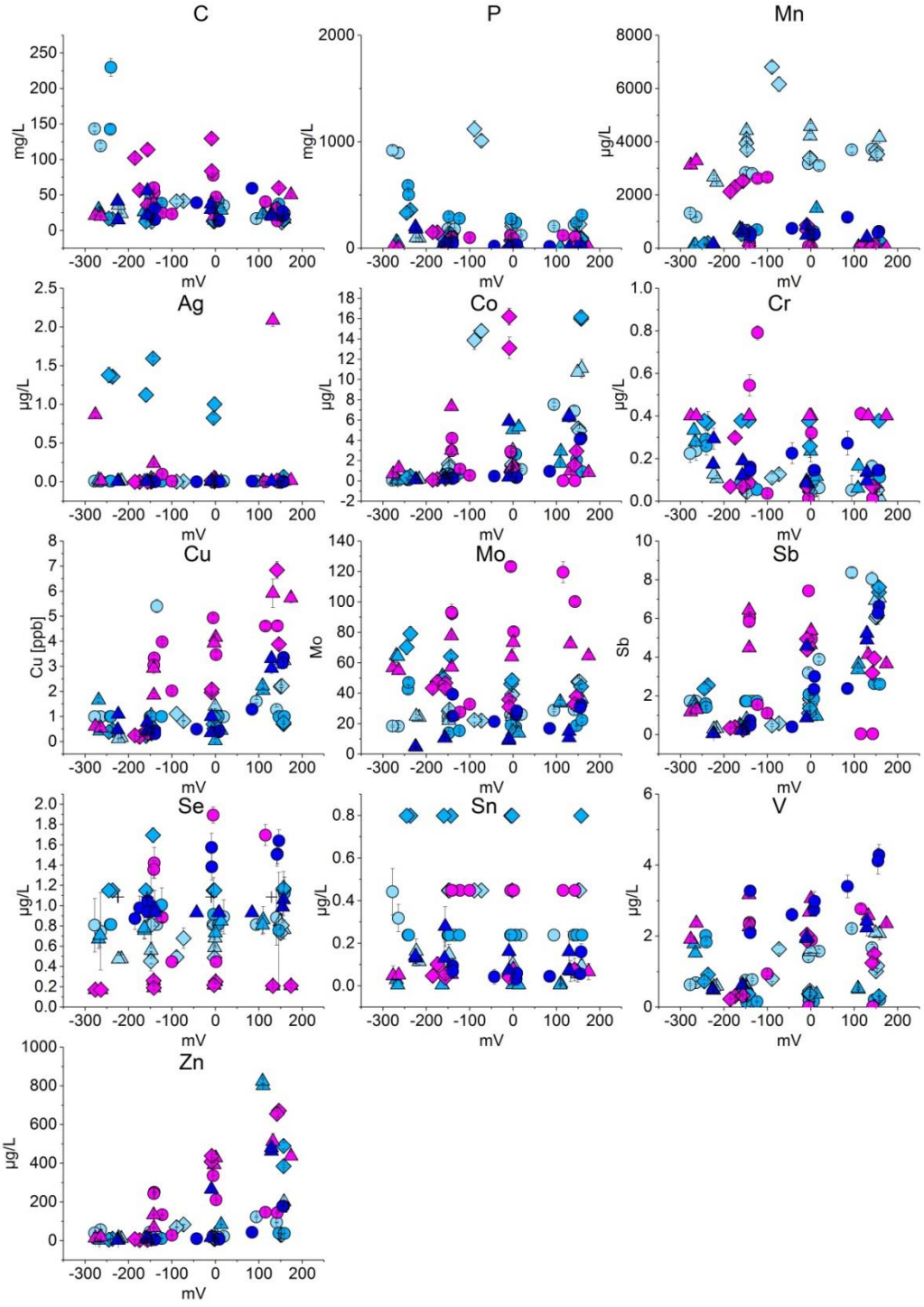


Figure A3. 7: Concentrations of C, P, Mn, Ag, Co, Cr, Cu, Mo, Sb, Se, Sn, V, Zn as a function of E_h (●, ●, ●, ● for sampling site 1, 2, 3 and 4; ●, ▲, ♦ representing the 3 repetitions) during the resuspension experiments.

The results of individual measurements are given in Table A3. 126-A3. 143, section 9.

AIII.VII Indices for evaluation of sequential extraction

AIII.VII.I Enrichment factor

Enrichment factor (EF) as estimation of anthropogenic enrichment of an element is calculated as

$$EF = \frac{[X/Fe]_{Sample}}{[X/Fe]_{Crust}}$$

where $[X/Fe]_{Sample}$ refers to the ratio of of the content of the target element and iron in the sample and $[X/Fe]_{Crust}$ refers to the ratio of trhe content of the target element and iron in the continental earth crust. Continental eath crust concentrations were taken from [1].

AIII.VII.II Geoaccumulation index

The geoaccumulation index (I_{Geo}) is computed, another measure of the enrichment of an element compared to the average earth crust concnetration is computed as

$$I_{Geo} = log_2(\frac{C_n}{1.5B_n})$$

Where Cn is the element concentration in the sediment sample and Bn is the geochemical background value in the continental earth crust (taken from [1]).

AIII.VII.III Contamination factor

The contamination factor is a measure of the risk an element to the environment in relation to its retention time. It is computed by division of the sum of the non-residual fractions (exchangeable + oxidizeable + reducible) by the residual fraction for each metal(loid). The results were interpreted following [2]: CF < 0 indicates low contamination, CF < 3 indicates moderate conatmination, CF < 6 indicates considerable contamination, CF > 6 high contamination.

AIII.VII.IV Risk assessment code

The risk assessment code (RAC) is computed in terms of percent contribution in the exchangeable fraction of the sequential extraction and may be classified as following [3]: RAC < 1% indicates no risk to the aquatic environment, RAC = 1-10% indicates low to the aquatic environment, RAC = 11-30% indicates medium risk to the aquatic environment, RAC = 31-50% indicates high risk to the aquatic environment and RAC > 50% indicates very high risk to the aquatic environment.

Table A3. 7: Enrichment Factor, Geoaccumulation Index, Contamination Factor and Risk Assessment Code for the elements As, Sb, Cd, Cr, Co, Cu, Pb, Mo, Ni, Se, Ag, Sn, V and Zn in samples of the 4 sampling sites.

		Enrichment Factor (EF)	Interpretation EF	Geoaccumulation Index (I_{geo})	Interpretation I_{geo}	Contamination Factor (CF)	Interpretation CF	Risk Assessment Code (RAC)	Interpretation RAC
			ENRICHMENT is:		CONTAMINATION is:		CONTAMINATION is:		RISK is:
As	Sampling Site 1	14.33	SEVERE	2.77	moderate-heavy	0.17	LOW	3.36	NO
	Sampling Site 2	11.37	SEVERE	2.53	moderate-heavy	0.10	LOW	2.22	NO
	Sampling Site 3	10.08	SEVERE	1.18	moderate	0.31	LOW	6.98	NO
	Sampling Site 4	11.74	SEVERE	2.71	moderate-heavy	0.18	LOW	2.81	NO
Sb	Sampling Site 1	0.04	NO	-5.84	uncontaminated	11.83	HIGH	18.13	MEDIUM
	Sampling Site 2	0.04	NO	-5.70	uncontaminated	85.98	HIGH	12.70	VERY HIGH
	Sampling Site 3	0.06	NO	-6.14	uncontaminated	22.74	HIGH	10.48	MEDIUM
	Sampling Site 4	0.04	NO	-5.57	uncontaminated	1.84	MODERATE	11.36	LOW
Cd	Sampling Site 1	68.41	EXTREMELY SEVERE	5.03	extreme	6.55	HIGH	51.20	LOW
	Sampling Site 2	35.93	VERY SEVERE	4.19	heavy-extreme	32.63	HIGH	66.80	HIGH
	Sampling Site 3	42.49	VERY SEVERE	3.26	heavy	3.32	CONSIDERABLE	46.52	LOW
	Sampling Site 4	63.21	EXTREMELY SEVERE	5.14	extreme	8.92	HIGH	54.62	LOW
Cr	Sampling Site 1	0.54	NO	-1.95	uncontaminated	0.13	LOW	0.34	NO
	Sampling Site 2	0.74	NO	-1.42	uncontaminated	0.15	LOW	0.46	NO
	Sampling Site 3	0.86	NO	-2.38	uncontaminated	0.04	LOW	0.44	NO
	Sampling Site 4	0.58	NO	-1.64	uncontaminated	0.15	LOW	0.29	NO
Co	Sampling Site 1	0.71	NO	-1.56	uncontaminated	3.91	CONSIDERABLE	21.13	LOW
	Sampling Site 2	0.92	NO	-1.10	uncontaminated	2.17	MODERATE	24.21	LOW
	Sampling Site 3	0.66	NO	-2.76	uncontaminated	2.31	MODERATE	24.29	LOW
	Sampling Site 4	0.50	NO	-1.83	uncontaminated	4.08	CONSIDERABLE	22.51	LOW
Cu	Sampling Site 1	1.64	MINOR	-0.36	uncontaminated	39.16	HIGH	3.04	HIGH
	Sampling Site 2	1.68	MINOR	-0.23	uncontaminated	26.80	HIGH	4.44	MEDIUM
	Sampling Site 3	1.15	MINOR	-1.95	uncontaminated	16.07	HIGH	7.01	MEDIUM
	Sampling Site 4	1.70	MINOR	-0.08	uncontaminated	28.00	HIGH	2.81	MEDIUM
Pb	Sampling Site 1	26.19	VERY SEVERE	3.64	heavy	0.13	LOW	3.86	NO
	Sampling Site 2	24.17	SEVERE	3.62	heavy	0.16	LOW	8.32	NO
	Sampling Site 3	15.20	SEVERE	1.77	moderate	0.23	LOW	7.94	NO
	Sampling Site 4	39.81	VERY SEVERE	4.47	heavy-extreme	0.13	LOW	4.78	NO
Mo	Sampling Site 1	1.05	MINOR	-1.00	uncontaminated	0.48	LOW	1.13	NO
	Sampling Site 2	1.96	MINOR	-0.01	uncontaminated	0.30	LOW	0.72	NO
	Sampling Site 3	4.26	MODERATE	-0.06	uncontaminated	1.65	MODERATE	48.60	LOW
	Sampling Site 4	1.02	MINOR	-0.81	uncontaminated	0.19	LOW	1.14	NO
Ni	Sampling Site 1	0.37	NO	-2.52	uncontaminated	1.16	MODERATE	11.00	LOW
	Sampling Site 2	0.51	NO	-1.94	uncontaminated	0.83	LOW	12.54	NO
	Sampling Site 3	0.51	NO	-3.13	uncontaminated	0.71	LOW	12.27	NO
	Sampling Site 4	0.38	NO	-2.25	uncontaminated	0.98	LOW	9.81	NO
Se	Sampling Site 1	36.70	VERY SEVERE	4.13	heavy-extreme	1.43	MODERATE	1.65	LOW
	Sampling Site 2	44.02	VERY SEVERE	4.48	heavy-extreme	1.17	MODERATE	1.11	LOW
	Sampling Site 3	43.06	VERY SEVERE	3.27	heavy	2.89	MODERATE	2.62	LOW
	Sampling Site 4	33.26	VERY SEVERE	4.22	heavy-extreme	1.43	MODERATE	2.00	LOW
Ag	Sampling Site 1	25.94	VERY SEVERE	3.63	heavy	0.03	LOW	0.45	NO
	Sampling Site 2	35.02	VERY SEVERE	4.15	heavy-extreme	0.03	LOW	0.32	NO
	Sampling Site 3	20.32	SEVERE	2.19	moderate-heavy	0.15	LOW	1.22	NO
	Sampling Site 4	29.74	VERY SEVERE	4.05	heavy-extreme	0.03	LOW	0.28	NO
Sn	Sampling Site 1	6.90	MODERATELY SEVERE	1.72	moderate	0.09	LOW	0.11	NO
	Sampling Site 2	7.05	MODERATELY SEVERE	1.84	moderate	0.01	LOW	0.12	NO
	Sampling Site 3	3.34	MODERATE	-0.42	uncontaminated	0.06	LOW	0.43	NO
	Sampling Site 4	7.62	MODERATELY SEVERE	2.09	moderate-heavy	0.02	LOW	0.08	NO
V	Sampling Site 1	0.56	NO	-1.90	uncontaminated	0.11	LOW	0.87	NO
	Sampling Site 2	0.83	NO	-1.24	uncontaminated	0.13	LOW	0.05	NO
	Sampling Site 3	0.69	NO	-2.69	uncontaminated	0.16	LOW	0.75	NO
	Sampling Site 4	0.49	NO	-1.88	uncontaminated	0.11	LOW	0.38	NO
Zn	Sampling Site 1	15.79	SEVERE	2.91	moderate-heavy	15.78	HIGH	52.70	MEDIUM
	Sampling Site 2	17.34	SEVERE	3.14	heavy	6.46	HIGH	59.55	LOW
	Sampling Site 3	9.78	MODERATELY SEVERE	1.14	moderate	17167.32	HIGH	61.54	VERY HIGH
	Sampling Site 4	13.87	SEVERE	2.95	moderate-heavy	16.73	HIGH	57.06	MEDIUM

AIII.VIII Interstitial Water Equilibrium Sediment Benchmarks

In the approach to evaluate dissolved concentrations in sediment pore water developed by the US Environmental Protection Agency [4], measured concentrations are converted to interstitial water benchmark units (IWBU) by dividing the individual concentration of Cd, Cu, Pb, Ni and Zn by their respective Water Quality Criteria Final Chronic Value (WQC FCV). If the sum is less than 1, it is assumed that no risk for benthic organisms originates from the considered elements.

$$\sum_i \frac{[\boldsymbol{M_{i,d}}]}{\boldsymbol{FCV_{i,d}}} \leq \mathbf{1.0}$$

where:

$$\sum_i \frac{[\boldsymbol{M_{i,d}}]}{\boldsymbol{FCV_{i,d}}} = \frac{[\boldsymbol{M_{Cd,d}}]}{[\boldsymbol{FCV_{Cd,d}}]} + \frac{[\boldsymbol{M_{Cu,d}}]}{[\boldsymbol{FCV_{Cu,d}}]} + \frac{[\boldsymbol{M_{Pb,d}}]}{[\boldsymbol{FCV_{Pb,d}}]} + \frac{[\boldsymbol{M_{Ni,d}}]}{[\boldsymbol{FCV_{Ni,d}}]} + \frac{[\boldsymbol{M_{Zn,d}}]}{[\boldsymbol{FCV_{Zn,d}}]}$$

and $[M_{Cd,d}]$, $[M_{Cu,d}]$, $[M_{Pb,d}]$, $[M_{Ni,d}]$, $[M_{Zn,d}]$ are the dissolved concentrations of Cd, Cu, Pb, Ni and Zn and $[FCV_{Cd,d}]$, $[FCV_{Cu,d}]$, $[FCV_{Pb,d}]$, $[FCV_{Ni,d}]$, $[FCV_{Zn,d}]$ are their final chronic values given in table A3. 8.

Table A3. 8: Water quality criteria final chronic value based on dissolved concentration of metal as published by US.EPA [4].

Metal	Cd	Cu	Pb	Ni	Zn
Saltwater FCV (µg/L)	9.3	3.1	8.1	8.2	81

Table A3. 9: Summed interstitial water benchmark units for suction-based pore water samples of the sampling site 1, 2, 3 and 4. Exceedances of the assessment criteria are marked in red.

	Sampling Site 1									
Depth	Sediment core 1			Sediment core 2			Sediment core 3			
(cm)	Profil 1	Profil 2	Profil 3	Profil 1	Profil 2	Profil 3	Profil 1	Profil 2	Profil 3	MAX
-4	0.31	3.54	8.48	0.62	1.86	1.89	8.44	3.22	2.82	8.48
-3	7.16	4.57	6.80	0.72	1.48	2.29	5.11	3.31	3.75	7.16
-2	3.91	1.80	6.07	0.68	1.10	2.31	3.80	3.30	4.23	6.07
-1	3.49	2.87	5.58	0.55	1.75	2.32	2.35	3.10	4.54	5.58
0	5.41	1.52	3.76	0.38	1.25	1.44	1.39	2.37	3.40	5.41
1	0.84	0.51	0.26	0.22	0.65	1.22		1.51	2.64	2.64
2	0.90	0.34	0.25	0.22	0.42	0.61	0.98	1.88	1.55	1.88
3	0.47	1.45	0.20	0.28	0.38	0.39	0.59	1.24	1.20	1.45
4	1.15	0.25	0.20	0.17	0.27	0.30	0.70	1.63	0.73	1.63
5	0.53	0.24	0.18	0.15	0.25	0.59	0.55	1.09	0.20	1.09
6	0.63	0.15	0.20	0.14	0.35	0.27	0.43	0.74	0.81	0.81
7	0.52	0.21	0.77	0.20	0.42	0.22	0.37	0.48	0.92	0.92
8	0.70	0.15	0.22	0.20	0.24	0.18	0.48	0.73	0.80	0.80
9	0.87	0.29	0.19	0.19	0.26	0.20	0.36	0.51	0.66	0.87
10	0.88	0.30	0.29	0.36	0.25	0.21	0.47	0.45	0.56	0.88
11	0.70	0.24	0.18	0.29	0.29	0.19	0.42	0.42	0.53	0.70
12	0.81	0.21	0.18	0.29	0.24	0.23	1.06	0.52	0.44	1.06
13	0.95	0.23	0.16	0.32	0.25	0.19	3.08	0.48	0.38	3.08
14	1.29	0.18	0.20	0.63	0.25	0.48	0.37	0.46	0.44	1.29
15	2.88	0.16	0.18	0.33	0.25	0.31	0.99	1.06	0.42	2.88

	Sampling Site 2									
Depth	Sediment core 1			Sediment core 2			Sediment core 3			
(cm)	Profil 1	Profil 2	Profil 3	Profil 1	Profil 2	Profil 3	Profil 1	Profil 2	Profil 3	MAX
-4	4.01	1.62	4.36	0.33	1.42	1.29	2.46	1.90	1.39	4.36
-3	3.46	2.00	2.02	0.42	1.29	2.24	1.99	2.53	2.01	3.46
-2	2.57	1.10	0.74	0.47	2.12	2.56	2.22	2.48	2.00	2.57
-1	2.80	0.69	0.78	0.54	2.49	3.10	1.79	1.85	2.17	3.10
0	2.94	0.25	0.38	0.39	1.56	2.80	1.17	1.85	1.64	2.94
1	1.90	0.18	0.25	0.33	0.79	1.35	0.84	0.79	1.86	1.90
2	1.74	0.23	0.25	0.24	0.73	2.11	0.73	0.32	2.00	2.11
3	3.29	0.30	0.22	0.24	0.70	2.19	0.23	0.24	0.48	3.29
4	3.95	0.81	0.21	0.28	0.58	2.63	0.20	0.20	0.34	3.95
5	5.00	0.24	0.25	0.28	0.46	2.48	0.15	0.20	0.29	5.00
6	1.08	0.15	2.43	0.30	0.39	2.01	0.16	0.22	0.28	2.43
7	1.12	0.79	0.23	0.49	0.30	0.64	0.15	0.25	0.15	1.12
8	0.94	0.09	0.20	0.22	0.39	0.36		0.11	0.16	0.94
9	1.38	1.45	0.86	0.28	0.27	0.32	0.16	0.19	0.17	1.45
10	0.94	0.25	0.17	0.29	0.40	0.26	0.12	0.13	0.18	0.94
11	1.05	0.22	0.32	0.37	0.39	0.21	0.09	0.16	0.30	1.05
12	1.03	0.39	0.47	0.36	0.35	0.23	0.12	0.12	0.14	1.03
13	1.05	0.24	0.20	0.23	0.37	0.27	0.09	0.15	0.34	1.05
14	0.95	0.17	0.20	0.42	0.35	0.29	0.06	0.06	0.14	0.95
15	0.95	0.22	0.07	0.50	0.43	0.32	0.17	0.23	0.14	0.95

	Sampling Site 3									
Depth	Sediment core 1			Sediment core 2			Sediment core 3			
(cm)	Profil 1	Profil 2	Profil 3	Profil 1	Profil 2	Profil 3	Profil 1	Profil 2	Profil 3	MAX
-4	1.12	1.08	2.04	1.83	1.83	1.21	0.62	1.55	12.23	12.23
-3	1.59	0.98	1.60	2.12	1.96	1.39	0.90	1.75	4.68	4.68
-2	2.05	1.51	2.11	2.17	2.36	1.17	1.49	1.24	4.53	4.53
-1	1.63	1.33	2.03	2.42	2.04	1.17	1.07	1.36	3.67	3.67
0	1.21	0.67	1.20	1.84	1.48	0.89	1.07	1.55	3.56	3.56
1	0.83	0.34	0.68	1.55	0.69	0.80	1.02	0.98	1.18	1.55
2	0.50	0.30	0.39	0.70	0.64	0.67	0.70	0.73	1.09	1.09
3	0.39	0.38	0.34	0.51	0.58	0.48	0.34	0.68	0.94	0.94
4	0.32	0.47	1.57	0.58	2.91	0.57	0.33	0.33	0.94	2.91
5	0.28	0.68	0.43	0.45	0.47	0.38	0.33	0.33	0.94	0.94
6	0.86	0.27	0.22	0.35	0.43	0.47	0.33	0.33	1.11	1.11
7	0.24	0.22	0.43	0.35	0.66	0.42	0.34	0.46	0.95	0.95
8	0.21	0.21		0.41		0.47	0.33	0.33	0.91	0.91
9	0.19	0.25	0.52	0.47	0.63	0.34	0.41	0.58	0.81	0.81
10	0.18	0.38	0.10	0.64	0.25	0.45	0.42	0.34	0.81	0.81
11	0.32	0.37	0.14	1.14	1.34	0.28	0.34	0.07	0.81	1.34
12	1.99	0.42	0.06	0.08		0.32	0.33	0.34	2.61	2.61
13	0.21	0.18	0.06	0.96		0.44	0.33	0.34	0.81	0.96
14	0.20		0.06	0.01		0.05	0.34	0.34	0.81	0.81
15	0.20		0.65				0.33	0.34	0.81	0.81

	Sampling Site 4									
Depth	Sediment core 1			Sediment core 2			Sediment core 3			
(cm)	Profil 1	Profil 2	Profil 3	Profil 1	Profil 2	Profil 3	Profil 1	Profil 2	Profil 3	MAX
-4	2.02	0.58	2.44	2.36	1.08	0.63	0.52	1.69	3.47	3.47
-3	0.73	0.64	0.75	2.01	0.95	0.87	0.51	2.01	2.96	2.96
-2	0.36	0.97	2.59	1.20	1.02	1.90	0.52	3.46	1.45	3.46
-1	0.27	0.58	2.61	1.80	1.02	0.49	0.39	2.96	0.68	2.96
0	0.33	0.43	1.04	1.50	0.58	0.29	0.37	3.12	1.21	3.12
1	0.25	0.39	0.68	1.15	0.30	0.41	0.26	1.19	1.52	1.52
2	0.29	0.31	0.34	1.11	0.27	0.60	0.30	1.26	0.07	1.26
3	0.19	0.54	0.37	1.05	0.24	0.29	0.11	1.04	0.07	1.05
4	0.17	0.33	0.25	1.15	0.23	0.79	0.20	0.92	0.08	1.15
5	0.22	0.20	0.25	1.11	0.24	1.05	0.21	0.93	1.76	1.76
6	0.20	0.30	0.78	1.00	0.24	0.47	0.22	0.90	0.39	1.00
7	0.38	0.32	0.17	1.15	0.23	0.47	0.27	0.91	1.91	1.91
8		0.12	0.11	1.78	0.23	0.58	0.21	0.13	0.07	1.78
9	1.06	0.12	0.12	1.25	0.41	0.36	0.43	0.35	1.58	1.58
10	0.31	0.63	0.16	1.34	0.50	1.05	0.12	0.90	0.39	1.34
11	0.29	0.14	0.11	1.97	0.50	0.74	0.12	0.19	0.39	1.97
12	0.24	0.15	0.14	1.59	0.41	0.32	0.26	0.48	0.39	1.59
13	0.20	0.58	0.15	1.79		0.38	0.20	0.53	0.39	1.79
14	0.22	0.00	0.20	1.36		0.44	0.12	0.48	0.39	1.36
15	0.29	0.62	0.14	0.65		0.47		0.87	0.39	0.87

AIII.IX Results of individual measurements

AIII.IX.I Metal(loid) content in the different fractions of the sequential extraction

Table A3. 10: Metal(loid) content in the different fractions of the sequential extraction.

			Ag		As		Cd		Co		Cr		Cu		Fe		Mn	
			Conc.	RSD	Conc.	RSD	Conc.	RSD	Conc.	RSD	Conc.	RSD	Conc.	RSD	Conc.	RSD	Conc.	RSD
			mg/kg	%	mg/kg	%	mg/kg	%	mg/kg	%	mg/kg	%	mg/kg	%	mg/kg	%	mg/kg	%
Exchangable	Sampling Site 1	Sediment Core 1	0.01	8.22	0.39	4.27	3.61	3.30	2.45	1.23	0.14	1.76	1.94	2.15	627.08	1.61	307.74	2.10
		Sediment Core 2	0.01	9.95	0.71	6.46	3.44	7.64	2.78	4.34	0.13	9.91	2.15	1.62	709.45	1.10	311.47	1.69
		Sediment Core 3	0.01	22.16	0.76	5.23	4.23	6.51	2.83	7.64	0.14	8.17	2.33	4.92	902.94	4.59	335.50	0.84
Acid reduceable		Sediment Core 1	0.01	2.34	1.46	2.06	1.78	3.27	2.60	3.11	0.26	4.07	1.12	6.71	3409.86	4.39	78.61	1.94
		Sediment Core 2	0.01	9.84	1.71	5.30	1.78	7.22	2.65	5.35	0.29	4.13	1.10	1.62	3166.06	1.37	59.22	1.33
		Sediment Core 3	0.01	3.17	1.73	5.90	2.11	6.85	2.63	5.04	0.30	5.07	1.10	5.56	3398.98	4.63	84.68	0.51
Oxidizable		Sediment Core 1	0.02	40.74	0.30	8.40	0.65	7.55	4.80	5.69	3.84	6.87	81.71	2.53	327.73	3.63	216.43	1.68
		Sediment Core 2	0.02	11.15	0.26	24.11	0.77	7.58	4.85	3.11	3.72	3.38	85.44	3.76	291.29	3.31	211.28	1.37
		Sediment Core 3	0.03	9.27	0.55	7.26	0.75	10.28	4.75	6.27	4.61	1.38	81.92	3.54	740.56	2.47	245.91	3.16
Residual (calculated)		Sediment Core 1	1.27		16.23		0.95		2.47		36.05		1.78		34211.83		31.34	
		Sediment Core 2	1.37		16.07		0.68		2.76		36.21		1.81		34263.08		79.84	
		Sediment Core 3	1.42		15.19		1.30		2.52		33.07		1.74		33021.39		40.49	
Exchangable	Sampling Site 2	Sediment Core 1	0.01	7.18	0.43	6.08	2.58	7.15	3.98	7.29	0.27	7.90	3.32	1.14	465.62	1.72	88.67	0.15
		Sediment Core 2	0.01	6.32	0.36	4.85	2.89	2.76	4.11	2.07	0.29	2.22	2.93	2.07	502.28	2.57	116.72	3.68
		Sediment Core 3	0.01	5.36	0.23	7.64	2.75	5.33	4.38	1.15	0.24	2.57	3.98	3.65	511.57	3.42	105.34	0.95
Acid reduceable		Sediment Core 1	0.01	9.14	0.57	4.65	0.61	6.38	1.07	4.56	0.44	5.21	0.83	3.70	2832.47	4.06	12.56	5.29
		Sediment Core 2	0.01	26.08	0.52	5.00	0.72	3.83	1.31	5.01	0.13	7.23	0.83	7.62	3389.45	6.81	14.34	1.49
		Sediment Core 3	0.01	8.99	0.40	5.47	0.67	9.57	1.65	5.05	0.11	7.52	0.88	3.69	4088.88	2.72	18.94	8.73
Oxidizable		Sediment Core 1	0.04	7.19	0.67	3.72	0.61	7.96	6.14	2.38	8.11	3.14	75.46	2.48	1396.95	2.31	196.32	1.41
		Sediment Core 2	0.04	13.14	0.64	11.89	0.67	6.43	7.02	2.58	7.79	2.67	76.05	1.58	1336.21	1.09	193.74	0.93
		Sediment Core 3	0.03	26.86	0.27	11.12	0.44	2.35	5.76	4.04	5.54	3.24	72.24	1.67	235.11	2.11	163.09	0.77
Residual (calculated)		Sediment Core 1	2.16		14.12		0.67		7.49		48.39		0.97		37053.49		101.76	
		Sediment Core 2	2.17		12.64		0.03		6.25		47.83		1.49		34484.97		18.66	
		Sediment Core 3	1.52		15.88		0.01		3.15		52.44		1.02		36061.21		39.51	
Exchangable	Sampling Site 3	Sediment Core 1	0.01	5.08	0.40	2.64	0.90	2.06	1.26	5.27	0.09	5.88	1.32	4.29	419.39	3.03	217.42	2.75
		Sediment Core 2	0.01	10.29	0.52	2.62	0.97	4.50	1.36	3.28	0.15	2.61	1.84	4.77	417.23	4.49	128.12	4.45
		Sediment Core 3	0.01	19.00	0.37	3.98	1.13	8.18	1.43	5.90	0.16	4.41	1.73	2.83	357.66	2.40	151.78	3.48
Acid reduceable		Sediment Core 1	0.01	12.44	0.78	2.16	0.39	1.60	0.88	2.32	0.13	5.52	0.83	2.46	1615.15	0.96	20.56	1.24
		Sediment Core 2	0.01	3.37	0.93	3.25	0.26	3.72	0.72	2.88	0.11	3.43	0.83	7.26	1376.00	4.33	9.49	0.60
		Sediment Core 3	0.01	6.58	0.96	4.71	0.29	4.30	0.90	4.05	0.15	36.39	0.84	5.29	1550.46	2.78	11.60	4.36
Oxidizable		Sediment Core 1	0.05	13.45	0.13	17.91	0.34	10.65	1.66	4.53	0.91	6.19	52.09	2.59	31.66	2.51	43.05	0.78
		Sediment Core 2	0.06	26.08	0.14	28.60	0.36	11.38	1.48	7.86	0.99	11.44	50.67	2.66	45.67	3.43	40.28	0.94
		Sediment Core 3	0.05	21.44	0.11	36.21	0.31	5.30	1.93	1.11	0.73	5.04	49.60	3.07	35.49	3.26	48.55	1.81
Residual (calculated)		Sediment Core 1	0.39		4.27		0.63		1.55		26.33		3.45		14513.80		37.37	
		Sediment Core 2	0.46		5.26		0.37		1.95		28.94		3.05		16879.70		86.68	
		Sediment Core 3	0.49		4.48		0.50		1.53		29.76		2.91		16967.24		39.48	
Exchangable	Sampling Site 4	Sediment Core 1	0.00	10.86	0.50	5.70	4.91	3.85	2.51	1.78	0.15	2.08	2.57	4.16	614.23	2.80	218.20	0.96
		Sediment Core 2	0.00	13.96	0.54	6.18	3.96	2.83	2.43	7.56	0.14	7.33	2.44	1.99	511.34	2.57	231.27	2.34
		Sediment Core 3	0.01	15.66	0.46	1.96	4.15	5.12	2.20	3.89	0.13	3.22	2.19	1.72	658.51	2.54	257.70	0.14
Acid reduceable		Sediment Core 1	0.01	9.83	1.37	4.09	2.20	4.43	2.05	7.59	0.30	6.68	1.15	4.19	4246.41	4.79	53.74	0.88
		Sediment Core 2	0.01	8.01	1.74	5.06	1.83	5.75	1.56	5.03	0.25	9.91	1.01	3.57	3756.36	2.59	55.86	0.36
		Sediment Core 3	0.01	21.10	1.49	9.16	2.05	6.82	2.05	6.60	0.32	8.37	1.14	2.81	4072.46	2.42	64.50	2.01
Oxidizable		Sediment Core 1	0.02	14.20	0.78	2.60	0.77	7.56	4.41	3.05	6.37	2.41	88.79	2.00	926.94	2.51	225.91	3.29
		Sediment Core 2	0.01	13.58	0.39	2.29	0.82	7.22	4.12	1.32	5.42	3.72	77.96	0.95	536.87	0.67	237.30	0.71
		Sediment Core 3	0.07	4.31	0.81	12.46	0.74	1.89	4.15	2.68	6.59	4.34	78.99	2.42	905.40	3.19	214.25	1.35
Residual (calculated)		Sediment Core 1	2.00		14.91		1.33		2.02		40.68		0.75		39335.09		138.05	
		Sediment Core 2	1.74		14.83		0.45		2.29		44.21		0.00		40229.68		76.68	
		Sediment Core 3	1.73		15.31		0.62		1.93		43.16		0.13		38927.19		64.66	

Table A3. 10 continued.

			Mo		Ni		Pb		Sb		Se		Sn		V		Zn	
			Conc.	RSD	Conc.	RSD	Conc.	RSD	Conc.	RSD	Conc.	RSD	Conc.	RSD	Conc.	RSD	Conc.	RSD
			mg/kg	%	mg/kg	%	mg/kg	%	mg/kg	%	mg/kg	%	mg/kg	%	mg/kg	%	mg/kg	%
Exchangable	Sampling Site 1	Sediment Core 1	0.01	14.71	2.31	3.03	6.57	1.70	0.15	2.88	0.02	40.21	0.01	9.52	0.33	1.29	364.37	1.59
		Sediment Core 2	0.01	6.34	2.43	1.17	11.80	0.75	0.06	9.93	0.02	40.81	0.01	12.32	0.42	6.02	416.25	1.05
		Sediment Core 3	0.01	18.08	2.50	3.73	12.15	2.36	0.07	14.33	0.03	24.66	0.01	5.81	0.49	7.13	473.14	4.45
Acid reduceable		Sediment Core 1	0.01	27.30	2.29	2.40	16.96	1.87	0.08	8.50	0.02	44.44	0.03	12.40	3.91	2.08	170.92	4.79
		Sediment Core 2	0.35	7.26	2.40	0.16	21.19	1.61	0.09	8.42	0.02	42.50	0.04	7.67	4.17	5.36	175.17	0.84
		Sediment Core 3	0.01	14.10	3.25	3.69	21.24	2.74	0.08	9.94	0.01	43.53	0.05	9.27	4.03	5.96	182.06	4.82
Oxidizable		Sediment Core 1	0.20	13.52	6.94	2.77	1.34	3.37	0.35	13.59	0.66	27.92	1.99	6.27	0.24	8.39	148.11	2.27
		Sediment Core 2	0.13	8.84	6.35	1.98	1.24	2.66	0.31	0.48	0.72	35.50	0.12	7.74	0.21	0.97	151.79	2.41
		Sediment Core 3	0.14	20.81	6.87	3.70	1.09	4.60	0.26	15.26	0.81	16.38	0.17	13.69	0.52	1.60	152.39	3.59
Residual (calculated)		Sediment Core 1	0.64		9.40		229.38		0.06		0.66		7.87		41.93		76.80	
		Sediment Core 2	0.43		11.75		228.53		0.04		0.57		11.61		48.83		41.35	
		Sediment Core 3	0.76		9.41		235.62		0.03		0.39		12.13		39.33		20.79	
Exchangable	Sampling Site 2	Sediment Core 1	0.01	16.70	3.91	2.09	20.36	2.38	0.07	7.76	0.02	15.23	0.02	3.04	0.05	7.02	514.28	0.96
		Sediment Core 2	0.01	8.69	4.30	2.70	25.53	2.45	0.08	3.20	0.02	63.79	0.01	6.99	0.03	3.74	570.66	2.63
		Sediment Core 3	0.01	29.52	4.11	2.83	16.63	1.52	0.07	11.67	0.02	32.29	0.01	7.79	0.04	0.37	536.76	3.32
Acid reduceable		Sediment Core 1	0.02	17.66	1.43	0.24	11.44	2.70	0.10	6.75	0.02	96.84	0.01	18.70	6.06	3.84	86.15	3.67
		Sediment Core 2	0.06	2.21	1.52	3.08	14.45	2.87	0.09	8.59	0.02	14.24	0.01	7.26	6.41	4.45	107.86	6.10
		Sediment Core 3	0.03	10.08	1.98	3.43	10.36	3.78	0.11	2.89	0.01	57.28	0.01	8.58	8.54	5.64	104.86	1.84
Oxidizable		Sediment Core 1	0.36	16.94	8.55	1.61	1.53	2.77	0.39	0.58	0.90	14.13	0.23	8.76	2.13	4.40	145.02	1.88
		Sediment Core 2	0.29	14.86	9.14	3.25	1.56	1.64	0.47	2.05	0.84	1.04	0.16	12.15	1.96	5.26	166.64	0.96
		Sediment Core 3	0.42	8.53	9.87	3.07	1.11	4.78	0.33	3.22	0.86	7.17	0.07	8.81	0.23	5.06	123.26	2.13
Residual (calculated)		Sediment Core 1	1.54		18.44		248.03		0.00		0.78		13.17		68.06		302.47	
		Sediment Core 2	1.57		16.10		178.86		0.01		0.83		13.24		67.90		48.79	
		Sediment Core 3	1.05		19.24		242.64		0.00		0.71		10.05		66.93		161.72	
Exchangable	Sampling Site 3	Sediment Core 1	0.02	6.00	1.68	1.77	3.65	2.12	0.05	11.71	0.02	21.79	0.01	2.94	0.13	7.81	128.70	2.90
		Sediment Core 2	1.54	2.40	1.76	1.21	6.30	0.65	0.04	3.94	0.01	23.05	0.01	7.45	0.32	4.42	139.68	4.49
		Sediment Core 3	0.95	6.53	1.83	2.24	7.31	2.69	0.04	4.40	0.02	22.43	0.01	21.26	0.18	4.63	157.84	2.75
Acid reduceable		Sediment Core 1	0.07	6.78	1.28	0.63	4.99	0.89	0.07	2.88	0.02	20.00	0.01	4.76	3.21	2.67	40.21	1.02
		Sediment Core 2	0.01	4.50	1.24	3.70	7.35	2.52	0.06	7.57	0.02	37.12	0.01	2.30	2.84	3.83	27.46	3.79
		Sediment Core 3	0.02	2.86	1.19	0.87	7.25	2.40	0.06	2.43	0.02	26.32	0.01	16.29	3.22	2.71	34.18	3.84
Oxidizable		Sediment Core 1	0.20	6.19	2.78	4.21	1.98	1.42	0.34	3.29	0.40	34.19	0.08	15.96	1.23	2.24	57.68	2.39
		Sediment Core 2	0.20	10.24	2.75	4.33	1.01	1.16	0.28	12.04	0.47	42.31	0.09	21.38	0.04	15.46	48.42	2.33
		Sediment Core 3	0.20	11.89	3.34	1.19	0.95	0.24	0.27	6.33	0.64	33.60	0.08	25.36	0.06	8.47	55.81	3.03
Residual (calculated)		Sediment Core 1	0.14		7.36		56.84		0.03		0.24		0.75		22.03		16.65	
		Sediment Core 2	-1.32		8.72		59.31		0.01		0.24		3.80		24.45		22.21	
		Sediment Core 3	-0.77		9.16		58.31		0.01		0.07		2.91		25.72		3.40	
Exchangable	Sampling Site 4	Sediment Core 1	0.01	13.65	2.74	0.49	14.10	1.98	0.07	0.87	0.04	43.75	0.01	8.14	0.15	1.47	538.56	3.39
		Sediment Core 2	0.01	14.62	2.56	1.69	13.79	1.79	0.08	10.45	0.02	26.75	0.01	12.27	0.22	8.26	401.37	1.98
		Sediment Core 3	0.01	7.11	2.51	1.54	10.38	2.75	0.07	5.32	0.02	68.42	0.01	9.47	0.19	3.54	456.63	2.57
Acid reduceable		Sediment Core 1	0.01	5.88	2.75	1.07	18.40	4.03	0.07	5.65	0.02	49.75	0.05	7.74	4.04	8.12	184.92	4.42
		Sediment Core 2	0.01	21.19	2.18	0.80	13.00	2.36	0.08	3.48	0.02	60.08	0.05	9.94	3.77	6.01	138.21	3.20
		Sediment Core 3	0.01	28.17	2.74	0.62	17.22	2.33	0.06	10.44	0.02	81.86	0.05	5.78	3.85	7.24	167.84	2.31
Oxidizable		Sediment Core 1	0.15	8.10	8.22	4.43	1.14	1.37	0.30	10.99	0.78	9.61	0.23	9.38	0.81	3.16	147.13	3.20
		Sediment Core 2	0.13	20.83	8.19	5.09	1.01	2.05	0.23	8.20	0.76	10.58	0.16	33.67	0.44	0.52	143.85	0.90
		Sediment Core 3	0.15	20.75	7.61	6.39	1.06	1.15	0.27	4.92	0.77	10.94	0.25	3.20	0.82	1.73	129.16	3.18
Residual (calculated)		Sediment Core 1	1.04		12.53		240.03		0.16		0.56		12.47		44.26		16.71	
		Sediment Core 2	0.83		14.14		234.98		0.24		0.61		15.78		44.96		99.96	
		Sediment Core 3	0.72		13.49		235.69		0.26		0.55		14.97		43.38		49.13	

AIII.IX.II Concentrations in suction-based sediment pore water samples

AIII.IX.II.I Concentrations in suction-based pore water samples of sampling site 1

Table A3. 11: Carbon concentrations across the SWI of the sediment cores of sampling site 1 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in mg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**3004**	15	**626**	27	**564**	32	**536**	31	**348**	9	**988**	89	**703**	25	33	1	**123**	7
-3	**1559**	3	**559**	28	**518**	22	**558**	27	**475**	33	**950**	36	**825**	23	**73**	4	**123**	4
-2	**1022**	5	**574**	54	**493**	16	**498**	37	**341**	9	**840**	32	**938**	21	55	2	**143**	4
-1	**894**	5	**601**	25	**503**	47	**508**	21	**272**	12	**812**	48	**448**	20	**81**	4	**129**	5
0	**1707**	5	**456**	10	**350**	12	**563**	29	**305**	21	**741**	54	**328**	16	67	2	**131**	3
1	**1407**	4	**616**	22	**502**	26	**657**	27	**436**	17	**784**	34	**no sample***		67	3	**134**	6
2	**1260**	7	**591**	20	**604**	19	**805**	49	**393**	15	**861**	27	**385**	17	**73**	3	**145**	4
3	**1016**	5	**577**	17	**630**	15	**674**	25	**490**	12	**837**	46	**391**	15	17	0	**297**	17
4	**1064**	3	**938**	15	**516**	20	**562**	26	**556**	21	**1144**	48	**385**	11	**114**	4	**365**	14
5	**991**	6	**730**	18	**487**	13	**619**	18	**566**	22	**977**	29	**716**	18	**121**	5	**344**	13
6	**867**	3	**982**	39	**617**	21	**553**	47	**697**	18	**639**	26	**719**	31	**139**	2	**380**	20
7	**821**	2	**916**	38	**654**	28	**448**	32	**776**	72	**1121**	82	**646**	17	**131**	3	**423**	11
8	**803**	2	**786**	11	**957**	42	**592**	28	**1363**	107	**1184**	54	**690**	39	**264**	7	**481**	20
9	**866**	7	**655**	15	**592**	30	**727**	42	**1200**	61	**1247**	81	**746**	35	**256**	7	**491**	21
10	**930**	2	**730**	18	**1476**	95	**629**	40	**1262**	22	**1435**	83	**830**	37	**277**	17	**406**	14
11	**923**	3	**784**	24	**970**	21	**585**	17	**1289**	44	**1323**	63	**725**	18	**272**	9	**432**	11
12	**767**	4	**981**	20	**829**	27	**710**	35	**1357**	86	**1507**	37	**685**	32	**171**	2	**337**	8
13	**675**	4	**953**	24	**850**	42	**721**	38	**1485**	50	**1643**	64	**679**	20	**271**	10	**267**	4
14	**1097**	7	**1628**	18	**732**	48	**627**	22	**1445**	97	**1477**	71	**659**	17	**263**	10	**437**	14
15	**531**	4	**979**	18	**726**	51	**1574**	104	**1368**	84	**3894**	276	**641**	15	**364**	12	**295**	6
LoD	7.64		2.43		5.77		3.60		14.49		9.80		26.02		26.02		26.02	
LoQ	20.07		5.67		14.68		9.80		41.68		20.30		67.54		67.54		67.54	
* insufficient sample volume for ICP measurement																		

Table A3. 12: Phosphorous concentrations across the SWI of the sediment cores of sampling site 1 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**85**	3	**189**	6	**187**	7	**64**	4	**30**	2	**276**	10	**149**	2	**405**	18	**404**	21
-3	**40**	0	**138**	1	**172**	2	**86**	7	**20**	1	**255**	7	**261**	10	**416**	20	**383**	6
-2	**31**	2	**203**	3	**299**	12	**122**	10	**22**	2	**213**	4	**290**	9	**362**	13	**369**	8
-1	**26**	1	**300**	6	**402**	18	**228**	13	**22**	2	**217**	7	**244**	11	**404**	14	**360**	12
0	**925**	38	**729**	25	**603**	26	**537**	30	**1010**	32	**234**	10	**24**	1	**388**	15	**275**	7
1	**1167**	45	**2417**	59	**2732**	114	**2601**	36	**4775**	134	**1381**	63	**no sample***		**207**	12	**38**	1
2	**1208**	82	**3772**	126	**4645**	262	**4068**	214	**5623**	203	**1199**	27	**34**	1	**24**	1	**37**	1
3	**554**	39	**6016**	115	**6486**	229	**5741**	314	**8736**	601	**4066**	141	**87**	3	**22**	1	**360**	13
4	**293**	9	**8573**	478	**6984**	405	**6424**	360	**7678**	157	**8680**	57	**1773**	49	**136**	5	**4144**	109
5	**371**	25	**8364**	168	**7568**	426	**5130**	281	**8728**	347	**12630**	624	**4801**	188	**811**	19	**6720**	196
6	**864**	46	**10426**	518	**9990**	355	**3668**	360	**6847**	412	**8226**	499	**5173**	129	**4858**	139	**4251**	106
7	**1455**	58	**11393**	565	**11012**	661	**4448**	251	**6767**	116	**8297**	281	**4853**	128	**6639**	227	**7605**	458
8	**1957**	44	**8955**	453	**7428**	219	**4492**	213	**7706**	212	**8682**	180	**5142**	281	**7784**	312	**11817**	293
9	**2876**	286	**9700**	511	**7249**	475	**5258**	339	**7698**	375	**10437**	371	**6289**	317	**7347**	274	**12085**	481
10	**3744**	77	**11148**	435	**8229**	531	**6466**	456	**8569**	141	**11284**	524	**6822**	201	**9598**	235	**11666**	612
11	**4242**	183	**15364**	366	**6822**	147	**7991**	378	**12172**	856	**12180**	860	**7024**	405	**11141**	456	**14603**	440
12	**3465**	214	**9553**	296	**7184**	507	**9038**	483	**11719**	763	**12727**	759	**8308**	302	**10359**	137	**11622**	400
13	**3704**	160	**10619**	240	**7485**	373	**11419**	512	**12187**	500	**14137**	837	**8318**	324	**12789**	532	**11128**	219
14	**4331**	220	**12771**	549	**8420**	127	**12447**	589	**13286**	641	**16172**	968	**4488**	168	**12333**	494	**12927**	327
15	**5954**	601	**12987**	327	**10360**	260	**11212**	468	**12724**	562	**16928**	874	**4419**	112	**12281**	314	**11921**	268
LoD	6.56		8.56		2.18		1.20		1.45		1.15		0.99		0.99		0.99	
LoQ	17.18		19.86		4.83		2.14		3.49		2.49		2.71		2.71		2.71	
* insufficient sample volume for ICP measurement																		

Table A3. 13: Sulfur concentrations across the SWI of the sediment cores of sampling site 1 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in mg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**813**	54	**569**	10	**502**	32	**262**	11	**432**	13	**447**	19	**420**	11	**444**	19	**495**	23
-3	**558**	25	**493**	5	**390**	15	**279**	14	**377**	27	**466**	24	**451**	8	**486**	23	**511**	29
-2	**377**	30	**487**	18	**370**	20	**284**	18	**268**	18	**436**	22	**416**	23	**467**	31	**524**	36
-1	**333**	25	**435**	6	**321**	3	**283**	11	**378**	19	**440**	19	**371**	16	**511**	26	**542**	21
0	**502**	19	**355**	9	**234**	10	**277**	13	**368**	17	**347**	5	**271**	11	**522**	18	**456**	8
1	**339**	15	**366**	15	**283**	11	**276**	7	**347**	16	**372**	12	**no sample***		**431**	21	**467**	13
2	**342**	26	**347**	19	**285**	17	**264**	14	**303**	12	**346**	15	**278**	17	**504**	27	**448**	8
3	**298**	23	**290**	17	**248**	7	**259**	5	**294**	10	**316**	10	**243**	11	**440**	22	**522**	14
4	**289**	11	**312**	15	**223**	12	**253**	15	**193**	5	**301**	5	**214**	10	**404**	10	**399**	14
5	**283**	22	**245**	3	**202**	11	**248**	16	**181**	8	**260**	11	**234**	6	**273**	14	**323**	14
6	**274**	10	**276**	15	**208**	4	**248**	20	**219**	14	**238**	17	**199**	9	**271**	5	**267**	11
7	**281**	10	**261**	15	**201**	11	**240**	13	**219**	9	**226**	10	**174**	1	**234**	4	**255**	15
8	**258**	5	**238**	8	**219**	6	**231**	10	**204**	14	**224**	5	**156**	8	**232**	9	**236**	11
9	**266**	20	**216**	4	**173**	11	**220**	11	**164**	3	**206**	7	**144**	8	**181**	8	**191**	8
10	**244**	8	**202**	5	**221**	13	**211**	16	**155**	3	**204**	5	**140**	7	**169**	8	**167**	3
11	**234**	9	**221**	8	**168**	5	**195**	10	**176**	10	**186**	14	**129**	6	**153**	6	**170**	5
12	**221**	7	**210**	7	**156**	3	**187**	10	**153**	8	**182**	7	**126**	5	**131**	7	**116**	5
13	**196**	6	**169**	5	**143**	6	**181**	8	**139**	6	**169**	8	**126**	5	**131**	5	**88**	5
14	**189**	10	**188**	9	**130**	3	**161**	8	**122**	4	**159**	10	**128**	6	**100**	7	**88**	4
15	**169**	7	**135**	3	**120**	3	**150**	6	**116**	6	**144**	7	**123**	5	**109**	4	**71**	1
LoD	1.13		0.11		0.28		0.46		0.06		0.14		0.43		0.43		0.43	
LoQ	3.31		0.18		0.67		1.23		0.08		0.31		1.05		1.05		1.05	
* insufficient sample volume for ICP measurement																		

Table A3. 14: Manganese concentrations across the SWI of the sediment cores of sampling site 1 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**103**	2	**74**	6	**59**	2	**7**	0	**81**	3	**2**	0	**81**	2	**49**	2	**18**	1
-3	**62**	2	**70**	6	**67**	2	**25**	1	**42**	1	**2**	0	**46**	3	**110**	5	**14**	1
-2	**41**	2	**313**	72	**291**	12	**150**	2	**48**	1	**3**	0	**37**	1	**363**	8	**9**	0
-1	**78**	2	**933**	20	**639**	30	**427**	16	**47**	2	**3**	0	**457**	30	**1152**	37	**8**	1
0	**695**	28	**924**	23	**636**	29	**806**	15	**544**	13	**148**	3	**1567**	26	**1722**	47	**374**	29
1	**899**	21	**1038**	32	**993**	36	**964**	12	**1437**	46	**1190**	44	**no sample***		**2196**	67	**2475**	113
2	**886**	27	**1027**	38	**1063**	35	**1079**	21	**1480**	40	**1427**	49	**1618**	38	**2551**	46	**2665**	50
3	**1147**	36	**987**	17	**987**	33	**1121**	17	**1611**	32	**1339**	49	**1542**	47	**2373**	103	**3173**	45
4	**1552**	31	**1077**	36	**808**	16	**1095**	15	**1153**	38	**1161**	26	**1298**	49	**2575**	53	**2916**	82
5	**1444**	32	**1077**	11	**826**	13	**1019**	12	**1219**	28	**1004**	17	**1423**	71	**1888**	62	**2672**	66
6	**1489**	15	**1108**	22	**830**	17	**800**	7	**830**	25	**536**	12	**1094**	25	**1901**	92	**1910**	73
7	**1154**	14	**1112**	21	**846**	11	**736**	9	**824**	22	**557**	19	**919**	54	**1584**	33	**2160**	92
8	**915**	13	**1007**	20	**573**	24	**752**	15	**885**	12	**526**	8	**753**	19	**1723**	53	**2182**	123
9	**934**	9	**1031**	12	**622**	11	**797**	15	**847**	52	**644**	17	**752**	10	**1299**	17	**1695**	56
10	**899**	18	**1141**	15	**682**	29	**839**	7	**904**	19	**597**	17	**828**	27	**1352**	48	**1404**	51
11	**921**	14	**1239**	41	**555**	17	**863**	9	**983**	46	**651**	12	**821**	28	**1252**	27	**1528**	26
12	**797**	50	**783**	17	**602**	12	**877**	24	**843**	19	**618**	14	**922**	44	**1071**	37	**1028**	55
13	**689**	9	**873**	10	**621**	17	**933**	18	**920**	19	**673**	12	**935**	25	**1293**	43	**917**	17
14	**668**	10	**1032**	20	**691**	29	**976**	12	**878**	30	**688**	24	**443**	18	**1023**	56	**1007**	37
15	**697**	17	**1045**	9	**728**	23	**820**	13	**781**	36	**673**	22	**398**	22	**1131**	69	**869**	23
LoD	0.09		0.14		0.58		0.13		0.21		0.14		0.24		0.24		0.24	
LoQ	0.23		0.32		1.62		0.31		0.48		0.26		0.61		0.61		0.61	
* insufficient sample volume for ICP measurement																		

Table A3. 15: Iron concentrations across the SWI of the sediment cores of sampling site 1 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**75**	2	**51**	20	**77**	4	**8**	0	**18**	0	**14**	1	**40**	0	**63**	2	**52**	2
-3	**54**	1	**95**	19	**48**	2	**13**	1	**10**	0	**12**	0	**39**	1	**56**	2	**51**	4
-2	**33**	2	**42**	22	**49**	1	**11**	0	**9**	0	**12**	0	**36**	1	**59**	1	**49**	2
-1	**31**	1	**70**	1	**45**	2	**10**	0	**16**	0	**13**	0	**30**	2	**58**	2	**56**	2
0	**86**	4	**954**	44	**590**	12	**405**	6	**1209**	32	**183**	5	**1298**	39	**52**	2	**43**	3
1	**39**	1	**2261**	114	**1225**	54	**3738**	122	**6945**	433	**9327**	408	**no sample***		**52**	1	**13600**	744
2	**39**	2	**2573**	84	**1613**	56	**5100**	158	**3853**	165	**8838**	201	**5807**	165	**589**	10	**29527**	1097
3	**25**	1	**3878**	89	**4660**	150	**6034**	243	**4556**	223	**8677**	383	**1570**	53	**7512**	427	**41130**	663
4	**23**	1	**4885**	167	**7214**	326	**6446**	192	**3469**	48	**6354**	243	**158**	6	**12061**	431	**31950**	1167
5	**26**	1	**5043**	218	**9278**	247	**7394**	307	**3789**	163	**4459**	128	**152**	6	**1775**	69	**22230**	763
6	**42**	0	**5634**	172	**8956**	199	**6427**	179	**81**	4	**77**	3	**110**	3	**4615**	263	**330**	19
7	**72**	1	**6031**	153	**8060**	348	**4935**	118	**51**	1	**90**	1	**86**	8	**4283**	98	**334**	18
8	**52**	1	**1462**	68	**806**	24	**168**	2	**77**	2	**104**	1	**70**	2	**1682**	32	**485**	29
9	**71**	2	**2520**	53	**1287**	18	**114**	2	**121**	7	**709**	20	**82**	2	**571**	14	**467**	21
10	**75**	2	**3724**	134	**666**	17	**197**	3	**393**	6	**412**	5	**115**	4	**821**	39	**437**	16
11	**88**	2	**4952**	195	**505**	17	**374**	5	**1469**	55	**1124**	30	**130**	4	**549**	15	**528**	16
12	**44**	3	**152**	3	**878**	21	**727**	18	**1825**	67	**1013**	21	**216**	11	**350**	16	**340**	19
13	**46**	1	**882**	128	**1226**	17	**1385**	28	**2219**	42	**1568**	25	**235**	9	**447**	15	**362**	11
14	**46**	1	**1207**	42	**1500**	55	**2567**	13	**2265**	85	**2545**	20	**35**	2	**414**	27	**441**	16
15	**73**	7	**1990**	73	**1773**	57	**216**	4	**858**	17	**1866**	45	**48**	2	**439**	28	**404**	9
LoD	0.41		1.55		0.59		0.37		0.43		0.16		0.34		0.34		0.34	
LoQ	0.97		4.08		1.64		0.85		1.13		0.38		0.82		0.82		0.82	
* insufficient sample volume for ICP measurement																		

Table A3. 16: Arsenic concentrations across the SWI of the sediment cores of sampling site 1 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**2.966**	0.109	**2.499**	0.022	**2.365**	0.247	**1.082**	0.072	**1.920**	0.084	**2.093**	0.121	**1.317**	0.037	**2.704**	0.088	**2.713**	0.160
-3	**1.978**	0.093	**2.258**	0.072	**1.938**	0.030	**1.163**	0.101	**1.781**	0.170	**2.195**	0.093	**1.761**	0.085	**3.536**	0.209	**2.830**	0.049
-2	**1.395**	0.118	**2.554**	0.091	**2.472**	0.214	**1.582**	0.157	**1.290**	0.066	**2.111**	0.074	**1.927**	0.021	**3.999**	0.070	**2.866**	0.098
-1	**1.489**	0.073	**3.188**	0.169	**3.541**	0.161	**2.308**	0.119	**1.730**	0.044	**2.175**	0.091	**3.767**	0.198	**5.948**	0.091	**3.134**	0.125
0	**7.813**	0.283	**5.004**	0.270	**3.018**	0.131	**3.883**	0.309	**5.534**	0.323	**2.636**	0.128	**3.148**	0.187	**7.910**	0.233	**2.610**	0.109
1	**11.157**	0.405	**6.267**	0.314	**3.939**	0.219	**4.876**	0.121	**11.656**	0.405	**9.124**	0.328	**no sample***		**5.956**	0.272	**2.335**	0.102
2	**12.316**	0.540	**4.763**	0.210	**4.481**	0.354	**4.513**	0.180	**6.177**	0.146	**6.288**	0.144	**2.550**	0.086	**1.653**	0.094	**2.011**	0.066
3	**12.066**	0.994	**3.546**	0.064	**5.765**	0.255	**4.126**	0.285	**4.740**	0.205	**5.451**	0.241	**2.885**	0.083	**1.179**	0.033	**4.020**	0.166
4	**6.856**	0.179	**3.628**	0.188	**6.902**	0.460	**3.640**	0.263	**2.889**	0.187	**4.850**	0.258	**3.761**	0.080	**1.721**	0.029	**5.080**	0.195
5	**5.048**	0.090	**2.985**	0.115	**5.304**	0.195	**3.258**	0.137	**2.660**	0.124	**4.241**	0.238	**5.129**	0.138	**1.868**	0.102	**4.701**	0.026
6	**4.197**	0.188	**3.254**	0.116	**4.607**	0.177	**2.804**	0.312	**2.978**	0.133	**3.934**	0.205	**4.649**	0.107	**3.246**	0.176	**2.978**	0.059
7	**3.387**	0.091	**3.144**	0.219	**4.018**	0.173	**3.482**	0.116	**3.050**	0.266	**3.724**	0.236	**4.281**	0.157	**3.863**	0.028	**4.360**	0.227
8	**2.684**	0.064	**2.708**	0.082	**3.716**	0.206	**2.357**	0.132	**3.084**	0.213	**3.644**	0.158	**4.258**	0.263	**3.916**	0.120	**4.738**	0.115
9	**2.925**	0.088	**2.947**	0.096	**3.083**	0.152	**2.001**	0.158	**2.556**	0.120	**3.390**	0.223	**4.397**	0.262	**3.317**	0.180	**4.246**	0.055
10	**3.084**	0.121	**2.950**	0.155	**4.162**	0.108	**2.058**	0.113	**2.662**	0.142	**3.274**	0.219	**4.381**	0.196	**4.009**	0.192	**3.639**	0.141
11	**3.281**	0.192	**3.637**	0.087	**3.179**	0.107	**2.054**	0.167	**3.253**	0.094	**3.235**	0.212	**4.198**	0.106	**4.204**	0.171	**4.248**	0.167
12	**3.280**	0.117	**2.826**	0.091	**2.731**	0.173	**2.207**	0.154	**3.087**	0.182	**3.010**	0.195	**4.222**	0.277	**3.814**	0.103	**3.117**	0.108
13	**2.943**	0.123	**2.449**	0.125	**2.998**	0.163	**2.392**	0.111	**2.709**	0.140	**3.018**	0.213	**4.322**	0.103	**4.451**	0.241	**2.810**	0.132
14	**2.781**	0.137	**2.839**	0.189	**2.489**	0.180	**2.114**	0.099	**2.546**	0.121	**2.943**	0.150	**4.404**	0.217	**3.832**	0.127	**3.203**	0.055
15	**2.516**	0.463	**2.296**	0.062	**2.686**	0.068	**2.033**	0.139	**2.436**	0.167	**2.938**	0.165	**4.401**	0.093	**4.221**	0.028	**2.801**	0.145
LoD	0.186		0.155		0.083		0.073		0.064		0.120		0.077		0.077		0.077	
LoQ	0.532		0.444		0.192		0.165		0.153		0.299		0.194		0.194		0.194	
* insufficient sample volume for ICP measurement																		

Table A3. 17: Antimony concentrations across the SWI of the sediment cores of sampling site 1 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.833**	0.044	**0.843**	0.034	0.941	0.140	**0.261**	0.011	**0.417**	0.023	**0.459**	0.036	**0.918**	0.025	**0.542**	0.029	**0.539**	0.021
-3	**0.599**	0.026	**0.675**	0.061	0.662	0.050	**0.257**	0.025	**0.391**	0.037	**0.505**	0.012	**0.919**	0.080	**0.587**	0.024	**0.568**	0.010
-2	**0.442**	0.044	**0.599**	0.031	0.545	0.037	**0.337**	0.029	**0.241**	0.016	**0.428**	0.042	**0.789**	0.025	**0.504**	0.024	**0.579**	0.048
-1	**0.349**	0.025	**0.469**	0.028	0.208	<LoD	**0.285**	0.023	**0.351**	0.029	**0.385**	0.017	**0.718**	0.010	**0.443**	0.039	**0.631**	0.030
0	**0.432**	0.024	**0.260**	0.006	0.208	<LoD	**0.259**	0.013	**0.368**	0.026	**0.372**	0.015	**0.448**	0.044	**0.441**	0.044	**0.548**	0.038
1	0.215	0.021	**0.265**	0.016	0.208	<LoD	**0.162**	0.012	**0.244**	0.022	**0.287**	0.029	**no sample***		**0.308**	0.022	**0.397**	0.041
2	0.216	0.015	**0.234**	0.016	0.208	<LoD	**0.138**	0.009	**0.179**	0.024	**0.120**	0.007	**0.351**	0.014	**0.310**	0.029	0.188	0.011
3	0.162	0.024	**0.230**	0.019	0.208	<LoD	0.114	0.010	**0.205**	0.021	**0.113**	0.006	**0.313**	0.029	0.225	0.014	**0.261**	0.023
4	0.143	0.015	**0.226**	0.019	0.208	<LoD	0.127	0.005	**0.131**	0.011	**0.138**	0.019	**0.312**	0.015	**0.250**	0.016	0.199	0.017
5	0.133	0.008	**0.205**	0.019	0.208	<LoD	0.122	0.021	**0.121**	0.009	**0.143**	0.013	**0.362**	0.029	0.221	0.020	0.190	0.008
6	0.129	0.009	**0.210**	0.011	0.208	<LoD	0.120	0.034	**0.163**	0.024	**0.124**	0.012	**0.308**	0.031	0.203	0.019	0.187	0.013
7	0.128	0.008	**0.193**	0.014	0.208	<LoD	0.122	0.015	**0.140**	0.024	**0.124**	0.014	**0.293**	0.022	0.191	0.023	**0.251**	0.023
8	0.108	0.012	**0.189**	0.017	0.208	<LoD	**0.145**	0.018	**0.159**	0.023	**0.143**	0.031	**0.284**	0.026	**0.253**	0.023	**0.283**	0.024
9	0.147	0.018	**0.182**	0.016	0.208	<LoD	0.123	0.022	**0.122**	0.016	**0.120**	0.007	**0.291**	0.025	0.200	0.021	**0.271**	0.047
10	0.146	0.011	**0.158**	0.009	0.208	<LoD	0.131	0.012	**0.121**	0.035	**0.147**	0.018	**0.295**	0.029	**0.232**	0.007	0.216	0.015
11	0.134	0.009	**0.223**	0.020	0.208	<LoD	**0.151**	0.014	**0.174**	0.008	**0.129**	0.018	**0.279**	0.021	**0.235**	0.020	**0.247**	0.024
12	0.122	0.017	**0.227**	0.022	0.208	<LoD	**0.156**	0.022	**0.157**	0.022	**0.131**	0.016	**0.285**	0.025	0.205	0.017	0.180	0.010
13	0.137	0.018	**0.218**	0.024	0.208	<LoD	**0.159**	0.037	**0.152**	0.015	**0.137**	0.022	**0.278**	0.018	**0.245**	0.024	0.155	0.017
14	0.119	0.014	**0.261**	0.018	0.208	<LoD	**0.168**	0.024	**0.143**	0.023	**0.140**	0.007	**0.276**	0.013	0.222	0.019	0.165	0.013
15	0.045	<LoD	**0.198**	0.019	0.208	<LoD	**0.151**	0.025	**0.158**	0.024	**0.150**	0.019	**0.300**	0.023	0.217	0.024	0.160	0.014
LoD	0.091		0.051		0.415		0.061		0.020		0.021		0.085		0.085		0.085	
LoQ	0.262		0.122		0.989		0.137		0.050		0.052		0.229		0.229		0.229	
* insufficient sample volume for ICP measurement																		

Table A3. 18: Cadmium concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.147**	0.004	**0.103**	0.007	**0.150**	0.030	**0.057**	0.004	**0.126**	0.007	**0.104**	0.006	**0.056**	0.005	**0.140**	0.004	**0.099**	0.006
-3	**0.098**	0.009	**0.114**	0.014	**0.125**	0.018	**0.105**	0.008	**0.129**	0.012	**0.186**	0.015	**0.197**	0.007	**0.447**	0.019	**0.385**	0.029
-2	**0.065**	0.004	**0.213**	0.013	**0.159**	0.018	**0.153**	0.007	**0.099**	0.006	**0.182**	0.016	**0.277**	0.026	**0.603**	0.038	**0.410**	0.039
-1	0.058	0.006	**0.230**	0.011	**0.170**	0.004	**0.090**	0.006	**0.136**	0.011	**0.182**	0.009	**0.663**	0.018	**0.801**	0.046	**0.418**	0.024
0	**0.068**	0.007	**0.118**	0.006	**0.066**	0.010	**0.055**	0.004	**0.117**	0.010	**0.223**	0.020	**0.507**	0.027	**0.527**	0.014	**0.705**	0.007
1	0.024	0.003	0.016	0.003	**0.009**	0.003	**0.020**	0.002	**0.047**	0.005	**0.486**	0.042	**no sample***		**0.524**	0.027	**1.332**	0.059
2	0.010	<LoD	0.023	0.004	**0.012**	0.005	**0.023**	0.001	**0.014**	0.001	**0.099**	0.002	**0.354**	0.026	**0.387**	0.024	**0.608**	0.022
3	0.010	<LoD	**0.050**	0.005	**0.013**	0.007	**0.028**	0.001	**0.017**	0.004	**0.043**	0.003	**0.169**	0.017	**0.428**	0.015	**0.268**	0.017
4	0.010	<LoD	0.033	0.006	0.005	0.004	**0.022**	0.002	**0.012**	0.005	**0.031**	0.005	**0.101**	0.006	**0.237**	0.008	**0.115**	0.009
5	0.010	<LoD	0.025	0.003	0.007	0.004	**0.021**	0.001	**0.016**	0.004	**0.034**	0.003	**0.082**	0.008	**0.076**	0.007	**0.074**	0.005
6	0.010	<LoD	0.036	0.004	**0.019**	0.008	**0.019**	0.001	0.008	0.005	0.014	0.005	**0.060**	0.006	**0.252**	0.013	**0.047**	0.004
7	0.010	<LoD	**0.041**	0.007	**0.156**	0.018	**0.021**	0.002	0.009	0.002	0.015	0.004	**0.049**	0.003	**0.064**	0.003	**0.094**	0.008
8	0.010	<LoD	0.025	0.004	**0.012**	0.005	**0.018**	0.001	**0.011**	0.003	0.017	0.001	**0.046**	0.003	**0.059**	0.006	**0.096**	0.008
9	0.010	<LoD	0.027	0.005	**0.011**	0.008	**0.019**	0.002	**0.012**	0.006	**0.025**	0.003	**0.043**	0.003	**0.059**	0.003	**0.080**	0.008
10	0.010	<LoD	0.031	0.006	**0.246**	0.005	**0.022**	0.001	**0.016**	0.004	**0.024**	0.003	**0.046**	0.003	**0.063**	0.006	**0.070**	0.005
11	0.010	<LoD	**0.053**	0.006	**0.014**	0.004	**0.034**	0.004	**0.030**	0.009	**0.022**	0.002	**0.048**	0.006	**0.070**	0.007	**0.094**	0.006
12	0.010	<LoD	0.020	0.005	**0.013**	0.007	**0.032**	0.006	**0.029**	0.007	**0.023**	0.001	**0.056**	0.002	**0.073**	0.006	**0.074**	0.006
13	0.010	<LoD	**0.050**	0.005	**0.015**	0.005	**0.044**	0.004	**0.033**	0.005	**0.040**	0.004	**0.062**	0.006	**0.077**	0.007	**0.058**	0.006
14	0.010	<LoD	**0.038**	0.013	**0.019**	0.003	**0.051**	0.002	**0.035**	0.008	**0.040**	0.003	**0.030**	0.006	**0.068**	0.006	**0.079**	0.006
15	**0.112**	0.031	0.036	0.003	**0.025**	0.005	**0.038**	0.004	**0.033**	0.006	**0.051**	0.008	**0.038**	0.003	**0.065**	0.005	**0.063**	0.005
LoD	0.021		0.014		0.003		0.004		0.004		0.006		0.004		0.004		0.004	
LoQ	0.059		0.037		0.009		0.011		0.010		0.017		0.010		0.010		0.010	
* insufficient sample volume for ICP measurement																		

Table A3. 19: Chromium concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.217**	0.033	**0.304**	0.000	**0.224**	0.046	0.303	0.034	**1.046**	0.092	**0.363**	0.034	0.413	0.021	**0.892**	0.067	0.453	0.054
-3	0.138	0.013	**0.303**	0.029	**0.174**	0.045	**0.602**	0.057	0.164	0.020	**0.342**	0.026	0.443	0.044	0.201	<LoD	0.445	0.035
-2	0.083	0.009	**0.239**	0.016	**0.155**	0.024	**0.709**	0.054	0.073	<LoD	**0.345**	0.023	0.201	<LoD	0.201	<LoD	0.201	<LoD
-1	0.072	0.017	**0.306**	0.031	**0.180**	0.013	**0.772**	0.043	0.175	0.018	**0.342**	0.025	0.441	0.016	0.201	<LoD	0.439	0.052
0	0.000	0.000	**0.405**	0.045	0.141	0.022	**0.714**	0.043	0.281	0.028	**0.387**	0.049	0.201	<LoD	0.201	<LoD	0.201	<LoD
1	0.131	0.033	**0.624**	0.036	**0.411**	0.039	**0.927**	0.068	**0.491**	0.018	**0.538**	0.048	**no sample***		0.201	<LoD	0.201	<LoD
2	0.087	0.019	**0.820**	0.030	**0.470**	0.053	**0.957**	0.060	**0.596**	0.053	**0.580**	0.053	0.539	0.077	0.201	<LoD	0.490	0.024
3	0.104	0.030	**0.937**	0.069	**0.438**	0.033	**0.971**	0.008	**0.738**	0.055	**0.712**	0.024	0.623	0.044	0.451	0.042	**0.998**	0.086
4	**0.172**	0.025	**1.260**	0.094	**0.463**	0.044	**0.891**	0.065	**0.663**	0.056	**0.933**	0.073	0.778	0.064	0.681	0.019	**1.383**	0.057
5	0.112	0.005	**1.049**	0.099	**0.707**	0.042	**0.811**	0.057	**0.763**	0.073	**1.232**	0.081	**1.171**	0.008	**0.905**	0.030	**1.555**	0.060
6	0.130	0.019	**1.415**	0.102	**0.911**	0.082	**0.801**	0.063	**0.647**	0.043	**0.873**	0.088	**1.129**	0.074	**1.374**	0.057	**1.094**	0.052
7	**0.194**	0.014	**1.394**	0.102	0.000	0.000	**0.913**	0.093	**0.608**	0.036	**0.962**	0.091	**1.045**	0.044	**1.395**	0.071	**2.071**	0.087
8	**0.237**	0.013	**1.036**	0.046	**0.762**	0.080	**0.941**	0.080	**0.840**	0.064	**1.033**	0.022	**1.028**	0.059	**1.570**	0.066	**2.731**	0.168
9	**0.325**	0.027	**1.111**	0.070	**0.767**	0.016	**0.990**	0.063	**0.871**	0.052	**1.192**	0.116	**1.182**	0.073	**1.690**	0.111	**2.858**	0.158
10	**0.436**	0.039	**1.363**	0.113	**1.088**	0.080	**1.244**	0.121	**1.009**	0.046	**1.256**	0.089	**2.232**	0.049	**1.821**	0.123	**2.338**	0.094
11	**0.427**	0.025	**2.153**	0.145	**0.819**	0.017	**1.356**	0.142	**1.501**	0.074	**1.440**	0.089	**1.317**	0.075	**2.171**	0.137	**2.959**	0.061
12	**0.363**	0.036	**1.275**	0.068	**0.996**	0.109	**1.608**	0.122	**1.526**	0.117	**1.553**	0.111	**1.500**	0.075	**2.003**	0.076	**2.266**	0.060
13	**0.530**	0.046	**1.264**	0.085	**1.068**	0.088	**2.092**	0.167	**1.608**	0.126	**1.665**	0.058	**1.531**	0.051	**2.484**	0.171	**2.168**	0.099
14	**0.447**	0.034	**1.613**	0.043	**1.097**	0.062	**1.859**	0.140	**1.798**	0.130	**1.963**	0.138	**0.912**	0.058	**2.476**	0.103	**2.604**	0.086
15	**0.642**	0.059	**1.559**	0.035	**1.322**	0.074	**1.764**	0.078	**1.594**	0.053	**2.143**	0.172	**4.371**	0.084	**2.446**	0.067	**2.510**	0.211
LoD	0.050		0.073		0.072		0.136		0.147		0.076		0.402		0.402		0.402	
LoQ	0.139		0.203		0.146		0.351		0.408		0.206		0.822		0.822		0.822	
* insufficient sample volume for ICP measurement																		

Table A3. 20: Cobalt concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.600**	0.067	**0.427**	0.038	**0.419**	0.013	**0.177**	0.015	**0.345**	0.038	**0.199**	0.021	**0.411**	0.024	**0.320**	0.024	**0.341**	0.045
-3	**0.430**	0.014	**0.430**	0.023	**0.355**	0.033	**0.191**	0.023	**0.272**	0.026	**0.210**	0.017	**0.348**	0.033	**0.343**	0.031	**0.372**	0.042
-2	**0.276**	0.022	**0.617**	0.046	**0.427**	0.036	**0.253**	0.020	**0.210**	0.014	**0.172**	0.007	**0.331**	0.029	**0.394**	0.037	**0.382**	0.032
-1	**0.278**	0.018	**0.752**	0.064	**0.626**	0.044	**0.430**	0.039	**0.309**	0.027	**0.174**	0.018	**0.748**	0.044	**0.682**	0.039	**0.394**	0.020
0	**0.502**	0.017	**0.766**	0.071	**0.401**	0.044	**0.823**	0.046	**0.891**	0.061	**0.271**	0.022	**4.300**	0.199	**1.191**	0.055	**0.452**	0.029
1	**0.271**	0.019	**0.443**	0.031	**0.407**	0.022	**0.557**	0.053	**1.311**	0.074	**1.950**	0.173	**no sample***		**4.563**	0.224	**2.886**	0.034
2	**0.254**	0.020	**0.411**	0.030	**0.320**	0.024	**0.283**	0.047	**0.772**	0.047	**0.968**	0.058	**1.661**	0.098	**5.202**	0.208	**2.550**	0.063
3	**0.203**	0.018	**0.390**	0.037	**0.281**	0.028	**0.208**	0.036	**0.559**	0.044	**0.443**	0.023	**0.935**	0.038	**3.666**	0.092	**1.656**	0.043
4	**0.200**	0.013	**0.551**	0.014	**0.285**	0.022	**0.214**	0.012	**0.442**	0.044	**0.329**	0.025	**0.738**	0.026	**2.209**	0.067	**0.979**	0.046
5	**0.188**	0.006	**0.452**	0.026	**0.354**	0.033	**0.156**	0.017	**0.459**	0.032	**0.381**	0.036	**0.871**	0.038	**1.076**	0.041	**2.031**	0.039
6	**0.204**	0.022	**0.528**	0.050	**0.395**	0.038	**0.184**	0.007	**0.612**	0.033	**0.518**	0.025	**0.798**	0.042	**0.994**	0.045	**0.925**	0.059
7	**0.254**	0.017	**0.550**	0.025	**0.601**	0.023	**0.222**	0.018	**0.707**	0.050	**0.536**	0.044	**0.716**	0.066	**0.928**	0.087	**1.087**	0.081
8	**0.287**	0.022	**0.537**	0.015	**0.546**	0.027	**0.329**	0.031	**0.742**	0.053	**0.516**	0.046	**0.731**	0.063	**1.040**	0.051	**1.350**	0.083
9	**0.352**	0.022	**0.543**	0.038	**0.532**	0.046	**0.335**	0.031	**0.670**	0.059	**0.594**	0.051	**0.784**	0.048	**0.877**	0.035	**1.182**	0.061
10	**0.364**	0.021	**0.613**	0.031	**0.808**	0.049	**0.426**	0.011	**0.759**	0.049	**0.710**	0.056	**0.852**	0.043	**1.105**	0.059	**1.059**	0.092
11	**0.402**	0.023	**0.855**	0.060	**0.643**	0.049	**0.466**	0.035	**0.894**	0.061	**0.691**	0.059	**0.805**	0.043	**1.154**	0.052	**1.369**	0.054
12	**0.449**	0.019	**0.892**	0.055	**0.712**	0.068	**0.531**	0.055	**0.920**	0.043	**0.778**	0.073	**0.800**	0.061	**1.126**	0.094	**1.140**	0.059
13	**0.510**	0.028	**0.733**	0.051	**0.827**	0.054	**0.680**	0.045	**0.897**	0.072	**0.746**	0.073	**0.791**	0.044	**1.374**	0.044	**1.000**	0.086
14	**0.533**	0.050	**0.921**	0.036	**0.787**	0.058	**0.766**	0.048	**0.917**	0.074	**0.732**	0.046	**0.843**	0.083	**1.281**	0.032	**1.201**	0.113
15	**0.570**	0.155	**0.839**	0.084	**0.818**	0.051	**0.758**	0.044	**0.895**	0.044	**0.804**	0.104	**0.846**	0.047	**1.293**	0.066	**1.037**	0.062
LoD	0.021		0.030		0.018		0.014		0.011		0.009		0.007		0.007		0.007	
LoQ	0.060		0.084		0.047		0.038		0.029		0.020		0.019		0.019		0.019	
* insufficient sample volume for ICP measurement																		

Table A3. 21: Copper concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**64.45**	1.72	**8.72**	1.20	**20.88**	0.79	**1.47**	0.02	**4.30**	0.19	**2.96**	0.10	**6.00**	0.18	**7.29**	0.16	**6.21**	0.37
-3	**21.64**	0.64	**11.64**	0.80	**17.30**	0.94	**1.54**	0.10	**3.62**	0.16	**3.41**	0.24	**6.63**	0.38	**7.69**	0.36	**7.24**	0.61
-2	**11.77**	0.60	**4.38**	4.24	**15.77**	0.49	**1.51**	0.07	**2.70**	0.06	**3.37**	0.07	**6.53**	0.17	**7.22**	0.33	**7.49**	0.45
-1	**10.51**	0.27	**6.32**	0.13	**15.40**	0.46	**1.04**	0.06	**4.05**	0.28	**3.41**	0.20	**3.74**	0.18	**6.45**	0.34	**6.66**	0.30
0	**15.14**	0.63	**3.66**	0.12	**10.66**	0.53	**0.56**	0.05	**2.75**	0.09	**1.91**	0.14	**0.83**	0.04	**4.59**	0.20	**4.91**	0.35
1	**2.27**	0.08	0.59	0.06	0.20	<LoD	0.25	0.08	**0.96**	0.04	**0.59**	0.03	**no sample***		**1.96**	0.09	**0.75**	0.05
2	**2.37**	0.08	0.51	0.04	0.20	<LoD	**0.28**	0.04	**0.57**	0.05	**0.16**	0.02	**1.17**	0.08	**1.82**	0.12	0.27	<LoD
3	**1.16**	0.03	**4.01**	0.09	0.20	<LoD	**0.46**	0.04	**0.56**	0.02	**0.19**	0.03	0.63	0.05	**0.79**	0.05	0.27	<LoD
4	**3.20**	0.19	0.38	0.05	0.20	<LoD	0.20	0.07	**0.52**	0.04	**0.24**	0.04	**0.78**	0.04	**1.02**	0.03	0.55	0.03
5	**1.49**	0.06	0.35	0.03	0.20	<LoD	0.14	0.06	**0.42**	0.04	**0.26**	0.00	**0.84**	0.06	**1.21**	0.07	0.57	0.04
6	**1.81**	0.04	0.13	<LoD	0.20	<LoD	0.14	0.06	**0.41**	0.03	**0.26**	0.04	0.63	0.02	**0.76**	0.04	0.56	0.04
7	**1.48**	0.05	0.33	0.02	**45.87**	3.37	0.23	0.04	**0.49**	0.03	0.15	0.06	0.61	0.04	0.71	0.04	**1.55**	0.09
8	**1.89**	0.06	0.13	<LoD	0.20	<LoD	0.19	0.07	**0.43**	0.04	**0.22**	0.02	**1.03**	0.03	**1.35**	0.08	**1.39**	0.08
9	**2.34**	0.03	0.58	0.02	0.20	<LoD	0.20	0.00	**0.46**	0.04	**0.24**	0.01	**0.73**	0.03	**0.87**	0.03	**1.18**	0.09
10	**2.54**	0.06	0.58	0.03	0.20	<LoD	**0.28**	0.01	**0.44**	0.03	**0.27**	0.02	**0.77**	0.06	0.64	0.03	**1.05**	0.04
11	**2.03**	0.07	0.30	0.02	0.20	<LoD	**0.35**	0.04	**0.54**	0.05	**0.25**	0.04	**0.84**	0.06	0.61	0.04	**0.89**	0.07
12	**2.30**	0.22	0.34	0.04	0.20	<LoD	**0.38**	0.02	**0.44**	0.03	**0.31**	0.04	**2.78**	0.13	**0.87**	0.04	**0.80**	0.05
13	**2.65**	0.09	0.30	0.08	0.20	<LoD	**0.33**	0.03	**0.44**	0.02	**0.19**	0.02	**8.59**	0.50	**0.79**	0.08	0.68	0.05
14	**3.81**	0.12	0.13	<LoD	0.20	<LoD	**1.17**	0.11	**0.45**	0.04	**0.30**	0.03	**0.72**	0.03	**0.77**	0.06	**0.76**	0.05
15	**7.66**	1.40	0.13	<LoD	0.20	<LoD	**0.56**	0.05	**0.42**	0.03	**0.34**	0.04	**2.03**	0.15	**0.77**	0.05	**0.77**	0.06
LoD	0.32		0.27		0.40		0.13		0.13		0.10		0.54		0.54		0.54	
LoQ	0.73		0.61		0.84		0.28		0.33		0.15		0.71		0.71		0.71	
* insufficient sample volume for ICP measurement																		

Table A3. 22: Lead concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.103**	0.010	0.045	0.031	**0.188**	0.016	**0.119**	0.017	**0.171**	0.012	**0.059**	0.007	**0.074**	0.006	**0.068**	0.008	0.009	<LoD
-3	**0.062**	0.006	0.069	0.030	**0.351**	0.023	**0.082**	0.011	**0.088**	0.003	**0.131**	0.015	0.042	0.003	0.041	0.003	0.019	0.002
-2	0.052	0.004	0.015	<LoD	**0.165**	0.009	**0.072**	0.009	**0.101**	0.006	**0.076**	0.009	0.037	0.006	**0.148**	0.010	0.009	<LoD
-1	0.038	0.003	0.078	0.004	**0.193**	0.012	**0.110**	0.026	**0.179**	0.010	**0.080**	0.012	**0.055**	0.004	0.030	0.004	**0.230**	0.010
0	0.034	0.003	0.058	0.005	**0.121**	0.013	**0.084**	0.011	**0.095**	0.006	**0.046**	0.006	0.009	<LoD	0.030	0.005	0.031	0.004
1	0.011	<LoD	0.043	0.003	**0.100**	0.012	**0.058**	0.009	**0.069**	0.006	**0.069**	0.012	**no sample***		0.021	0.002	0.009	<LoD
2	0.029	0.002	0.047	0.004	0.054	0.013	**0.064**	0.004	**0.054**	0.004	**0.063**	0.011	**0.050**	0.009	**0.109**	0.009	0.009	<LoD
3	**0.063**	0.005	0.040	0.002	0.040	0.007	**0.200**	0.014	**0.157**	0.015	**0.047**	0.013	0.019	0.002	0.030	0.002	0.009	<LoD
4	**0.082**	0.008	0.054	0.003	0.079	0.011	**0.101**	0.013	**0.029**	0.002	**0.048**	0.011	0.041	0.005	**0.066**	0.006	0.023	0.003
5	0.011	<LoD	0.051	0.002	0.040	0.009	**0.072**	0.010	**0.087**	0.005	**0.073**	0.010	**0.071**	0.003	**0.221**	0.008	**0.098**	0.007
6	0.011	<LoD	0.031	0.004	**0.116**	0.011	**0.093**	0.009	**0.027**	0.005	**0.044**	0.005	0.027	0.003	**1.009**	0.014	0.009	<LoD
7	0.011	<LoD	0.034	0.002	**0.261**	0.021	**0.112**	0.009	**0.054**	0.002	**0.041**	0.004	0.027	0.006	0.046	0.008	**0.051**	0.005
8	0.027	0.004	**0.115**	0.005	0.032	0.004	**0.137**	0.005	**0.056**	0.005	**0.055**	0.006	**0.082**	0.002	**0.275**	0.019	**0.047**	0.001
9	0.037	0.006	0.046	0.004	0.042	0.006	**0.099**	0.010	**0.073**	0.005	**0.060**	0.012	**0.070**	0.004	**0.053**	0.002	**0.065**	0.004
10	0.031	0.003	0.068	0.003	**0.095**	0.008	**0.199**	0.021	**0.080**	0.009	**0.049**	0.007	0.035	0.002	0.036	0.004	**0.057**	0.006
11	0.023	0.003	0.055	0.004	0.059	0.004	**0.148**	0.009	**0.140**	0.006	**0.054**	0.007	0.041	0.003	**0.074**	0.009	**0.060**	0.004
12	**0.063**	0.002	0.015	<LoD	0.058	0.006	**0.147**	0.006	**0.028**	0.003	**0.066**	0.006	**0.079**	0.006	**0.112**	0.008	**0.060**	0.004
13	0.042	0.008	**0.142**	0.006	0.035	0.005	**0.130**	0.008	**0.039**	0.003	**0.065**	0.011	**1.130**	0.028	**0.078**	0.007	0.038	0.002
14	**0.056**	0.005	0.036	0.003	0.061	0.005	**0.577**	0.030	**0.062**	0.006	**0.078**	0.004	**0.135**	0.016	**0.083**	0.008	**0.047**	0.004
15	**0.322**	0.052	0.040	0.003	0.049	0.004	**0.123**	0.011	**0.061**	0.006	**0.067**	0.008	**0.325**	0.023	**0.073**	0.007	**0.069**	0.007
LoD	0.022		0.030		0.029		0.005		0.006		0.012		0.018		0.018		0.018	
LoQ	0.056		0.080		0.081		0.012		0.015		0.031		0.046		0.046		0.046	
* insufficient sample volume for ICP measurement																		

Table A3. 23: Molybdenum concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**16.225**	1.006	**14.848**	0.416	**9.840**	0.949	**3.879**	0.306	**6.582**	0.264	**6.276**	0.345	**7.628**	0.247	**7.610**	0.223	**8.662**	0.292
-3	**11.388**	0.460	**13.111**	0.301	**7.680**	0.232	**4.288**	0.268	**5.787**	0.513	**6.466**	0.134	**8.100**	0.265	**8.038**	0.340	**9.071**	0.521
-2	**7.455**	0.578	**12.999**	0.211	**7.658**	0.474	**4.661**	0.371	**4.025**	0.229	**5.817**	0.251	**7.582**	0.413	**7.300**	0.355	**9.063**	0.567
-1	**6.828**	0.497	**10.944**	0.085	**6.151**	0.422	**4.476**	0.345	**5.957**	0.220	**5.838**	0.139	**6.345**	0.210	**7.872**	0.252	**9.552**	0.366
0	**10.501**	0.424	**8.903**	0.375	**3.629**	0.108	**4.340**	0.254	**5.939**	0.350	**4.394**	0.121	**3.854**	0.076	**7.893**	0.130	**7.187**	0.185
1	**7.287**	0.283	**8.224**	0.369	**3.807**	0.224	**3.415**	0.061	**4.510**	0.095	**3.668**	0.165	**no sample***		**5.900**	0.237	**5.134**	0.084
2	**7.482**	0.485	**5.930**	0.316	**3.073**	0.127	**2.480**	0.142	**2.318**	0.135	**2.201**	0.128	**2.130**	0.118	**5.581**	0.372	**3.468**	0.108
3	**6.279**	0.483	**3.702**	0.161	**2.455**	0.161	**1.915**	0.113	**1.215**	0.060	**1.730**	0.060	**0.968**	0.077	**3.714**	0.171	**2.248**	0.086
4	**5.622**	0.162	**3.384**	0.190	**1.843**	0.124	**1.855**	0.167	**0.448**	0.015	**1.402**	0.050	**0.452**	0.016	**2.212**	0.057	**0.604**	0.015
5	**4.570**	0.318	**2.598**	0.070	**1.095**	0.064	**2.307**	0.139	**0.236**	0.019	**0.548**	0.018	**0.361**	0.031	**0.758**	0.025	**2.195**	0.061
6	**3.315**	0.204	**2.703**	0.106	**0.970**	0.080	**2.678**	0.204	**0.253**	0.017	**0.330**	0.022	0.239	0.015	**0.428**	0.016	**1.107**	0.044
7	**2.652**	0.104	**2.347**	0.171	**7.422**	0.566	**1.911**	0.130	0.175	0.033	0.232	0.020	0.159	0.005	**0.287**	0.012	**0.910**	0.057
8	**2.097**	0.063	0.326	0.020	**0.994**	0.050	**0.955**	0.092	0.154	0.022	0.205	0.029	0.132	0.011	0.250	0.007	**0.493**	0.039
9	**2.188**	0.083	0.147	<LoD	**0.530**	0.029	**0.681**	0.064	0.141	0.009	0.169	0.028	0.120	0.012	0.178	0.023	**0.414**	0.021
10	**5.382**	0.257	0.147	<LoD	**0.979**	0.083	**0.504**	0.043	0.119	0.013	0.163	0.020	0.127	0.013	0.187	0.016	**0.298**	0.020
11	**2.129**	0.127	0.147	<LoD	**0.463**	0.042	**0.328**	0.023	0.160	0.008	0.167	0.026	0.116	0.007	0.184	0.011	**0.321**	0.028
12	**2.109**	0.081	0.147	<LoD	**0.315**	0.018	0.225	0.018	0.143	0.018	0.156	0.017	0.138	0.025	0.150	0.008	**0.301**	0.027
13	**1.973**	0.086	0.147	<LoD	**0.315**	0.022	0.207	0.013	0.136	0.010	0.147	0.019	0.144	0.012	0.190	0.018	0.259	0.030
14	**2.303**	0.155	0.147	<LoD	**0.288**	0.028	0.222	0.014	0.160	0.025	0.150	0.015	0.140	0.023	0.149	0.019	**0.306**	0.022
15	**2.508**	0.528	0.147	<LoD	**0.316**	0.015	0.160	0.021	**0.295**	0.028	0.161	0.022	0.217	0.025	0.145	0.008	**0.264**	0.018
LoD	0.162		0.294		0.079		0.098		0.081		0.105		0.096		0.096		0.096	
LoQ	0.468		0.829		0.213		0.283		0.231		0.295		0.261		0.261		0.261	
* insufficient sample volume for ICP measurement																		

Table A3. 24: Nickel concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**2.33**	0.15	**5.81**	0.75	**13.95**	0.67	**0.99**	0.09	**3.58**	0.20	**7.53**	0.14	**53.23**	3.38	**6.88**	0.65	**6.59**	0.37
-3	**1.34**	0.12	**6.48**	0.49	**9.53**	0.43	**1.66**	0.13	**2.34**	0.22	**9.45**	0.70	**24.18**	0.61	**6.35**	0.26	**11.26**	0.75
-2	**0.79**	0.10	**3.00**	2.82	**7.71**	0.32	**1.35**	0.12	**1.71**	0.13	**9.77**	0.22	**13.64**	0.40	**7.29**	0.41	**14.53**	0.76
-1	**0.74**	0.04	**6.55**	0.11	**4.66**	0.15	**1.57**	0.06	**3.37**	0.18	**9.77**	0.28	**8.72**	0.79	**7.62**	0.49	**19.05**	1.08
0	**4.18**	0.29	**2.59**	0.17	**2.43**	0.03	**1.48**	0.13	**2.78**	0.18	**6.48**	0.24	**8.74**	0.37	**6.79**	0.34	**14.25**	1.26
1	**0.83**	0.08	**2.58**	0.08	**1.51**	0.10	**1.07**	0.08	**2.71**	0.27	**7.96**	0.29	**no sample***		**6.72**	0.22	**18.52**	0.79
2	**1.06**	0.07	1.36	0.10	**1.44**	0.12	**1.00**	0.03	**1.84**	0.11	**4.40**	0.40	**4.59**	0.25	**10.16**	0.30	**11.44**	0.43
3	**0.73**	0.12	1.17	0.04	**1.08**	0.08	**0.87**	0.08	**1.46**	0.10	**2.59**	0.16	**3.00**	0.17	**7.70**	0.53	**8.88**	0.43
4	**0.86**	0.04	0.94	0.06	**1.07**	0.10	**0.76**	0.06	**0.76**	0.03	**1.75**	0.13	**3.57**	0.67	**10.42**	0.31	**4.39**	0.26
5	**0.34**	0.02	0.99	0.08	**0.92**	0.07	**0.77**	0.05	**0.81**	0.07	**4.01**	0.22	**2.18**	0.13	**5.47**	0.37	0.00	0.00
6	**0.36**	0.02	0.79	0.05	**0.97**	0.09	**0.69**	0.05	**1.73**	0.13	**1.51**	0.12	**1.76**	0.21	**2.76**	0.25	**5.09**	0.42
7	**0.32**	0.02	0.77	0.02	**5.91**	0.32	**0.90**	0.07	**2.10**	0.16	**1.38**	0.10	1.38	0.10	**1.99**	0.19	**3.34**	0.19
8	**0.75**	0.05	0.72	0.06	**1.20**	0.12	**1.00**	0.09	**0.78**	0.06	**0.82**	0.02	1.11	0.07	**2.07**	0.06	**2.72**	0.24
9	**0.88**	0.05	0.81	0.08	**0.99**	0.06	**0.87**	0.08	**0.84**	0.07	**0.89**	0.02	0.94	0.16	**1.82**	0.13	**2.13**	0.16
10	**0.44**	0.02	0.88	0.06	**1.52**	0.07	**1.97**	0.07	**0.77**	0.06	**0.90**	0.07	**1.72**	0.53	**1.91**	0.18	**1.67**	0.17
11	**0.33**	0.04	1.06	0.07	**0.85**	0.04	**1.25**	0.10	**0.78**	0.06	**0.83**	0.08	1.15	0.11	**1.66**	0.12	**1.87**	0.14
12	**0.46**	0.02	0.76	0.02	**0.87**	0.09	**1.17**	0.06	**0.77**	0.11	**0.99**	0.09	1.22	0.14	**1.76**	0.09	1.40	0.10
13	**0.74**	0.07	0.92	0.13	**0.76**	0.05	**1.59**	0.12	**0.79**	0.08	**1.00**	0.10	1.29	0.11	**1.65**	0.10	1.19	0.12
14	**0.48**	0.06	1.04	0.05	**1.00**	0.07	**1.43**	0.09	**0.81**	0.06	**3.01**	0.19	0.94	0.14	**1.57**	0.13	1.44	0.04
15	**2.91**	0.43	0.85	0.06	**0.85**	0.04	**1.06**	0.04	**0.86**	0.06	**1.53**	0.14	**2.41**	0.18	**6.50**	0.62	1.26	0.14
LoD	0.06		0.70		0.07		0.09		0.10		0.12		0.54		0.54		0.54	
LoQ	0.15		1.70		0.16		0.25		0.26		0.28		1.45		1.45		1.45	
* insufficient sample volume for ICP measurement																		

Table A3. 25: Selenium concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	0.605	0.052	**1.028**	0.343	0.153	<LoD	0.561	0.187	0.415	<LoD	**0.905**	0.483	0.348	<LoD	0.348	<LoD	0.348	<LoD
-3	0.236	<LoD	**1.319**	0.285	0.153	<LoD	0.509	0.130	0.415	<LoD	**0.949**	0.145	0.348	<LoD	0.348	<LoD	0.785	0.337
-2	0.236	<LoD	**1.644**	0.160	0.153	<LoD	0.636	0.130	0.415	<LoD	**0.698**	0.273	0.348	<LoD	0.348	<LoD	0.910	0.463
-1	0.236	<LoD	**1.500**	0.133	0.153	<LoD	0.658	0.053	0.415	<LoD	**0.901**	0.278	0.348	<LoD	0.348	<LoD	0.348	<LoD
0	0.236	<LoD	**1.466**	0.234	0.331	0.241	0.556	0.150	0.415	<LoD	**0.940**	0.364	0.348	<LoD	0.759	0.210	0.348	<LoD
1	0.236	<LoD	**1.329**	0.242	0.153	<LoD	0.698	0.181	0.415	<LoD	**1.164**	0.374	**no sample***		0.348	<LoD	0.348	<LoD
2	0.236	<LoD	**2.004**	0.213	0.369	0.489	0.602	0.109	0.415	<LoD	**1.268**	0.274	0.348	<LoD	0.348	<LoD	0.348	<LoD
3	0.236	<LoD	**1.915**	0.281	0.542	0.170	0.681	0.109	0.415	<LoD	**1.113**	0.289	0.348	<LoD	0.348	<LoD	0.866	0.105
4	0.236	<LoD	**2.035**	0.249	0.153	<LoD	0.600	0.198	0.415	<LoD	**1.343**	0.470	0.348	<LoD	0.766	0.191	1.014	0.176
5	0.236	<LoD	**1.826**	0.240	0.153	<LoD	0.711	0.327	0.415	<LoD	**1.595**	0.207	0.348	<LoD	0.879	0.413	1.031	0.271
6	0.485	0.096	**1.858**	0.566	0.377	0.230	0.680	0.222	0.415	<LoD	**1.377**	0.177	0.348	<LoD	0.348	<LoD	0.941	0.445
7	0.236	<LoD	**2.149**	0.233	0.511	0.238	0.699	0.372	0.415	<LoD	**1.736**	0.517	0.348	<LoD	0.811	0.268	1.276	0.547
8	0.236	<LoD	**2.154**	0.110	0.553	0.351	**0.801**	0.099	0.415	<LoD	**1.396**	0.224	0.348	<LoD	0.809	0.223	1.585	0.403
9	0.656	0.156	**1.670**	0.131	0.361	0.230	0.795	0.252	0.415	<LoD	**1.477**	0.490	0.348	<LoD	0.788	0.111	1.213	0.161
10	0.733	0.163	**2.149**	0.272	**0.855**	0.318	**0.973**	0.298	0.415	<LoD	**1.730**	0.417	0.348	<LoD	0.934	0.182	0.925	0.388
11	0.769	0.140	**2.336**	0.172	0.552	0.138	**1.204**	0.292	0.415	<LoD	**1.669**	0.513	0.348	<LoD	1.295	0.182	1.070	0.244
12	0.873	0.222	**2.114**	0.230	0.410	0.233	**0.900**	0.238	0.415	<LoD	**1.501**	0.084	0.348	<LoD	0.827	0.266	0.943	0.076
13	1.113	0.126	**2.316**	0.213	0.722	0.566	**1.160**	0.230	0.415	<LoD	**1.655**	0.494	0.348	<LoD	0.852	0.163	0.828	0.139
14	1.055	0.186	**2.502**	0.387	**0.925**	0.165	**1.124**	0.324	0.415	<LoD	**1.604**	0.298	0.348	<LoD	0.842	0.303	0.978	0.270
15	**1.628**	0.742	**2.409**	0.349	**0.817**	0.158	**1.181**	0.158	0.415	<LoD	**1.931**	0.377	0.348	<LoD	0.846	0.248	1.052	0.539
LoD	0.472		0.157		0.307		0.330		0.830		0.237		0.697		0.697		0.697	
LoQ	1.290		0.276		0.795		0.800		2.082		0.626		1.847		1.847		1.847	
* insufficient sample volume for ICP measurement																		

Table A3. 26: Silver concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.137**	0.005	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.024	0.003	**0.080**	0.007	**0.079**	0.005
-3	0.019	0.001	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	**0.044**	0.003	**0.057**	0.004	**0.037**	0.003
-2	0.024	0.002	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	**0.056**	0.006	**0.059**	0.003	**0.042**	0.006
-1	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.017	0.003	0.036	0.003	**0.043**	0.005
0	**0.038**	0.002	0.062	<LoD	**0.530**	0.030	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.007	<LoD	0.025	0.002	0.026	0.005
1	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	**no sample***		0.015	0.003	0.007	<LoD
2	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.014	0.002	0.030	0.005	0.007	<LoD
3	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.023	0.003	0.007	<LoD	0.007	<LoD
4	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	**0.049**	0.007	0.023	0.006	0.007	<LoD
5	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.033	0.004	0.007	<LoD	0.021	0.005
6	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.033	0.004	0.021	0.004	0.007	<LoD
7	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.035	0.007	0.035	0.004	**0.079**	0.006
8	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	**0.041**	0.004	0.007	<LoD	**0.134**	0.008
9	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	**0.055**	0.005	0.007	<LoD	**0.155**	0.011
10	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	**0.064**	0.011	0.007	<LoD	**0.129**	0.009
11	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	**0.073**	0.004	0.020	0.004	**0.171**	0.017
12	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	**0.104**	0.010	0.034	0.002	**0.128**	0.011
13	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	**0.099**	0.007	**0.049**	0.005	**0.118**	0.010
14	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.032	0.005	**0.052**	0.005	**0.119**	0.010
15	0.029	0.034	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.037	0.007	**0.043**	0.006	**0.113**	0.004
LoD	0.015		0.124		0.192		0.090		0.105		0.043		0.013		0.013		0.013	
LoQ	0.038		0.168		0.257		0.180		0.132		0.067		0.037		0.037		0.037	
* insufficient sample volume for ICP measurement																		

Table A3. 27: Tin concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	0.225	0.042	0.163	0.066	0.057	<LoD	**0.498**	0.138	0.138	0.113	0.099	0.084	0.045	<LoD	0.177	0.052	0.100	0.100
-3	0.118	0.037	0.061	<LoD	0.057	<LoD	**0.295**	0.104	0.111	0.035	0.039	<LoD	0.045	<LoD	0.045	<LoD	0.114	0.083
-2	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.308**	0.093	0.076	0.048	0.039	<LoD	0.110	0.022	0.110	0.071	0.045	<LoD
-1	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.345**	0.097	0.135	0.059	0.170	0.138	0.100	0.061	0.136	0.049	0.045	<LoD
0	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.426**	0.157	**0.240**	0.078	0.039	<LoD	0.178	0.128	0.090	0.068	0.045	<LoD
1	**0.421**	0.039	0.133	0.057	0.057	<LoD	**0.395**	0.099	**0.404**	0.130	**0.278**	0.226	**no sample***		0.045	<LoD	0.045	<LoD
2	0.055	<LoD	0.228	0.031	0.132	0.062	**0.541**	0.041	**0.337**	0.136	**0.216**	0.144	0.109	0.060	0.045	<LoD	0.130	0.053
3	0.055	<LoD	**1.178**	0.045	0.168	0.069	**0.847**	0.266	**0.493**	0.081	**0.230**	0.154	0.215	0.095	0.099	0.035	**0.344**	0.068
4	0.055	<LoD	**0.718**	0.060	**0.212**	0.198	**0.599**	0.152	**0.428**	0.101	**0.381**	0.209	**0.315**	0.104	**0.296**	0.094	**0.539**	0.077
5	0.055	<LoD	**0.726**	0.061	**0.326**	0.109	**0.457**	0.048	**0.521**	0.083	**0.736**	0.283	**0.572**	0.063	**0.261**	0.045	**0.735**	0.180
6	0.055	<LoD	**0.687**	0.028	**0.346**	0.086	**0.595**	0.212	**0.200**	0.057	**0.387**	0.140	**0.543**	0.047	0.000	0.000	**0.370**	0.103
7	0.219	0.032	**0.853**	0.053	**4.858**	0.734	**0.834**	0.310	**0.240**	0.092	**0.486**	0.103	**0.567**	0.073	**0.748**	0.172	**1.210**	0.168
8	0.128	0.038	**0.409**	0.025	**0.415**	0.123	**0.733**	0.197	**0.404**	0.126	**0.564**	0.211	**0.495**	0.133	**0.832**	0.142	**1.603**	0.263
9	0.241	0.088	**0.577**	0.061	**0.306**	0.138	**0.562**	0.244	**0.443**	0.151	**0.465**	0.106	**0.633**	0.152	**0.976**	0.107	**1.466**	0.182
10	0.231	0.037	**0.723**	0.078	**7.553**	0.500	**0.758**	0.203	**0.561**	0.102	**0.685**	0.142	**0.651**	0.195	**0.927**	0.097	**1.309**	0.127
11	**0.366**	0.029	**1.211**	0.083	**0.509**	0.138	**0.817**	0.097	**1.039**	0.261	**0.687**	0.073	**0.728**	0.088	**1.385**	0.343	**1.493**	0.135
12	0.198	0.042	**0.556**	0.084	**0.436**	0.126	**1.123**	0.167	**1.016**	0.206	**0.632**	0.180	**0.854**	0.119	**1.323**	0.291	**1.227**	0.076
13	0.288	0.009	**0.607**	0.085	**0.653**	0.183	**1.338**	0.246	**1.019**	0.165	**0.858**	0.047	**0.904**	0.063	**1.323**	0.344	**1.124**	0.127
14	0.300	0.107	**0.719**	0.073	**0.655**	0.274	**1.505**	0.281	**1.157**	0.335	**1.456**	0.270	**0.462**	0.078	**1.521**	0.273	**1.315**	0.073
15	**1.950**	0.311	**0.791**	0.106	**0.781**	0.172	**1.051**	0.224	**1.054**	0.264	**1.229**	0.308	**0.679**	0.133	**1.369**	0.333	**1.308**	0.177
LoD	0.110		0.122		0.113		0.101		0.056		0.078		0.090		0.090		0.090	
LoQ	0.309		0.294		0.190		0.220		0.141		0.210		0.254		0.254		0.254	

* insufficient sample volume for ICP measurement

Table A3. 28: Titanium concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	0.225	0.042	0.163	0.066	0.057	<LoD	**0.498**	0.138	0.138	0.113	0.099	0.084	0.045	<LoD	0.177	0.052	0.100	0.100
-3	0.118	0.037	0.061	<LoD	0.057	<LoD	**0.295**	0.104	0.111	0.035	0.039	<LoD	0.045	<LoD	0.045	<LoD	0.114	0.083
-2	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.308**	0.093	0.076	0.048	0.039	<LoD	0.110	0.022	0.110	0.071	0.045	<LoD
-1	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.345**	0.097	0.135	0.059	0.170	0.138	0.100	0.061	0.136	0.049	0.045	<LoD
0	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.426**	0.157	**0.240**	0.078	0.039	<LoD	0.178	0.128	0.090	0.068	0.045	<LoD
1	**0.421**	0.039	0.133	0.057	0.057	<LoD	**0.395**	0.099	**0.404**	0.130	**0.278**	0.226	**no sample***		0.045	<LoD	0.045	<LoD
2	0.055	<LoD	0.228	0.031	0.132	0.062	**0.541**	0.041	**0.337**	0.136	**0.216**	0.144	0.109	0.060	0.045	<LoD	0.130	0.053
3	0.055	<LoD	**1.178**	0.045	0.168	0.069	**0.847**	0.266	**0.493**	0.081	**0.230**	0.154	0.215	0.095	0.099	0.035	**0.344**	0.068
4	0.055	<LoD	**0.718**	0.060	**0.212**	0.198	**0.599**	0.152	**0.428**	0.101	**0.381**	0.209	**0.315**	0.104	**0.296**	0.094	**0.539**	0.077
5	0.055	<LoD	**0.726**	0.061	**0.326**	0.109	**0.457**	0.048	**0.521**	0.083	**0.736**	0.283	**0.572**	0.063	**0.261**	0.045	**0.735**	0.180
6	0.055	<LoD	**0.687**	0.028	**0.346**	0.086	**0.595**	0.212	**0.200**	0.057	**0.387**	0.140	**0.543**	0.047	0.000	0.000	**0.370**	0.103
7	0.219	0.032	**0.853**	0.053	**4.858**	0.734	**0.834**	0.310	**0.240**	0.092	**0.486**	0.103	**0.567**	0.073	**0.748**	0.172	**1.210**	0.168
8	0.128	0.038	**0.409**	0.025	**0.415**	0.123	**0.733**	0.197	**0.404**	0.126	**0.564**	0.211	**0.495**	0.133	**0.832**	0.142	**1.603**	0.263
9	0.241	0.088	**0.577**	0.061	**0.306**	0.138	**0.562**	0.244	**0.443**	0.151	**0.465**	0.106	**0.633**	0.152	**0.976**	0.107	**1.466**	0.182
10	0.231	0.037	**0.723**	0.078	**7.553**	0.500	**0.758**	0.203	**0.561**	0.102	**0.685**	0.142	**0.651**	0.195	**0.927**	0.097	**1.309**	0.127
11	**0.366**	0.029	**1.211**	0.083	**0.509**	0.138	**0.817**	0.097	**1.039**	0.261	**0.687**	0.073	**0.728**	0.088	**1.385**	0.343	**1.493**	0.135
12	0.198	0.042	**0.556**	0.084	**0.436**	0.126	**1.123**	0.167	**1.016**	0.206	**0.632**	0.180	**0.854**	0.119	**1.323**	0.291	**1.227**	0.076
13	0.288	0.009	**0.607**	0.085	**0.653**	0.183	**1.338**	0.246	**1.019**	0.165	**0.858**	0.047	**0.904**	0.063	**1.323**	0.344	**1.124**	0.127
14	0.300	0.107	**0.719**	0.073	**0.655**	0.274	**1.505**	0.281	**1.157**	0.335	**1.456**	0.270	**0.462**	0.078	**1.521**	0.273	**1.315**	0.073
15	**1.950**	0.311	**0.791**	0.106	**0.781**	0.172	**1.051**	0.224	**1.054**	0.264	**1.229**	0.308	**0.679**	0.133	**1.369**	0.333	**1.308**	0.177
LoD	0.110		0.122		0.113		0.101		0.056		0.078		0.090		0.090		0.090	
LoQ	0.309		0.294		0.190		0.220		0.141		0.210		0.254		0.254		0.254	

* insufficient sample volume for ICP measurement

Table A3. 29: Vanadium concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.673**	0.016	0.392	0.007	**0.345**	0.008	**0.400**	0.025	**0.236**	0.011	**0.800**	0.010	0.056	<LoD	**1.415**	0.062	**0.616**	0.043
-3	**0.469**	0.008	0.408	0.009	**0.335**	0.013	**0.508**	0.031	**0.283**	0.026	**1.082**	0.022	**0.436**	0.027	**2.304**	0.117	**0.995**	0.020
-2	**0.320**	0.025	**0.845**	0.023	**0.789**	0.046	**0.801**	0.061	**0.230**	0.015	**1.072**	0.050	**0.996**	0.016	**2.274**	0.058	**1.043**	0.031
-1	**0.294**	0.017	**1.585**	0.045	**1.038**	0.055	**1.122**	0.067	**0.411**	0.019	**1.201**	0.044	**1.895**	0.043	**2.482**	0.079	**1.188**	0.044
0	**0.879**	0.039	**1.535**	0.075	**0.615**	0.029	**1.352**	0.086	**1.196**	0.059	**1.717**	0.083	**0.680**	0.046	**2.696**	0.049	**1.180**	0.053
1	**0.652**	0.018	**3.225**	0.154	**1.434**	0.064	**1.865**	0.045	**1.894**	0.080	**1.965**	0.051	**no sample***		**1.482**	0.072	**0.676**	0.022
2	**0.699**	0.017	**5.171**	0.320	**1.928**	0.124	**1.934**	0.136	**1.814**	0.042	**1.832**	0.081	**0.825**	0.024	**0.513**	0.027	**1.085**	0.023
3	**0.446**	0.040	**5.713**	0.186	**1.898**	0.099	**1.924**	0.112	**2.417**	0.077	**2.589**	0.089	**1.578**	0.049	**0.676**	0.034	**2.898**	0.090
4	**0.365**	0.019	**7.506**	0.398	**1.790**	0.112	**1.755**	0.095	**1.963**	0.041	**3.858**	0.115	**3.435**	0.099	**1.733**	0.038	**4.502**	0.179
5	**0.428**	0.013	**5.725**	0.145	**2.305**	0.104	**1.433**	0.079	**2.321**	0.075	**5.279**	0.133	**5.484**	0.179	**2.346**	0.054	**5.317**	0.097
6	**0.683**	0.025	**6.903**	0.419	**3.045**	0.102	**1.239**	0.116	**2.557**	0.058	**4.715**	0.395	**5.297**	0.183	**4.422**	0.100	**4.827**	0.164
7	**0.986**	0.055	**6.560**	0.511	**3.888**	0.199	**1.706**	0.112	**3.120**	0.109	**5.229**	0.227	**5.175**	0.187	**5.318**	0.142	**7.887**	0.459
8	**1.212**	0.042	**5.060**	0.140	**3.732**	0.118	**2.144**	0.152	**3.602**	0.116	**5.430**	0.205	**5.321**	0.247	**6.558**	0.220	**9.301**	0.143
9	**1.663**	0.065	**5.054**	0.098	**3.304**	0.188	**2.478**	0.181	**3.480**	0.090	**5.679**	0.360	**5.842**	0.232	**5.714**	0.264	**8.650**	0.290
10	**1.877**	0.046	**5.518**	0.201	**4.586**	0.202	**3.000**	0.197	**3.883**	0.087	**5.349**	0.183	**6.190**	0.196	**7.463**	0.273	**7.763**	0.218
11	**2.044**	0.072	**7.656**	0.314	**3.387**	0.112	**3.551**	0.232	**4.975**	0.174	**5.787**	0.340	**6.023**	0.154	**8.529**	0.263	**9.440**	0.191
12	**2.140**	0.097	**6.149**	0.223	**3.676**	0.155	**4.019**	0.216	**4.966**	0.334	**5.928**	0.329	**6.023**	0.262	**7.755**	0.101	**7.440**	0.170
13	**2.356**	0.075	**5.651**	0.143	**3.919**	0.145	**4.673**	0.230	**4.870**	0.175	**6.276**	0.219	**6.131**	0.252	**9.067**	0.266	**6.702**	0.232
14	**2.401**	0.067	**7.049**	0.360	**3.866**	0.058	**5.100**	0.320	**4.780**	0.132	**6.685**	0.294	**5.964**	0.205	**8.303**	0.337	**7.962**	0.090
15	**2.560**	0.433	**6.111**	0.099	**4.250**	0.094	**4.952**	0.246	**4.766**	0.116	**7.370**	0.394	**5.981**	0.198	**8.481**	0.191	**7.127**	0.214
LoD	0.079		0.146		0.065		0.051		0.024		0.035		0.112		0.112		0.112	
LoQ	0.218		0.410		0.176		0.146		0.068		0.098		0.294		0.294		0.294	
* insufficient sample volume for ICP measurement																		

Table A3. 30: Zink concentrations across the SWI of the sediment cores of sampling site 1. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3		Profil 1		Profil 2		Profil 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**30.51**	1.56	**10.01**	1.35	**22.90**	1.29	**5.95**	0.44	**12.35**	0.48	**4.91**	0.43	**5.70**	0.26	**14.38**	1.27	**4.02**	0.30
-3	**16.50**	0.64	**14.07**	0.81	**26.62**	1.80	**9.34**	0.70	**9.39**	0.24	**4.98**	0.20	**4.92**	0.30	**10.45**	0.60	**4.99**	0.31
-2	**14.07**	1.17	**12.38**	11.55	**44.70**	1.60	**21.87**	0.53	**13.76**	0.39	**9.38**	0.33	**5.00**	0.44	**29.46**	0.62	**5.14**	0.68
-1	**16.39**	0.44	**39.53**	0.85	**42.45**	1.09	**24.45**	0.98	**17.90**	0.93	**8.10**	0.54	**8.77**	0.57	**15.37**	0.41	**7.82**	0.89
0	**21.93**	0.83	**45.88**	1.67	**31.38**	1.43	**17.46**	0.82	**30.92**	0.74	**12.33**	0.44	**13.33**	0.93	**25.21**	0.80	**12.38**	0.68
1	**10.34**	0.44	**7.44**	0.21	**11.49**	0.64	**5.92**	0.43	**24.12**	0.71	**82.77**	2.83	**no sample***		**38.36**	1.68	**59.66**	3.35
2	**13.76**	0.82	**17.60**	0.68	**8.90**	0.35	**8.05**	0.48	**7.44**	0.34	**8.63**	0.56	**20.22**	1.36	**29.55**	1.02	**56.11**	2.23
3	**50.96**	1.74	**13.57**	0.29	**5.17**	0.31	**12.93**	0.80	**6.50**	0.30	**5.88**	0.21	**11.97**	0.84	**42.55**	2.35	**65.79**	1.72
4	**18.18**	0.82	**15.13**	0.44	**11.20**	0.44	**13.13**	0.41	**7.69**	0.27	**6.73**	0.15	**10.20**	0.58	**41.75**	0.43	**27.90**	1.15
5	**10.27**	0.21	**12.27**	0.38	**6.56**	0.55	**4.74**	0.43	**5.86**	0.32	**5.16**	0.44	**8.75**	0.42	**27.85**	1.85	**22.20**	1.23
6	**12.10**	0.51	**13.59**	0.25	**7.50**	0.41	**5.72**	0.27	**6.71**	0.40	**4.48**	0.34	**4.73**	0.39	**21.61**	1.46	**6.12**	0.35
7	**13.45**	0.58	**9.24**	0.35	**18.49**	0.70	**11.19**	0.46	**7.39**	0.47	**3.36**	0.20	**4.68**	0.35	**10.62**	0.65	**15.64**	0.68
8	**23.19**	0.68	**11.30**	0.26	**9.07**	0.75	**22.86**	1.15	**14.12**	0.75	**4.62**	0.39	**9.87**	0.77	**20.93**	0.60	**13.15**	0.68
9	**20.71**	0.85	**11.12**	0.35	**8.48**	0.45	**12.61**	0.57	**16.30**	1.43	**3.45**	0.22	**12.21**	1.09	**14.09**	0.72	**10.26**	0.39
10	**17.70**	0.42	**12.59**	0.64	**10.32**	0.60	**12.39**	0.47	**4.24**	0.33	**4.14**	0.38	**5.77**	0.39	**8.55**	0.41	**11.49**	0.55
11	**17.66**	0.78	**15.25**	0.41	**11.44**	0.47	**14.05**	0.33	**6.43**	0.51	**3.74**	0.32	**6.85**	0.30	**13.62**	0.71	**10.01**	0.42
12	**32.18**	2.69	**7.23**	0.41	**8.00**	0.63	**11.31**	0.38	**5.70**	0.31	**5.85**	0.19	0.00	0.00	**17.88**	0.86	**7.74**	0.21
13	**21.94**	0.77	**13.54**	1.75	**7.99**	0.45	**16.57**	0.89	**5.20**	0.50	**6.29**	0.28	**27.98**	1.48	**13.69**	0.60	**9.69**	0.38
14	**18.44**	0.93	**11.28**	0.36	**12.09**	0.68	**15.62**	0.24	**4.29**	0.30	**5.00**	0.35	**14.93**	0.56	**15.93**	1.15	**8.77**	0.49
15	**79.91**	9.98	**13.96**	0.44	**21.89**	1.06	**13.73**	0.97	**5.94**	0.37	**4.73**	0.31	**45.29**	1.91	**13.69**	0.67	**10.00**	0.33
LoD	0.16		0.24		0.21		0.12		0.09		0.09		0.13		0.13		0.13	
LoQ	0.45		0.67		0.56		0.31		0.23		0.24		0.34		0.34		0.34	
* insufficient sample volume for ICP measurement																		

Table A3. 31: Phosphate concentrations across the SWI of the sediment cores of sampling site 1. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
-4	0.30	0.09	missing**	0.04	0.05	0.05	missing**	0.05	0.05
-3	0.25	0.24	2.30	0.14	0.20	0.25	missing**	0.20	0.25
-2	0.30	0.14	2.40	0.04	0.05	0.10	1.377	0.05	0.10
-1	0.30	0.11	2.50	missing**	0.20	0.10	1.377	0.20	0.10
0	0.80	0.91	2.80	0.19	0.80	0.25	0.197	0.80	0.25
1	1.20	1.11	5.25	0.84	2.50	missing**	0.103	2.50	0.15
2	0.35	2.35	5.50	1.60	4.90	0.15	missing*	4.90	missing**
3	0.30	3.20	6.25	1.70	7.85	1.00	0.197	7.85	1.00
4	0.10	10.21	5.85	6.10	6.85	7.25	2.853	6.85	7.25
5	0.20	4.40	8.25	2.40	10.80	2.80	6.553	10.80	2.80
6	0.55	3.15	10.50	4.30	10.10	2.80	7.903	10.10	2.80
7	1.00	4.20	13.70	8.90	7.40	7.95	7.453	7.40	7.95
8	1.75	5.50	10.50	5.80	11.00	6.05	8.304	11.00	6.05
9	4.65	4.25	5.90	7.30	11.95	5.50	10.354	11.95	5.50
10	6.05	3.40	14.90	9.55	10.15	15.10	11.454	10.15	15.10
11	6.70	11.45	7.70	21.05	13.30	8.50	14.004	13.30	8.50
12	1.55	5.36	9.40	12.35	15.95	9.55	15.254	15.95	9.55
13	3.15	3.31	10.45	5.10	13.15	9.25	13.754	13.15	9.25
14	8.95	22.86	12.75	14.10	20.45	14.10	missing**	20.45	14.10
15	missing**	8.91	12.80	8.35	17.60	14.65	missing**	17.60	14.65
*** insufficient sample volume**									
**** handling error**									

Table A3. 32: Sulfate concentrations across the SWI of the sediment cores of sampling site 1. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
-4	240.75	374.85	507.85	430.25	791.65	512.90	missing**	321.25	591.30
-3	236.45	324.55	270.75	164.05	700.85	261.95	missing**	918.70	405.10
-2	279.00	759.45	612.30	771.40	704.40	403.75	635.75	794.00	594.70
-1	280.05	385.75	508.90	missing**	700.55	552.55	755.45	432.65	257.00
0	446.40	362.40	606.55	305.55	724.60	294.25	898.30	965.50	307.15
1	380.45	426.25	574.90	910.30	585.70	390.80	767.60	413.15	498.05
2	153.25	428.65	451.75	396.60	636.05	453.85	721.10	819.30	546.65
3	327.80	396.55	414.85	266.35	671.35	473.35	806.00	730.75	525.90
4	299.15	1132.65	381.60	697.65	577.25	679.75	556.45	647.45	192.30
5	386.55	402.35	468.05	222.90	561.20	172.05	538.75	missing**	207.45
6	245.05	244.60	521.90	168.25	569.70	223.70	513.50	564.10	190.70
7	345.45	327.35	621.45	244.20	532.20	400.35	462.95	350.95	221.45
8	352.35	341.55	465.95	177.00	546.15	307.15	403.50	171.30	416.15
9	620.45	297.35	205.70	212.85	491.15	218.50	392.95	513.35	168.65
10	548.90	224.65	572.10	216.60	444.95	484.60	344.50	193.30	134.85
11	509.35	515.30	303.80	336.80	425.50	257.00	358.55	251.50	161.75
12	196.10	293.25	299.45	173.95	399.70	268.05	346.25	137.50	151.75
13	308.35	201.25	271.80	51.05	362.85	226.95	300.15	222.65	250.55
14	553.45	691.45	297.30	118.40	349.95	279.35	missing**	224.15	97.65
15	missing**	190.65	241.40	65.55	324.55	199.45	missing**	252.25	139.05
*** insufficient sample volume**									
**** handling error**									

Table A3. 33: Ammonium concentrations across the SWI of the sediment cores of sampling site 1. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
4	2.82	0.39	3.27	3.70	2.36	2.93	2.58	1.71	3.37
3	1.68	2.13	2.71	1.11	2.95	3.24	1.71	0.80	2.42
2	3.26	2.26	2.04	4.92	2.46	3.20	1.25	0.44	3.71
1	3.70	3.06	2.34	4.01	2.62	3.37	1.63	2.30	3.63
0	3.17	3.85	4.39	4.86	3.22	3.72	3.67	1.20	2.94
1	4.07	4.03	5.22	5.15	5.13	4.32	missing*	3.84	5.00
2	4.88	4.72	3.55	6.85	7.67	4.82	3.73	5.13	7.22
3	4.24	5.68	4.57	7.73	10.12	5.36	6.78	7.32	9.29
4	4.99	6.57	7.04	13.98	12.01	5.31	9.94	9.64	10.58
5	4.66	7.52	6.56	13.28	13.82	6.33	11.30	missing**	15.02
6	5.01	7.36	8.43	13.04	12.60	6.20	11.25	12.72	15.52
7	5.79	8.02	7.80	13.78	12.00	7.49	12.41	10.40	15.50
8	6.08	8.70	6.75	18.90	15.65	8.79	13.38	11.87	13.75
9	6.68	8.77	8.85	24.24	16.45	8.22	15.50	16.30	16.92
10	7.37	9.86	9.55	11.54	16.25	9.41	16.24	12.25	15.99
11	8.97	14.14	10.03	18.23	19.54	10.53	19.44	14.59	18.78
12	7.11	11.24	11.04	11.20	18.34	10.43	18.15	13.64	19.06
13	8.54	11.44	10.19	9.79	20.98	12.39	19.12	13.23	19.66
14	9.03	12.33	12.39	18.24	18.47	11.66	13.47	14.55	19.33
15	missing**	13.73	14.17	20.20	23.37	11.95	missing**	14.06	24.21
*** insufficient sample volume**									
**** handling error**									

AIII.IX.II.II Concentrations in suction-based pore water samples of sampling site 2

Table A3. 34: Carbon concentrations across the SWI of the sediment cores of sampling site 2 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in mg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**469**	17	**624**	34	**596**	26	**418**	23	**260**	16	**66**	2	**427**	10	**75**	3	**170**	7
-3	**402**	11	**737**	23	**581**	25	**455**	24	**192**	12	**75**	3	**700**	30	**84**	3	**168**	12
-2	**214**	6	**625**	28	**425**	17	**426**	19	**387**	21	**72**	4	**754**	25	**71**	1	**150**	11
-1	**203**	8	**992**	13	**650**	57	**295**	10	**422**	30	**84**	3	**361**	5	**79**	2	**92**	5
0	**253**	5	**954**	19	**587**	43	**386**	12	**491**	19	**100**	7	**382**	13	**63**	3	**79**	4
1	**186**	3	**805**	20	**503**	18	**632**	51	**532**	21	**231**	21	**504**	17	**67**	2	**98**	2
2	**219**	7	**596**	15	**521**	9	**860**	32	**680**	40	**258**	19	**627**	31	**88**	2	**168**	9
3	**146**	10	**759**	25	**447**	15	**843**	53	**596**	26	**136**	7	**489**	16	**175**	3	**169**	7
4	**70**	9	**890**	22	**446**	23	**800**	52	**680**	36	**303**	15	**731**	18	**304**	8	**222**	8
5	**72**	11	**1004**	14	**434**	28	**693**	25	**1039**	53	**379**	11	**680**	22	**247**	8	**202**	13
6	**153**	2	**1014**	38	**521**	16	**721**	13	**1157**	22	**154**	7	**1692**	80	**258**	10	**176**	7
7	**163**	6	**1065**	16	**832**	17	**677**	30	**744**	16	**120**	10	**1644**	57	**346**	26	**176**	5
8	**136**	6	**898**	39	**640**	40	**1542**	71	**646**	26	**124**	8	**no sample***		**244**	8	**159**	8
9	**129**	2	**808**	14	**351**	17	**1710**	61	**584**	16	**126**	5	**2571**	99	**537**	20	**166**	7
10	**141**	4	**1019**	21	**499**	21	**1801**	81	**549**	21	**122**	7	**640**	31	**460**	25	**160**	5
11	**146**	13	**872**	10	**252**	13	**1467**	39	**584**	45	**220**	1	**1418**	51	**509**	18	**167**	5
12	**105**	5	**692**	7	**107**	6	**861**	27	**662**	20	**225**	11	**1286**	46	**542**	17	**153**	5
13	**67**	6	**721**	15	**231**	19	**723**	51	**757**	24	**98**	6	**1494**	31	**515**	14	**159**	7
14	**137**	8	**253**	8	**251**	9	**914**	15	**781**	15	**91**	3	**1435**	75	**320**	9	**177**	5
15	**48**	2	**733**	14	**202**	14	**1345**	50	**467**	45	**137**	8	**1382**	36	**465**	22	**142**	6
LoD	7.64		2.43		5.77		3.60		14.49		9.80		6.15		6.15		6.15	
LoQ	20.07		5.67		14.68		9.80		41.68		20.30		15.09		15.09		15.09	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 35: Phosphorous concentrations across the SWI of the sediment cores of sampling site 2 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**62**	2	**54**	2	**54**	1	**69**	4	**77**	2	**396**	19	**296**	9	**2888**	157	**253**	13
-3	**51**	2	**36**	1	**116**	6	**66**	4	**37**	2	**144**	4	**223**	11	**195**	10	**189**	12
-2	**35**	1	**32**	1	**110**	3	**122**	8	**33**	1	**44**	4	**241**	10	**2673**	72	**86**	8
-1	**33**	1	**148**	3	**127**	3	**182**	11	**94**	5	**65**	5	**162**	3	**156**	10	**141**	8
0	**38**	1	**1547**	33	**1349**	75	**131**	8	**793**	22	**1693**	78	**99**	4	**1182**	63	**94**	4
1	**28**	1	**2822**	66	**1757**	82	**1426**	97	**4178**	130	**10244**	166	**1533**	53	**1033**	30	**855**	25
2	**36**	2	**3810**	152	**364**	10	**3296**	113	**8446**	165	**12568**	745	**4827**	251	**3228**	70	**3740**	169
3	**52**	3	**6119**	88	**1072**	31	**3241**	216	**9540**	452	**12053**	393	**6364**	266	**8430**	464	**5901**	313
4	**122**	30	**8419**	292	**2677**	133	**4462**	268	**14337**	171	**16954**	755	**8947**	442	**12865**	673	**8748**	415
5	**258**	76	**10243**	440	**4265**	111	**6842**	145	**14071**	922	**17625**	807	**6126**	281	**13279**	662	**8615**	637
6	**265**	4	**13381**	99	**5798**	263	**10536**	580	**5077**	133	**9164**	682	**9885**	367	**18787**	1174	**5809**	149
7	**266**	12	**16891**	621	**7902**	216	**15099**	696	**4380**	121	**9382**	522	**10036**	279	**24213**	1464	**5999**	255
8	**1534**	118	**11401**	528	**2375**	103	**12025**	153	**4481**	99	**9089**	262	**no sample***		**6222**	340	**8215**	372
9	**3492**	109	**15990**	964	**5333**	190	**12264**	628	**4533**	163	**9264**	351	**19401**	989	**20246**	858	**7969**	757
10	**4874**	108	**17582**	491	**5425**	87	**11390**	528	**6001**	170	**9382**	553	**13403**	312	**13846**	787	**10974**	282
11	**6259**	388	**17327**	897	**4597**	131	**12916**	652	**6352**	68	**10742**	265	**15491**	154	**19445**	831	**13656**	543
12	**2341**	80	**6655**	134	**4860**	202	**12796**	594	**7009**	227	**12152**	689	**13987**	741	**14186**	638	**7427**	485
13	**2437**	64	**6497**	50	**6896**	204	**15773**	826	**10679**	648	**11984**	317	**15667**	1021	**18368**	721	**7843**	624
14	**2893**	88	**7202**	133	**6991**	206	**18334**	610	**15550**	1054	**18575**	733	**7956**	589	**10537**	387	**12244**	267
15	**3386**	152	**9013**	358	**9935**	537	**17780**	693	**14859**	427	**20654**	1260	**9567**	199	**22627**	700	**14975**	831
LoD	6.56		8.56		2.18		1.20		1.45		1.15		2.24		2.24		2.24	
LoQ	17.18		19.86		4.83		2.14		3.49		2.49		6.10		6.10		6.10	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 36: Sulfur concentrations across the SWI of the sediment cores of sampling site 2 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in mg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**1078**	71	**667**	27	**518**	8	**335**	14	**331**	12	**474**	18	**384**	18	**501**	21	**512**	32
-3	**1084**	50	**579**	19	**455**	24	**344**	13	**284**	11	**512**	19	**408**	28	**532**	18	**511**	31
-2	**702**	38	**524**	18	**385**	17	**350**	17	**420**	19	**456**	13	**521**	30	**465**	18	**499**	40
-1	**678**	38	**562**	18	**412**	15	**341**	14	**419**	18	**540**	21	**408**	17	**434**	23	**449**	28
0	**743**	45	**474**	16	**396**	19	**342**	14	**421**	28	**485**	25	**366**	12	**474**	25	**404**	29
1	**482**	21	**356**	9	**344**	11	**355**	29	**372**	16	**442**	14	**441**	14	**385**	16	**460**	28
2	**494**	24	**307**	10	**309**	5	**318**	12	**371**	12	**425**	27	**409**	20	**317**	9	**461**	26
3	**386**	20	**304**	16	**267**	8	**302**	19	**317**	12	**320**	3	**286**	17	**307**	15	**330**	11
4	**369**	52	**318**	24	**234**	14	**287**	17	**344**	6	**368**	10	**256**	9	**278**	12	**294**	10
5	**412**	68	**285**	12	**220**	5	**267**	8	**241**	13	**316**	17	**227**	11	**200**	10	**240**	15
6	**363**	13	**274**	16	**213**	9	**241**	6	**198**	3	**248**	18	**228**	11	**214**	13	**246**	5
7	**368**	16	**255**	9	**219**	5	**212**	10	**189**	6	**230**	17	**199**	7	**230**	15	**207**	10
8	**339**	28	**227**	16	**193**	8	**194**	4	**161**	5	**213**	2	**no sample***		**62**	6	**186**	4
9	**326**	11	**202**	9	**187**	8	**174**	5	**151**	5	**198**	9	**227**	10	**242**	11	**168**	4
10	**304**	10	**193**	6	**187**	5	**152**	7	**134**	5	**182**	10	**146**	5	**180**	8	**153**	3
11	**305**	25	**173**	6	**172**	3	**136**	4	**124**	3	**174**	5	**156**	3	**285**	8	**138**	4
12	**287**	12	**168**	6	**157**	4	**117**	6	**113**	3	**153**	9	**139**	6	**173**	8	**130**	5
13	**258**	7	**162**	5	**145**	3	**101**	2	**108**	5	**138**	3	**161**	9	**202**	3	**114**	6
14	**242**	8	**149**	4	**129**	8	**86**	2	**100**	6	**128**	4	**130**	6	**124**	4	**101**	3
15	**236**	9	**133**	3	**121**	3	**77**	3	**78**	3	**115**	5	**121**	5	**220**	5	**95**	5
LoD	1.13		0.11		0.28		0.46		0.06		0.14		0.27		0.27		0.27	
LoQ	3.31		0.18		0.67		1.23		0.08		0.31		0.63		0.63		0.63	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 37: Manganese concentrations across the SWI of the sediment cores of sampling site 2 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**170**	5	**190**	5	**30**	1	**3**	0	**30**	2	**2**	0	**11**	1	**191**	7	**2**	0
-3	**131**	3	**264**	5	**259**	13	**4**	0	**81**	3	**2**	0	**9**	1	**7**	0	**2**	0
-2	**83**	2	**452**	3	**304**	12	**16**	0	**194**	3	**2**	0	**37**	1	**191**	7	**2**	0
-1	**381**	23	**1287**	22	**343**	16	**272**	3	**143**	2	**3**	0	**125**	3	**46**	2	**3**	0
0	**1677**	39	**2050**	54	**392**	14	**991**	6	**312**	5	**140**	5	**190**	5	**289**	7	**70**	4
1	**1747**	64	**1686**	49	**436**	16	**707**	10	**432**	23	**339**	6	**513**	13	**477**	19	**381**	16
2	**2307**	80	**1112**	27	**538**	13	**620**	11	**497**	8	**380**	8	**612**	24	**459**	14	**703**	34
3	**1758**	34	**923**	20	**513**	9	**604**	8	**451**	14	**307**	11	**524**	18	**484**	15	**575**	20
4	**285**	17	**716**	19	**472**	10	**547**	9	**598**	6	**421**	17	**539**	15	**401**	24	**544**	15
5	**404**	23	**512**	11	**426**	9	**500**	6	**401**	18	**407**	6	**252**	4	**313**	5	**444**	8
6	**1141**	32	**461**	11	**346**	17	**422**	10	**118**	3	**150**	3	**202**	5	**342**	18	**205**	8
7	**1224**	24	**421**	8	**344**	10	**364**	4	**79**	4	**114**	3	**165**	4	**384**	15	**156**	3
8	**650**	20	**208**	2	**126**	3	**156**	4	**54**	2	**73**	1	**no sample***		**95**	2	**147**	7
9	**519**	14	**222**	3	**116**	3	**111**	2	**38**	1	**52**	1	**265**	11	**285**	8	**112**	2
10	**391**	5	**193**	3	**113**	2	**67**	1	**33**	1	**34**	1	**192**	5	**193**	2	**141**	6
11	**350**	3	**154**	3	**72**	2	**56**	1	**23**	0	**24**	1	**183**	5	**205**	7	**152**	6
12	**172**	4	**51**	1	**55**	1	**44**	1	**17**	1	**22**	1	**154**	3	**97**	3	**56**	2
13	**123**	8	**36**	1	**48**	2	**48**	0	**21**	1	**20**	1	**122**	1	**94**	3	**37**	1
14	**91**	1	**30**	1	**44**	1	**54**	1	**25**	1	**26**	1	**40**	1	**35**	1	**43**	1
15	**83**	1	**27**	0	1	1	**37**	0	**21**	1	**24**	1	**42**	1	**51**	3	**40**	1
LoD	0.09		0.14		0.58		0.13		0.21		0.14		0.19		0.19		0.19	
LoQ	0.23		0.32		1.62		0.31		0.48		0.26		0.51		0.51		0.51	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 38: Iron concentrations across the SWI of the sediment cores of sampling site 2 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**586**	17	**34**	1	**40**	1	**7**	0	**153**	2	**79**	1	**25**	1	**100**	4	**18**	1
-3	**200**	10	**51**	1	**31**	1	**5**	0	**171**	2	**76**	1	**21**	1	**1079**	36	**18**	1
-2	**146**	6	**108**	2	**426**	13	**3**	0	**231**	4	**76**	1	**34**	0	**109**	3	**16**	1
-1	**1124**	69	**4796**	158	**737**	25	**9**	0	**127**	1	**90**	1	**23**	1	**18**	1	**18**	1
0	**3205**	106	**22808**	1083	**9448**	485	**1290**	10	**372**	6	**325**	9	**35**	1	**2994**	73	**289**	10
1	**1382**	44	**7831**	768	**3968**	193	**5715**	154	**209**	5	**1731**	33	**3436**	146	**4687**	360	**12070**	595
2	**546**	23	**2084**	52	**66**	1	**4694**	174	**155**	2	**210**	6	**6478**	268	**2222**	56	**19456**	985
3	**394**	9	**2325**	88	**62**	2	**1511**	25	**120**	2	**227**	5	**4815**	372	**399**	12	**10527**	590
4	**693**	42	**2623**	131	**63**	1	**60**	1	**150**	2	**310**	6	**4044**	126	**201**	10	**6253**	167
5	**741**	102	**2613**	132	**57**	1	**67**	1	**124**	7	**247**	10	**347**	8	**145**	2	**2781**	78
6	**812**	20	**2475**	47	**53**	2	**106**	2	**18**	1	**44**	0	**669**	9	**456**	18	**21**	1
7	**906**	20	**2265**	123	**67**	1	**264**	4	**19**	1	**40**	1	**519**	13	**1206**	51	**13**	0
8	**299**	8	**38**	2	**10**	0	**28**	1	**19**	0	**37**	1	**no sample***		**29**	1	**20**	1
9	**401**	7	**158**	2	**12**	1	**50**	1	**21**	0	**39**	1	**1523**	60	**50**	0	**24**	0
10	**258**	7	**163**	4	**10**	0	**25**	1	**28**	1	**35**	1	**1129**	12	**31**	1	**57**	3
11	**351**	7	**135**	5	**12**	1	**37**	1	**31**	1	**32**	1	**910**	19	**36**	1	**122**	5
12	**431**	6	**20**	1	**14**	0	**39**	1	**29**	1	**40**	1	**53**	2	**17**	1	**18**	1
13	**740**	44	**13**	0	**16**	1	**80**	2	**40**	0	**44**	1	**29**	1	**24**	1	**17**	0
14	**869**	12	**13**	0	**33**	1	**155**	3	**112**	4	**113**	1	**15**	0	**11**	0	**54**	1
15	**549**	12	**13**	0	0	<LoD	**134**	3	**117**	4	**162**	5	**18**	0	**25**	1	**83**	1
LoD	0.41		1.55		0.59		0.37		0.43		0.16		0.21		0.21		0.21	
LoQ	0.97		4.08		1.64		0.85		1.13		0.38		0.57		0.57		0.57	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 39: Arsenic concentrations across the SWI of the sediment cores of sampling site 2 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**3.810**	0.115	**2.422**	0.089	**1.923**	0.024	**1.360**	0.108	**1.029**	0.082	**1.447**	0.038	**0.868**	0.056	**1.770**	0.101	**1.654**	0.115
-3	**3.524**	0.162	**2.176**	0.059	**2.414**	0.141	**1.289**	0.075	**0.879**	0.035	**1.558**	0.110	**1.058**	0.075	**1.793**	0.081	**1.539**	0.143
-2	**2.234**	0.088	**2.311**	0.052	**2.445**	0.136	**1.234**	0.115	**1.297**	0.100	**1.335**	0.087	**1.387**	0.077	**1.589**	0.036	**1.527**	0.080
-1	**2.399**	0.148	**3.586**	0.118	**2.718**	0.110	**1.481**	0.085	**1.477**	0.131	**1.536**	0.063	**1.137**	0.044	**1.307**	0.101	**1.318**	0.093
0	**3.375**	0.190	**8.622**	0.436	**4.587**	0.246	**1.998**	0.131	**2.525**	0.158	**1.763**	0.071	**1.010**	0.041	**1.169**	0.109	**1.152**	0.069
1	**2.694**	0.076	**4.246**	0.168	**3.739**	0.178	**2.431**	0.163	**2.280**	0.176	**1.837**	0.067	**2.884**	0.114	**1.114**	0.030	**1.967**	0.073
2	**2.528**	0.041	**2.844**	0.044	**3.608**	0.238	**1.705**	0.077	**2.219**	0.110	**1.807**	0.082	**2.568**	0.149	**1.079**	0.037	**2.166**	0.059
3	**2.349**	0.104	**2.354**	0.078	**3.234**	0.168	**1.520**	0.115	**2.296**	0.132	**1.553**	0.085	**2.130**	0.082	**1.270**	0.072	**1.598**	0.062
4	**1.345**	0.673	**2.175**	0.077	**2.966**	0.168	**1.598**	0.092	**3.050**	0.244	**1.766**	0.099	**1.672**	0.061	**1.674**	0.156	**1.418**	0.049
5	**2.351**	1.084	**1.730**	0.103	**3.135**	0.131	**1.977**	0.070	**2.651**	0.206	**1.575**	0.129	**1.659**	0.080	**2.218**	0.121	**1.451**	0.091
6	**3.202**	0.128	**1.812**	0.126	**3.159**	0.199	**2.545**	0.160	**1.885**	0.100	**1.219**	0.087	**2.373**	0.161	**2.927**	0.122	**2.236**	0.078
7	**3.247**	0.140	**2.195**	0.150	**3.411**	0.146	**2.844**	0.102	**1.930**	0.122	**1.328**	0.123	**2.705**	0.069	**3.333**	0.256	**2.470**	0.115
8	**2.952**	0.162	**2.367**	0.132	**3.399**	0.183	**2.640**	0.109	**1.737**	0.105	**1.452**	0.069	**no sample***		**0.680**	0.061	**2.545**	0.119
9	**2.516**	0.075	**2.525**	0.082	**4.130**	0.188	**2.723**	0.064	**1.838**	0.059	**1.398**	0.133	**3.803**	0.142	**1.793**	0.138	**2.426**	0.074
10	**2.066**	0.041	**2.235**	0.100	**3.904**	0.169	**2.538**	0.164	**1.774**	0.054	**1.451**	0.098	**2.928**	0.162	**1.167**	0.074	**2.421**	0.042
11	**2.261**	0.123	**1.992**	0.065	**4.236**	0.130	**2.402**	0.086	**1.638**	0.153	**1.561**	0.076	**2.297**	0.077	**1.461**	0.062	**2.138**	0.066
12	**2.582**	0.137	**2.090**	0.078	**3.969**	0.255	**2.333**	0.135	**1.669**	0.090	**1.597**	0.155	**1.901**	0.119	**1.166**	0.031	**1.570**	0.057
13	**2.654**	0.065	**1.887**	0.073	**4.374**	0.199	**2.436**	0.127	**1.905**	0.134	**1.599**	0.040	**1.616**	0.091	**1.424**	0.082	**1.233**	0.049
14	**3.010**	0.155	**1.839**	0.092	**4.098**	0.108	**2.244**	0.145	**1.797**	0.085	**1.840**	0.128	**1.239**	0.063	**0.801**	0.080	**1.219**	0.039
15	**2.942**	0.153	**2.116**	0.073	**3.607**	0.094	**1.972**	0.069	**1.882**	0.067	**1.716**	0.140	**1.214**	0.034	**1.606**	0.041	**1.152**	0.105
LoD	0.186		0.155		0.083		0.073		0.064		0.120		0.081		0.081		0.081	
LoQ	0.532		0.444		0.192		0.165		0.153		0.299		0.199		0.199		0.199	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 40: Antimony concentrations across the SWI of the sediment cores of sampling site 2 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.771**	0.032	**0.595**	0.048	0.508	0.083	**0.201**	0.026	**0.218**	0.032	**0.252**	0.050	0.821	0.055	0.165	<LoD	0.165	<LoD
-3	**0.732**	0.040	**0.492**	0.019	0.208	<LoD	**0.189**	0.044	**0.164**	0.007	**0.277**	0.029	0.497	0.058	0.165	<LoD	0.165	<LoD
-2	**0.471**	0.013	**0.374**	0.030	0.208	<LoD	**0.164**	0.031	**0.266**	0.049	**0.220**	0.015	0.565	0.037	0.165	<LoD	0.165	<LoD
-1	**0.428**	0.042	**0.323**	0.028	0.208	<LoD	**0.143**	0.031	**0.252**	0.029	**0.253**	0.027	0.410	0.022	0.165	<LoD	0.165	<LoD
0	**0.353**	0.026	**0.281**	0.021	0.208	<LoD	0.112	0.027	**0.167**	0.022	**0.236**	0.013	0.165	<LoD	0.165	<LoD	0.165	<LoD
1	0.192	0.029	**0.196**	0.012	0.208	<LoD	0.085	0.020	**0.143**	0.009	**0.127**	0.011	0.165	<LoD	0.165	<LoD	0.165	<LoD
2	0.196	0.011	**0.183**	0.015	0.208	<LoD	0.078	0.015	**0.184**	0.025	**0.128**	0.017	0.165	<LoD	0.165	<LoD	0.165	<LoD
3	0.235	0.007	**0.166**	0.017	0.208	<LoD	0.076	0.014	**0.145**	0.027	**0.113**	0.016	0.165	<LoD	0.165	<LoD	0.165	<LoD
4	0.205	0.086	**0.201**	0.011	0.208	<LoD	0.084	0.005	**0.172**	0.011	**0.114**	0.021	0.165	<LoD	0.165	<LoD	0.165	<LoD
5	**0.281**	0.129	**0.153**	0.012	0.208	<LoD	0.113	0.019	**0.128**	0.026	**0.115**	0.012	0.165	<LoD	0.165	<LoD	0.165	<LoD
6	0.140	0.017	**0.159**	0.007	0.208	<LoD	**0.157**	0.023	**0.108**	0.015	**0.094**	0.021	0.165	<LoD	0.165	<LoD	0.165	<LoD
7	0.117	0.018	**0.191**	0.017	0.208	<LoD	**0.201**	0.012	**0.115**	0.013	**0.095**	0.028	0.165	<LoD	0.165	<LoD	0.165	<LoD
8	0.101	0.011	**0.218**	0.025	0.208	<LoD	**0.174**	0.008	**0.116**	0.016	**0.119**	0.014	**no sample***		0.165	<LoD	0.165	<LoD
9	0.098	0.008	**0.234**	0.017	0.208	<LoD	**0.182**	0.010	**0.119**	0.024	**0.104**	0.019	0.426	0.064	0.165	<LoD	0.165	<LoD
10	0.093	0.009	**0.212**	0.013	0.208	<LoD	**0.197**	0.018	**0.130**	0.007	**0.129**	0.013	0.165	<LoD	0.165	<LoD	0.165	<LoD
11	0.106	0.017	**0.212**	0.020	0.208	<LoD	**0.191**	0.018	**0.135**	0.021	**0.131**	0.045	0.165	<LoD	0.165	<LoD	0.165	<LoD
12	0.148	0.016	**0.228**	0.019	0.208	<LoD	**0.185**	0.012	**0.142**	0.022	**0.103**	0.018	0.165	<LoD	0.165	<LoD	0.165	<LoD
13	0.195	0.018	**0.213**	0.015	0.208	<LoD	**0.240**	0.024	**0.151**	0.004	**0.141**	0.023	0.165	<LoD	0.165	<LoD	0.165	<LoD
14	0.228	0.022	**0.224**	0.026	0.208	<LoD	**0.193**	0.004	**0.140**	0.009	**0.126**	0.013	0.165	<LoD	0.165	<LoD	0.165	<LoD
15	0.248	0.026	**0.211**	0.020	0.208	<LoD	**0.187**	0.017	**0.147**	0.005	**0.128**	0.025	0.165	<LoD	0.165	<LoD	0.165	<LoD
LoD	0.091		0.051		0.415		0.061		0.020		0.021		0.331		0.331		0.331	
LoQ	0.262		0.122		0.989		0.137		0.050		0.052		0.889		0.889		0.889	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 41: Cadmium concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.161**	0.015	**0.098**	0.009	**0.125**	0.016	**0.040**	0.004	**0.026**	0.007	0.003	<LoD	**0.039**	0.007	**0.046**	0.003	**0.010**	0.004
-3	**0.160**	0.013	**0.127**	0.016	**0.064**	0.011	**0.074**	0.004	**0.041**	0.003	**0.056**	0.004	**0.101**	0.007	**0.166**	0.014	**0.109**	0.018
-2	**0.100**	0.005	**0.069**	0.008	**0.013**	0.006	**0.034**	0.003	**0.081**	0.012	**0.093**	0.008	**0.258**	0.014	**0.218**	0.010	**0.085**	0.012
-1	**0.126**	0.004	0.032	0.004	**0.017**	0.008	**0.012**	0.002	**0.108**	0.013	**0.079**	0.009	**0.185**	0.017	**0.168**	0.018	**0.045**	0.009
0	**0.092**	0.007	0.007	<LoD	0.002	<LoD	**0.019**	0.002	**0.038**	0.005	**0.124**	0.010	**0.099**	0.012	**0.116**	0.004	0.005	0.002
1	0.024	0.003	0.007	<LoD	0.002	<LoD	**0.017**	0.002	**0.010**	0.004	**0.049**	0.002	**0.093**	0.012	**0.041**	0.003	**0.090**	0.014
2	0.010	<LoD	0.007	<LoD	0.002	<LoD	**0.015**	0.001	**0.012**	0.002	**0.032**	0.003	**0.044**	0.010	**0.019**	0.005	**0.100**	0.018
3	0.043	0.005	0.007	<LoD	0.002	<LoD	**0.015**	0.002	**0.010**	0.002	**0.022**	0.001	**0.011**	0.001	**0.009**	0.001	**0.035**	0.005
4	0.010	<LoD	0.017	0.002	0.002	<LoD	**0.014**	0.001	**0.011**	0.006	**0.023**	0.002	**0.011**	0.003	0.008	0.004	**0.031**	0.009
5	0.022	0.047	0.007	<LoD	0.002	<LoD	**0.016**	0.002	0.007	0.003	0.013	0.004	0.003	0.003	0.007	0.004	**0.015**	0.003
6	0.010	<LoD	0.007	<LoD	0.002	<LoD	**0.016**	0.001	0.002	<LoD	0.003	<LoD	0.005	0.005	**0.013**	0.004	**0.014**	0.004
7	0.010	<LoD	0.007	<LoD	0.002	<LoD	**0.020**	0.004	0.002	<LoD	0.010	0.002	**0.008**	0.003	**0.022**	0.005	**0.010**	0.003
8	0.010	<LoD	0.007	<LoD	0.002	<LoD	**0.015**	0.001	0.002	<LoD	0.003	<LoD	**no sample***		0.003	0.003	0.007	0.002
9	0.010	<LoD	0.007	<LoD	0.003	0.005	**0.020**	0.002	0.002	<LoD	0.003	<LoD	**0.013**	0.004	**0.020**	0.006	**0.020**	0.006
10	0.010	<LoD	0.015	0.004	**0.022**	0.008	**0.019**	0.002	0.002	<LoD	0.003	<LoD	**0.011**	0.003	**0.012**	0.006	**0.012**	0.002
11	0.010	<LoD	0.007	<LoD	0.002	<LoD	**0.048**	0.005	**0.143**	0.012	0.003	<LoD	**0.012**	0.003	**0.009**	0.004	**0.023**	0.005
12	0.010	<LoD	0.007	<LoD	0.002	<LoD	**0.011**	0.001	0.002	<LoD	0.003	<LoD	**0.016**	0.003	0.006	0.003	0.005	0.003
13	0.010	<LoD	0.007	<LoD	0.006	0.003	**0.016**	0.001	0.005	0.003	0.003	<LoD	**0.014**	0.004	**0.011**	0.001	**0.015**	0.001
14	0.010	<LoD	0.007	<LoD	0.004	0.003	**0.020**	0.002	0.002	<LoD	0.003	<LoD	0.002	<LoD	0.002	<LoD	**0.008**	0.005
15	0.010	<LoD	0.007	<LoD	**0.009**	0.003	**0.025**	0.002	0.007	0.005	0.010	0.003	0.004	0.003	**0.008**	0.005	**0.008**	0.001
LoD	0.021		0.014		0.003		0.004		0.004		0.006		0.003		0.003		0.003	
LoQ	0.059		0.037		0.009		0.011		0.010		0.017		0.008		0.008		0.008	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 42: Chromium concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.166**	0.019	**0.252**	0.005	**0.238**	0.020	0.279	0.019	0.152	0.045	**0.410**	0.025	0.057	<LoD	**0.365**	0.028	0.057	<LoD
-3	**0.169**	0.019	**0.218**	0.021	0.117	0.036	0.345	0.018	0.073	<LoD	**0.359**	0.033	0.057	<LoD	0.057	<LoD	0.057	<LoD
-2	0.104	0.019	0.188	0.016	0.117	0.050	0.316	0.046	0.212	0.085	**0.335**	0.036	0.057	<LoD	**0.311**	0.024	0.057	<LoD
-1	0.092	0.012	**0.223**	0.018	0.095	0.022	**0.398**	0.025	0.188	0.023	**0.336**	0.036	0.057	<LoD	0.057	<LoD	0.057	<LoD
0	0.083	0.014	**0.409**	0.019	**0.244**	0.008	**0.534**	0.051	0.239	0.066	**0.465**	0.040	0.057	<LoD	**0.421**	0.008	0.057	<LoD
1	0.025	<LoD	**0.411**	0.020	**0.301**	0.034	**0.691**	0.034	**0.935**	0.090	**1.914**	0.096	**0.247**	0.027	**0.212**	0.017	**0.226**	0.006
2	**0.149**	0.016	**0.663**	0.036	**0.575**	0.010	**1.064**	0.070	**1.784**	0.039	**1.650**	0.154	**0.720**	0.028	**0.523**	0.045	**0.813**	0.053
3	**0.335**	0.046	**1.758**	0.133	**4.332**	0.281	**1.084**	0.085	**1.755**	0.098	**1.740**	0.084	**0.751**	0.056	**1.201**	0.079	**1.031**	0.083
4	0.080	0.146	**3.021**	0.241	**1.697**	0.167	**1.328**	0.081	**2.568**	0.182	**2.733**	0.131	**1.396**	0.104	**2.073**	0.142	**1.796**	0.121
5	**0.161**	0.261	**1.648**	0.082	**1.259**	0.121	**1.559**	0.079	**2.331**	0.179	**3.007**	0.245	**0.734**	0.077	**2.049**	0.175	**1.777**	0.174
6	**0.272**	0.024	**2.292**	0.121	**1.244**	0.108	**2.218**	0.148	**0.959**	0.093	**1.345**	0.133	**1.277**	0.103	**3.501**	0.191	**0.794**	0.060
7	**0.288**	0.007	**3.058**	0.104	**1.753**	0.090	**2.898**	0.209	**0.914**	0.080	**1.528**	0.149	**1.159**	0.067	**4.562**	0.398	**0.942**	0.081
8	**0.450**	0.020	**1.431**	0.081	**0.675**	0.055	**2.011**	0.125	**0.909**	0.044	**1.530**	0.032	**no sample***		**0.951**	0.075	**1.176**	0.123
9	**0.826**	0.020	**2.605**	0.066	**1.042**	0.100	**2.302**	0.130	**1.050**	0.054	**1.647**	0.123	**2.707**	0.180	**4.235**	0.271	**1.387**	0.092
10	**0.653**	0.042	**3.799**	0.179	**0.977**	0.082	**2.120**	0.087	**1.308**	0.090	**1.822**	0.092	**2.112**	0.159	**2.865**	0.185	**2.093**	0.097
11	**0.811**	0.057	**3.276**	0.177	**1.165**	0.097	**2.460**	0.204	**1.463**	0.084	**2.068**	0.093	**2.184**	0.054	**4.171**	0.177	**3.058**	0.148
12	**0.513**	0.043	**1.612**	0.058	**1.099**	0.093	**2.554**	0.246	**1.608**	0.101	**2.537**	0.224	**2.624**	0.160	**2.894**	0.146	**1.615**	0.050
13	**0.559**	0.027	**1.341**	0.036	**1.197**	0.061	**3.817**	0.229	**2.438**	0.216	**2.618**	0.206	**3.092**	0.288	**4.244**	0.164	**1.869**	0.146
14	**0.505**	0.036	**1.633**	0.045	**1.731**	0.093	**4.453**	0.278	**3.601**	0.181	**4.029**	0.255	**1.123**	0.067	**2.623**	0.122	**2.982**	0.046
15	**0.618**	0.023	**1.972**	0.083	**2.386**	0.210	**4.479**	0.221	**3.442**	0.121	**4.962**	0.389	**1.586**	0.054	**6.250**	0.178	**4.002**	0.306
LoD	0.050		0.073		0.072		0.136		0.147		0.076		0.114		0.114		0.114	
LoQ	0.139		0.203		0.146		0.351		0.408		0.206		0.197		0.197		0.197	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 43: Cobalt concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.599**	0.053	**0.522**	0.046	**0.239**	0.022	**0.093**	0.008	**0.140**	0.011	**0.118**	0.012	**0.191**	0.014	**0.248**	0.012	**0.246**	0.054
-3	**0.529**	0.017	**0.609**	0.041	**0.481**	0.039	**0.110**	0.008	**0.164**	0.012	**0.132**	0.012	**0.197**	0.013	**0.244**	0.058	**0.234**	0.031
-2	**0.372**	0.022	**0.896**	0.055	**0.522**	0.038	**0.123**	0.003	**0.315**	0.024	**0.166**	0.023	**0.334**	0.023	**0.228**	0.027	**0.223**	0.026
-1	**0.715**	0.067	**2.057**	0.143	**0.621**	0.034	**0.461**	0.043	**0.275**	0.021	**0.158**	0.011	**0.583**	0.050	**0.236**	0.034	**0.206**	0.022
0	**2.703**	0.125	**2.350**	0.151	**0.696**	0.059	**2.290**	0.143	**0.526**	0.049	**0.579**	0.052	**0.885**	0.052	**0.742**	0.049	**0.525**	0.033
1	**2.776**	0.065	**1.457**	0.096	**0.719**	0.038	**1.941**	0.103	**0.617**	0.034	**0.848**	0.053	**1.468**	0.041	**0.817**	0.097	**1.441**	0.115
2	**2.961**	0.096	**1.171**	0.051	**0.929**	0.068	**1.098**	0.068	**0.771**	0.046	**0.918**	0.050	**1.208**	0.071	**0.689**	0.046	**1.426**	0.085
3	**2.029**	0.115	**1.139**	0.067	**0.858**	0.044	**0.809**	0.058	**0.619**	0.048	**0.846**	0.028	**0.686**	0.056	**0.773**	0.058	**0.850**	0.054
4	**0.360**	0.082	**1.353**	0.102	**0.889**	0.073	**0.685**	0.032	**0.920**	0.048	**1.082**	0.082	**0.767**	0.031	**0.963**	0.072	**0.973**	0.019
5	**0.667**	0.287	**1.089**	0.086	**0.928**	0.075	**0.674**	0.063	**0.782**	0.056	**1.077**	0.071	**0.872**	0.093	**0.877**	0.079	**0.862**	0.088
6	**1.682**	0.105	**1.003**	0.087	**0.813**	0.072	**0.742**	0.065	**0.793**	0.033	**0.843**	0.047	**0.966**	0.071	**1.133**	0.072	**0.993**	0.076
7	**1.683**	0.130	**1.012**	0.050	**0.946**	0.032	**0.892**	0.063	**0.996**	0.091	**0.857**	0.084	**0.910**	0.063	**1.302**	0.163	**0.977**	0.076
8	**1.091**	0.108	**0.911**	0.085	**0.825**	0.025	**1.007**	0.051	**0.986**	0.096	**0.904**	0.074	**no sample***		**0.337**	0.030	**0.956**	0.093
9	**1.064**	0.052	**0.885**	0.063	**0.986**	0.090	**1.115**	0.045	**0.966**	0.060	**0.953**	0.048	**1.341**	0.047	**1.354**	0.064	**0.884**	0.070
10	**0.844**	0.048	**1.025**	0.088	**0.985**	0.063	**1.101**	0.083	**1.034**	0.021	**0.968**	0.069	**1.109**	0.115	**0.894**	0.028	**1.070**	0.032
11	**0.914**	0.082	**0.995**	0.052	**1.013**	0.058	**1.228**	0.075	**1.082**	0.047	**1.081**	0.023	**1.139**	0.112	**1.328**	0.058	**1.067**	0.072
12	**0.868**	0.029	**1.036**	0.050	**0.968**	0.050	**1.201**	0.099	**1.153**	0.088	**1.189**	0.090	**1.007**	0.031	**1.172**	0.063	**1.217**	0.032
13	**0.829**	0.062	**1.028**	0.090	**0.975**	0.093	**1.289**	0.075	**1.413**	0.111	**1.176**	0.057	**1.144**	0.065	**1.496**	0.071	**1.196**	0.063
14	**0.797**	0.048	**1.022**	0.035	**1.130**	0.092	**1.341**	0.110	**1.269**	0.055	**1.324**	0.082	**1.050**	0.044	**0.768**	0.079	**1.266**	0.054
15	**0.948**	0.050	**1.070**	0.070	**1.203**	0.109	**1.453**	0.124	**1.206**	0.077	**1.273**	0.045	**1.049**	0.053	**1.722**	0.116	**1.342**	0.075
LoD	0.021		0.030		0.018		0.014		0.011		0.009		0.010		0.010		0.010	
LoQ	0.060		0.084		0.047		0.038		0.029		0.020		0.024		0.024		0.024	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 44: Copper concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**11.72**	0.61	**3.63**	0.15	**8.27**	0.26	**0.71**	0.05	**1.73**	0.07	**2.54**	0.11	**3.75**	0.24	**3.45**	0.17	**1.58**	0.10
-3	**10.09**	0.36	**4.90**	0.11	**3.82**	0.19	**0.82**	0.06	**1.26**	0.02	**2.42**	0.13	**3.57**	0.30	**4.33**	0.13	**1.52**	0.14
-2	**7.57**	0.14	**2.36**	0.03	**1.13**	0.09	**0.80**	0.04	**1.92**	0.10	**2.20**	0.05	**3.81**	0.24	**4.04**	0.23	**1.50**	0.11
-1	**8.18**	0.52	**1.10**	0.06	**1.05**	0.08	**0.92**	0.06	**2.22**	0.05	**2.66**	0.09	**2.60**	0.12	**2.78**	0.14	**1.54**	0.09
0	**8.41**	0.16	0.13	<LoD	0.20	<LoD	**0.36**	0.02	**1.15**	0.04	**1.91**	0.10	**1.39**	0.12	**1.37**	0.07	**0.65**	0.03
1	**5.44**	0.19	0.13	<LoD	0.20	<LoD	0.18	0.01	**0.74**	0.04	**0.67**	0.06	**0.45**	0.01	0.21	0.04	0.21	0.05
2	**4.35**	0.17	0.38	0.01	0.20	<LoD	0.17	0.04	**0.76**	0.04	**0.61**	0.03	**0.95**	0.06	0.07	<LoD	**2.49**	0.21
3	**6.66**	0.14	0.50	0.02	0.20	<LoD	0.26	0.05	**1.19**	0.08	**0.60**	0.05	0.07	<LoD	0.07	<LoD	0.16	0.08
4	**12.00**	0.74	**0.90**	0.08	0.20	<LoD	**0.36**	0.04	**0.81**	0.07	**0.95**	0.07	0.07	<LoD	0.07	<LoD	0.24	0.04
5	**14.65**	1.86	0.37	0.03	0.20	<LoD	**0.41**	0.03	**0.85**	0.05	**1.78**	0.07	0.07	<LoD	0.07	<LoD	0.27	0.04
6	**3.05**	0.06	0.13	<LoD	**6.89**	0.28	**0.34**	0.01	**0.68**	0.02	**0.36**	0.03	0.07	<LoD	0.07	<LoD	0.33	0.05
7	**3.15**	0.09	**2.03**	0.04	0.20	<LoD	**0.76**	0.03	**0.48**	0.04	**0.40**	0.04	0.07	<LoD	0.07	<LoD	0.07	<LoD
8	**2.70**	0.10	0.13	<LoD	0.20	<LoD	0.25	0.02	**0.67**	0.05	**0.38**	0.02	**no sample***		0.07	<LoD	0.07	<LoD
9	**3.26**	0.09	**3.94**	0.10	**2.17**	0.13	**0.31**	0.02	**0.45**	0.03	**0.45**	0.04	0.07	<LoD	0.07	<LoD	0.07	<LoD
10	**2.76**	0.04	0.33	0.03	0.20	<LoD	0.26	0.03	**0.55**	0.04	**0.32**	0.01	0.07	<LoD	0.07	<LoD	0.07	<LoD
11	**3.02**	0.16	0.29	0.02	0.54	0.09	**0.52**	0.05	**0.61**	0.06	**0.29**	0.03	0.07	<LoD	0.07	<LoD	0.26	0.05
12	**3.02**	0.10	**0.72**	0.07	0.20	<LoD	**0.48**	0.02	**0.53**	0.02	**0.29**	0.03	0.07	<LoD	0.07	<LoD	0.07	<LoD
13	**3.10**	0.13	0.59	0.01	0.20	<LoD	**0.29**	0.02	**0.51**	0.03	**0.36**	0.04	0.07	<LoD	0.07	<LoD	**0.49**	0.04
14	**2.78**	0.14	0.37	0.03	0.20	<LoD	**0.37**	0.05	**0.54**	0.05	**0.35**	0.02	0.07	<LoD	0.07	<LoD	0.07	<LoD
15	**2.77**	0.06	0.44	0.02	0.20	<LoD	**17.57**	0.46	**0.51**	0.05	**0.44**	0.04	0.07	<LoD	0.23	0.06	0.14	0.04
LoD	0.32		0.27		0.40		0.13		0.13		0.10		0.13		0.13		0.13	
LoQ	0.73		0.61		0.84		0.28		0.33		0.15		0.34		0.34		0.34	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 45: Lead concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.068**	0.006	0.062	0.003	**1.300**	0.045	**0.104**	0.014	**0.102**	0.007	**0.060**	0.007	**0.068**	0.009	**0.080**	0.015	**0.044**	0.011
-3	0.051	0.003	**0.184**	0.004	**0.407**	0.033	**0.104**	0.008	**0.090**	0.003	**0.048**	0.005	**0.037**	0.007	**0.035**	0.008	0.006	<LoD
-2	0.029	0.003	0.074	0.003	**0.105**	0.011	**0.082**	0.004	**0.039**	0.002	**0.039**	0.007	0.006	<LoD	**0.204**	0.006	**0.106**	0.021
-1	0.028	0.002	0.033	0.003	**0.151**	0.012	**0.079**	0.007	**0.051**	0.003	**0.059**	0.004	0.006	<LoD	**0.118**	0.016	**0.038**	0.009
0	0.047	0.006	0.030	0.002	0.036	0.005	**0.106**	0.018	**0.044**	0.003	**0.058**	0.004	0.006	<LoD	**0.107**	0.010	**0.041**	0.010
1	0.011	<LoD	0.015	<LoD	0.068	0.011	**0.088**	0.009	**0.051**	0.004	**0.072**	0.007	**0.203**	0.015	**0.058**	0.016	**0.034**	0.011
2	**0.191**	0.018	0.053	0.002	**0.315**	0.025	**0.095**	0.010	**0.142**	0.007	**0.254**	0.021	**0.219**	0.016	0.025	0.004	**0.430**	0.017
3	**0.932**	0.023	**0.182**	0.003	**0.135**	0.017	**0.124**	0.006	**0.090**	0.007	**0.115**	0.007	0.027	0.008	**0.056**	0.009	0.006	<LoD
4	**0.228**	0.077	**0.337**	0.010	0.048	0.006	**0.109**	0.015	**0.037**	0.002	**0.095**	0.012	**0.053**	0.006	**0.036**	0.013	0.006	<LoD
5	**0.662**	0.146	0.062	0.002	**0.611**	0.032	**0.128**	0.009	**0.067**	0.003	**0.123**	0.010	**0.033**	0.009	**0.162**	0.013	**0.074**	0.014
6	**0.056**	0.008	0.043	0.002	**0.984**	0.025	**0.298**	0.025	**0.062**	0.006	**0.066**	0.005	**0.033**	0.011	**0.039**	0.011	**0.071**	0.013
7	0.035	0.006	**0.151**	0.005	**0.107**	0.011	**0.625**	0.026	**0.060**	0.003	**0.113**	0.015	**0.043**	0.007	0.015	0.004	**0.073**	0.013
8	0.011	<LoD	0.015	<LoD	**0.405**	0.031	**0.204**	0.019	**0.075**	0.006	**0.168**	0.009	**no sample***		**0.037**	0.006	**0.066**	0.013
9	**0.058**	0.005	**0.516**	0.009	**0.628**	0.025	**0.368**	0.015	**0.056**	0.005	**0.111**	0.009	**0.046**	0.008	0.006	<LoD	**0.094**	0.008
10	0.011	<LoD	**0.199**	0.006	**0.253**	0.018	**0.470**	0.023	**0.106**	0.008	**0.063**	0.004	**0.049**	0.007	**0.032**	0.005	0.030	0.008
11	0.023	0.004	**0.262**	0.013	**0.551**	0.020	**0.388**	0.020	**0.240**	0.013	**0.049**	0.006	**0.031**	0.008	0.006	<LoD	**0.136**	0.010
12	0.039	0.002	**0.316**	0.004	**0.118**	0.010	**0.265**	0.017	**0.043**	0.002	**0.039**	0.011	**0.040**	0.009	0.025	0.011	0.023	0.008
13	0.031	0.016	**0.086**	0.005	**0.330**	0.027	**0.167**	0.010	**0.310**	0.019	**0.125**	0.022	0.025	0.006	**0.100**	0.008	**0.399**	0.026
14	0.041	0.006	0.072	0.001	**0.299**	0.015	**1.302**	0.014	**0.320**	0.022	**0.109**	0.017	**0.031**	0.009	0.006	<LoD	**0.252**	0.025
15	0.025	0.003	**0.232**	0.007	0.015	<LoD	**2.871**	0.050	**0.149**	0.014	**0.097**	0.008	**0.079**	0.016	**0.158**	0.014	**0.133**	0.014
LoD	0.022		0.030		0.029		0.005		0.006		0.012		0.012		0.012		0.012	
LoQ	0.056		0.080		0.081		0.012		0.015		0.031		0.030		0.030		0.030	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 46: Molybdenum concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**18.377**	0.950	**16.613**	0.477	**11.671**	0.619	**4.553**	0.225	**4.754**	0.320	**5.613**	0.299	**6.502**	0.134	**8.228**	0.279	**7.746**	0.273
-3	**17.246**	0.671	**14.030**	0.573	**8.161**	0.276	**5.210**	0.475	**4.040**	0.145	**6.013**	0.160	**6.952**	0.220	**8.464**	0.372	**8.031**	0.512
-2	**11.111**	0.512	**11.463**	0.304	**6.507**	0.441	**5.028**	0.330	**5.467**	0.374	**5.472**	0.252	**7.902**	0.349	**7.671**	0.347	**7.264**	0.657
-1	**11.015**	0.530	**10.784**	0.222	**7.735**	0.786	**4.707**	0.289	**5.482**	0.358	**6.275**	0.253	**6.144**	0.146	**6.466**	0.192	**7.102**	0.287
0	**10.632**	0.530	**7.718**	0.272	**6.262**	0.446	**3.461**	0.177	**3.590**	0.180	**4.984**	0.176	**5.338**	0.090	**5.982**	0.116	**5.303**	0.153
1	**5.506**	0.191	**4.309**	0.060	**3.113**	0.150	**1.398**	0.135	**1.332**	0.057	**1.888**	0.078	**3.324**	0.067	**2.187**	0.083	**3.891**	0.186
2	**4.769**	0.256	**2.551**	0.073	**1.690**	0.105	**0.563**	0.023	**0.514**	0.032	**1.102**	0.109	**0.955**	0.060	**0.741**	0.037	**1.099**	0.083
3	**3.395**	0.161	**2.351**	0.119	**0.726**	0.049	**0.414**	0.040	**0.265**	0.019	**0.449**	0.023	**0.306**	0.018	**0.353**	0.035	**0.244**	0.016
4	**6.773**	2.001	**2.468**	0.083	0.201	0.025	0.272	0.022	**0.349**	0.029	**0.456**	0.013	0.168	0.014	**0.246**	0.016	0.184	0.016
5	**6.465**	1.816	**2.287**	0.141	0.189	0.038	0.256	0.013	**0.364**	0.028	**0.468**	0.036	0.166	0.011	**0.309**	0.022	0.161	0.015
6	**2.017**	0.064	**2.387**	0.081	**0.224**	0.018	**0.304**	0.013	**0.231**	0.019	**0.332**	0.017	**0.292**	0.019	**0.465**	0.025	**0.301**	0.028
7	**2.086**	0.119	**7.462**	0.138	**0.290**	0.020	**0.388**	0.035	**0.289**	0.028	**0.355**	0.036	**0.287**	0.021	**0.501**	0.036	**0.247**	0.025
8	**2.016**	0.179	0.453	0.047	**0.273**	0.019	**0.398**	0.011	**0.267**	0.020	**0.315**	0.026	**no sample***		0.118	0.009	**0.282**	0.028
9	**2.170**	0.083	0.405	0.028	**0.352**	0.027	**0.411**	0.024	**0.348**	0.031	**0.587**	0.052	**0.465**	0.017	**0.446**	0.029	**0.317**	0.031
10	**1.897**	0.056	0.512	0.032	**0.309**	0.027	**0.354**	0.023	**0.252**	0.016	0.270	0.027	**0.388**	0.034	**0.276**	0.026	**0.327**	0.038
11	**2.138**	0.156	0.408	0.032	**0.376**	0.026	**0.384**	0.033	**0.238**	0.014	0.291	0.037	**0.357**	0.026	**0.348**	0.023	**0.313**	0.010
12	**2.139**	0.049	0.375	0.026	**0.315**	0.021	**0.352**	0.027	**0.280**	0.025	0.291	0.036	**0.329**	0.009	**0.274**	0.024	**0.252**	0.009
13	**2.380**	0.134	0.297	0.020	**0.352**	0.015	**0.413**	0.031	**0.276**	0.024	**0.319**	0.015	**0.286**	0.027	**0.284**	0.026	**0.528**	0.022
14	**2.469**	0.127	0.296	0.014	**0.350**	0.009	**0.378**	0.031	**0.298**	0.015	**0.359**	0.035	0.211	0.009	0.147	0.012	**0.252**	0.029
15	**2.587**	0.144	0.313	0.016	**0.377**	0.028	**0.306**	0.027	**0.278**	0.021	**0.344**	0.034	0.207	0.021	**0.311**	0.019	**0.303**	0.030
LoD	0.162		0.294		0.079		0.098		0.081		0.105		0.084		0.084		0.084	
LoQ	0.468		0.829		0.213		0.283		0.231		0.295		0.216		0.216		0.216	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 47: Nickel concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**1.68**	0.15	**3.56**	0.18	**12.43**	0.56	**0.67**	0.06	**6.94**	0.20	**3.74**	0.21	**10.13**	0.56	**6.32**	0.63	**7.16**	0.71
-3	**1.52**	0.14	**3.13**	0.12	**6.01**	0.25	**1.09**	0.08	**7.15**	0.38	**11.83**	0.29	**6.74**	0.34	**9.09**	0.22	**12.38**	0.60
-2	**0.92**	0.08	**2.65**	0.12	**2.98**	0.09	**1.58**	0.10	**12.22**	0.18	**15.03**	0.29	**7.86**	0.41	**9.25**	0.42	**12.23**	0.90
-1	**1.20**	0.06	**2.67**	0.11	**3.44**	0.17	**1.92**	0.12	**14.43**	0.46	**18.26**	0.35	**7.65**	0.33	**7.54**	0.46	**13.67**	0.74
0	**1.75**	0.12	1.70	0.05	**2.56**	0.21	**2.09**	0.22	**9.65**	0.48	**17.70**	0.32	**5.80**	0.13	**11.30**	0.27	**11.65**	0.65
1	**1.19**	0.11	1.07	0.06	**1.44**	0.10	**2.12**	0.19	**4.42**	0.14	**9.17**	0.44	**5.43**	0.22	**5.85**	0.28	**14.60**	0.80
2	**2.52**	0.16	0.80	0.04	**1.17**	0.08	**1.41**	0.05	**3.85**	0.20	**15.38**	0.34	**3.19**	0.09	**2.40**	0.22	**9.27**	0.45
3	**8.39**	0.16	0.96	0.06	**1.15**	0.03	**1.16**	0.06	**2.47**	0.10	**16.24**	0.49	**1.68**	0.06	**1.76**	0.17	**3.49**	0.23
4	**0.43**	0.08	**3.91**	0.09	**1.18**	0.06	**1.22**	0.09	**2.53**	0.12	**18.90**	0.75	**1.41**	0.12	**1.40**	0.09	**2.12**	0.10
5	**1.52**	0.65	0.92	0.05	**0.94**	0.05	**1.12**	0.10	**1.49**	0.10	**15.49**	0.25	**1.03**	0.07	**1.31**	0.08	**1.54**	0.12
6	**0.68**	0.05	0.81	0.01	**0.73**	0.07	**1.26**	0.09	**1.33**	0.04	**15.43**	0.33	**1.09**	0.07	**1.60**	0.08	**1.32**	0.10
7	**0.79**	0.08	0.92	0.07	**1.25**	0.12	**1.36**	0.04	**1.13**	0.10	**4.04**	0.16	**0.98**	0.09	**1.88**	0.14	**1.01**	0.06
8	**0.55**	0.06	0.35	<LoD	**0.67**	0.03	**0.95**	0.09	**1.34**	0.05	**1.75**	0.14	**no sample***		**0.67**	0.02	**1.03**	0.07
9	**2.60**	0.11	0.94	0.06	**0.68**	0.04	**1.10**	0.08	**0.98**	0.09	**1.34**	0.12	**1.07**	0.08	**1.37**	0.07	**1.14**	0.09
10	**0.41**	0.03	0.94	0.07	**0.63**	0.06	**1.19**	0.03	**1.74**	0.10	**1.21**	0.12	**0.74**	0.02	**0.84**	0.06	**1.27**	0.11
11	**0.56**	0.06	0.73	0.06	**0.65**	0.04	**1.23**	0.14	**1.19**	0.08	**0.90**	0.06	**0.52**	0.05	**1.08**	0.08	**1.63**	0.13
12	**0.44**	0.07	0.94	0.04	**3.24**	0.10	**1.37**	0.13	**1.39**	0.06	**1.09**	0.08	**0.72**	0.07	**0.74**	0.01	**0.97**	0.05
13	**0.38**	0.07	0.35	<LoD	**0.75**	0.07	**0.97**	0.04	**1.37**	0.07	**1.12**	0.09	**0.56**	0.05	**0.93**	0.09	**1.05**	0.11
14	**0.37**	0.04	0.35	<LoD	**0.79**	0.04	**1.13**	0.05	**1.15**	0.14	**1.35**	0.12	**0.26**	0.03	**0.33**	0.05	**0.73**	0.06
15	**0.44**	0.03	0.35	<LoD	0.03	<LoD	**1.20**	0.14	**1.99**	0.17	**1.33**	0.13	**1.17**	0.18	**1.13**	0.06	**0.62**	0.06
LoD	0.06		0.70		0.07		0.09		0.10		0.12		0.04		0.04		0.04	
LoQ	0.15		1.70		0.16		0.25		0.26		0.28		0.09		0.09		0.09	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 48: Selenium concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**1.395**	0.197	**1.964**	0.330	0.567	0.326	0.404	0.110	0.415	<LoD	**1.308**	0.366	0.308	<LoD	0.308	<LoD	0.308	<LoD
-3	**1.539**	0.121	**1.922**	0.374	0.405	0.404	0.596	0.373	0.415	<LoD	**1.306**	0.430	0.308	<LoD	0.308	<LoD	0.308	<LoD
-2	1.112	0.130	**1.650**	0.211	0.662	0.266	0.677	0.285	0.415	<LoD	**1.159**	0.386	0.308	<LoD	0.308	<LoD	0.308	<LoD
-1	1.160	0.218	**2.000**	0.245	0.795	0.265	0.579	0.256	0.415	<LoD	**0.817**	0.241	0.308	<LoD	0.308	<LoD	0.308	<LoD
0	1.254	0.270	**2.038**	0.183	0.682	0.393	0.576	0.073	0.415	<LoD	**1.146**	0.323	0.308	<LoD	0.308	<LoD	0.308	<LoD
1	0.923	0.213	**1.709**	0.244	0.528	0.095	0.656	0.282	0.415	<LoD	**1.513**	0.237	0.308	<LoD	0.308	<LoD	0.308	<LoD
2	1.008	0.175	**1.846**	0.247	0.419	0.306	0.749	0.225	0.415	<LoD	**1.697**	0.254	0.308	<LoD	0.308	<LoD	0.308	<LoD
3	0.677	0.272	**1.984**	0.300	0.711	0.277	0.545	0.171	0.415	<LoD	**1.382**	0.616	0.308	<LoD	0.308	<LoD	0.308	<LoD
4	**2.065**	2.624	**2.034**	0.418	0.153	<LoD	0.585	0.149	0.415	<LoD	**1.904**	0.249	0.308	<LoD	0.308	<LoD	0.308	<LoD
5	**2.676**	1.532	**2.030**	0.237	0.712	0.241	0.713	0.140	0.415	<LoD	**1.963**	0.254	0.308	<LoD	0.308	<LoD	0.308	<LoD
6	0.967	0.321	**2.032**	0.321	0.399	0.204	**0.862**	0.278	0.415	<LoD	**1.512**	0.336	0.308	<LoD	0.308	<LoD	0.308	<LoD
7	0.829	0.085	**2.148**	0.380	0.618	0.369	**0.925**	0.238	0.415	<LoD	**1.565**	0.369	0.308	<LoD	0.308	<LoD	0.308	<LoD
8	0.827	0.162	**2.230**	0.193	0.405	0.343	**0.807**	0.150	0.415	<LoD	**1.832**	0.306	**no sample***		0.308	<LoD	0.308	<LoD
9	0.922	0.154	**1.881**	0.334	0.153	<LoD	**1.049**	0.260	0.415	<LoD	**1.651**	0.320	0.308	<LoD	1.052	0.216	0.308	<LoD
10	0.875	0.189	**2.253**	0.287	0.763	0.352	**0.974**	0.418	0.415	<LoD	**1.856**	0.478	0.308	<LoD	0.308	<LoD	0.308	<LoD
11	1.095	0.167	**2.223**	0.423	0.639	0.270	**1.377**	0.185	0.415	<LoD	**1.773**	0.480	0.308	<LoD	0.654	0.186	0.308	<LoD
12	0.747	0.102	**2.053**	0.397	0.725	0.294	**0.953**	0.296	0.415	<LoD	**1.762**	0.550	0.308	<LoD	0.308	<LoD	0.308	<LoD
13	0.894	0.137	**2.091**	0.372	0.530	0.322	**1.168**	0.247	0.415	<LoD	**1.881**	0.476	0.630	0.264	0.626	0.363	0.308	<LoD
14	0.777	0.143	**1.864**	0.338	0.535	0.239	**1.138**	0.213	0.415	<LoD	**1.702**	0.290	0.308	<LoD	0.308	<LoD	0.308	<LoD
15	0.722	0.166	**2.007**	0.304	0.523	0.186	**0.997**	0.221	0.415	<LoD	**1.767**	0.140	0.308	<LoD	0.750	0.091	0.308	<LoD
LoD	0.472		0.157		0.307		0.330		0.830		0.237		0.615		0.615		0.615	
LoQ	1.290		0.276		0.795		0.800		2.082		0.626		1.502		1.502		1.502	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 49: Silver concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	0.037	0.008	0.062	<LoD	0.096	<LoD	0.045	<LoD	**0.505**	0.031	**0.112**	0.011	0.050	<LoD	0.050	<LoD	0.050	<LoD
-3	0.020	0.005	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.050	<LoD	0.050	<LoD	0.050	<LoD
-2	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.050	<LoD	0.050	<LoD	0.050	<LoD
-1	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.046	0.009	0.050	<LoD	0.050	<LoD	0.050	<LoD
0	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.050	<LoD	0.050	<LoD	0.050	<LoD
1	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.050	<LoD	0.050	<LoD	0.050	<LoD
2	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	**0.397**	0.008	**0.078**	0.005	0.050	<LoD	0.050	<LoD	0.050	<LoD
3	0.016	0.003	0.062	<LoD	0.096	<LoD	0.045	<LoD	**0.336**	0.006	**0.132**	0.006	0.050	<LoD	0.050	<LoD	0.050	<LoD
4	0.008	<LoD	**1.161**	0.040	0.096	<LoD	0.045	<LoD	**0.589**	0.037	**0.286**	0.012	0.050	<LoD	0.050	<LoD	0.050	<LoD
5	0.020	0.042	0.062	<LoD	0.096	<LoD	0.115	0.002	**0.790**	0.034	**0.384**	0.019	0.050	<LoD	0.050	<LoD	0.050	<LoD
6	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	**0.079**	0.004	0.050	<LoD	0.050	<LoD	0.050	<LoD
7	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.093	0.012	0.052	<LoD	**0.094**	0.007	0.050	<LoD	0.050	<LoD	0.050	<LoD
8	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	**0.134**	0.012	**0.104**	0.011	**no sample***		0.050	<LoD	0.050	<LoD
9	0.017	0.003	0.062	<LoD	0.096	<LoD	**0.181**	0.013	**0.152**	0.011	**0.139**	0.002	0.050	<LoD	0.050	<LoD	0.050	<LoD
10	0.016	0.004	0.062	<LoD	0.096	<LoD	0.045	<LoD	**0.166**	0.008	**0.169**	0.007	0.050	<LoD	0.050	<LoD	0.050	<LoD
11	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	**0.198**	0.019	**0.193**	0.010	0.050	<LoD	0.050	<LoD	0.050	<LoD
12	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	**0.239**	0.006	**0.223**	0.016	0.050	<LoD	0.050	<LoD	0.050	<LoD
13	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.118	0.017	0.021	<LoD	0.050	<LoD	0.050	<LoD	0.050	<LoD
14	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	0.021	<LoD	0.050	<LoD	0.050	<LoD	0.050	<LoD
15	0.008	<LoD	0.062	<LoD	0.096	<LoD	0.045	<LoD	0.052	<LoD	**0.081**	0.004	0.050	<LoD	0.050	<LoD	0.050	<LoD
LoD	0.015		0.124		0.192		0.090		0.105		0.043		0.100		0.100		0.100	
LoQ	0.038		0.168		0.257		0.180		0.132		0.067		0.134		0.134		0.134	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 50: Tin concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	0.055	<LoD	0.134	0.088	0.057	<LoD	**0.336**	0.091	**0.172**	0.103	0.143	0.097	0.103	0.068	**0.362**	0.077	0.090	0.069
-3	0.055	<LoD	0.142	0.062	0.129	0.090	**1.142**	0.269	0.028	<LoD	0.039	<LoD	0.038	<LoD	0.133	0.057	0.099	0.048
-2	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.376**	0.083	0.120	0.091	0.039	<LoD	0.139	0.069	**0.332**	0.151	0.129	0.084
-1	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.345**	0.065	**0.164**	0.097	0.039	<LoD	0.038	<LoD	0.038	<LoD	0.113	0.064
0	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.375**	0.067	0.095	0.056	0.039	<LoD	0.038	<LoD	**0.222**	0.077	0.038	<LoD
1	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.405**	0.079	**0.141**	0.050	**0.263**	0.083	0.038	<LoD	0.099	0.053	0.038	<LoD
2	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.538**	0.082	**0.246**	0.095	0.204	0.107	0.093	0.069	0.038	<LoD	0.099	0.019
3	**0.325**	0.041	0.178	0.351	0.057	<LoD	**0.344**	0.087	**0.247**	0.068	0.121	0.058	0.119	0.030	0.113	0.054	0.038	<LoD
4	0.055	<LoD	0.206	0.080	0.057	<LoD	**0.378**	0.153	**0.190**	0.083	**0.236**	0.188	0.149	0.058	0.136	0.043	0.038	<LoD
5	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.410**	0.066	0.137	0.050	0.171	0.098	0.123	0.047	0.096	0.075	0.096	0.092
6	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.460**	0.156	0.028	<LoD	0.104	0.097	0.113	0.078	**0.348**	0.136	0.038	<LoD
7	0.055	<LoD	0.235	0.084	0.057	<LoD	**0.592**	0.141	0.028	<LoD	**0.280**	0.153	0.129	0.071	**0.680**	0.188	0.038	<LoD
8	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.397**	0.112	0.028	<LoD	0.039	<LoD	**no sample***		0.116	0.082	0.099	0.067
9	0.055	<LoD	0.210	0.069	0.057	<LoD	**0.446**	0.148	0.028	<LoD	0.109	0.070	**0.415**	0.182	**0.365**	0.076	**0.298**	0.133
10	0.055	<LoD	0.219	0.093	**0.826**	0.091	**0.681**	0.111	0.028	<LoD	0.039	<LoD	**0.222**	0.069	0.143	0.025	**0.305**	0.142
11	0.055	<LoD	0.162	0.057	0.057	<LoD	**0.413**	0.094	**4.432**	0.595	0.039	<LoD	**0.312**	0.074	**0.222**	0.119	**0.378**	0.067
12	0.172	0.079	0.178	0.079	0.057	<LoD	**0.478**	0.170	0.028	<LoD	0.096	0.029	**0.401**	0.094	0.136	0.036	0.103	0.055
13	0.055	<LoD	0.061	<LoD	0.126	0.091	**0.558**	0.179	0.028	<LoD	0.039	<LoD	**0.421**	0.044	0.126	0.032	0.196	0.059
14	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.604**	0.183	**0.242**	0.099	0.093	0.092	0.038	<LoD	0.038	<LoD	0.113	0.034
15	0.055	<LoD	0.061	<LoD	0.057	<LoD	**0.566**	0.091	**0.283**	0.083	**0.233**	0.143	0.083	0.064	0.182	0.101	**0.219**	0.032
LoD	0.110		0.122		0.113		0.101		0.056		0.078		0.077		0.077		0.077	
LoQ	0.309		0.294		0.190		0.220		0.141		0.210		0.215		0.215		0.215	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 51: Titanium concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**1.180**	0.105	**0.554**	0.046	0.143	0.033	0.231	<LoD	**0.944**	0.070	0.305	0.086	0.137	<LoD	**1.291**	0.074	0.137	<LoD
-3	**1.271**	0.104	**0.552**	0.056	0.152	0.054	0.231	<LoD	**0.555**	0.051	0.294	0.054	0.137	<LoD	0.137	<LoD	0.137	<LoD
-2	**0.830**	0.039	0.097	0.023	0.109	0.036	0.231	<LoD	**1.157**	0.069	0.220	0.046	0.137	<LoD	**1.342**	0.145	0.137	<LoD
-1	**1.166**	0.095	0.177	0.013	0.184	0.019	0.231	<LoD	**1.030**	0.076	0.259	0.042	0.137	<LoD	0.137	<LoD	0.137	<LoD
0	**1.310**	0.093	**0.518**	0.012	**0.211**	0.019	0.231	<LoD	**1.901**	0.151	**1.209**	0.097	0.137	<LoD	**1.639**	0.212	0.137	<LoD
1	**0.762**	0.051	**0.363**	0.036	**0.404**	0.049	0.679	0.087	**4.159**	0.278	**7.193**	0.504	0.137	<LoD	0.137	<LoD	0.314	0.056
2	**0.935**	0.081	**1.641**	0.119	**0.847**	0.048	**1.432**	0.116	**7.381**	0.256	**6.316**	0.546	**0.843**	0.062	**0.758**	0.054	**1.286**	0.057
3	**0.688**	0.059	**1.590**	0.080	**1.483**	0.115	**1.734**	0.184	**6.729**	0.411	**8.955**	0.308	**1.645**	0.148	**2.502**	0.139	**2.480**	0.163
4	**1.822**	0.356	**2.186**	0.088	**2.078**	0.176	**3.621**	0.230	**9.682**	0.709	**16.881**	0.796	**3.752**	0.147	**6.004**	0.507	**5.152**	0.144
5	**3.700**	1.746	**3.716**	0.116	**3.139**	0.090	**5.178**	0.294	**9.219**	0.742	**18.946**	0.641	**1.004**	0.089	**5.618**	0.406	**4.494**	0.285
6	**1.547**	0.062	**5.459**	0.276	**3.722**	0.251	**7.656**	0.685	**2.169**	0.058	**3.795**	0.237	**2.474**	0.177	**14.051**	0.120	**1.299**	0.118
7	**1.414**	0.091	**10.268**	0.239	**4.951**	0.350	**12.106**	0.679	**1.762**	0.105	**3.838**	0.381	**2.192**	0.104	**21.702**	1.996	**1.833**	0.165
8	**1.530**	0.124	**2.108**	0.147	**1.090**	0.052	**4.244**	0.085	**2.722**	0.193	**4.343**	0.252	**no sample***		**4.309**	0.204	**3.001**	0.177
9	**2.597**	0.148	**5.548**	0.198	**1.532**	0.135	**5.595**	0.225	**3.006**	0.154	**5.077**	0.298	**6.696**	0.557	**17.532**	1.549	**3.550**	0.238
10	**2.767**	0.080	**10.809**	0.603	**1.547**	0.127	**4.597**	0.414	**2.630**	0.132	**5.340**	0.330	**5.156**	0.454	**11.270**	0.441	**7.163**	0.156
11	**4.070**	0.243	**10.370**	0.141	**1.709**	0.122	**5.714**	0.304	**3.303**	0.182	**5.732**	0.221	**6.928**	0.251	**15.835**	0.422	**12.221**	0.498
12	**3.118**	0.155	**1.826**	0.146	**2.157**	0.117	**5.985**	0.196	**3.188**	0.171	**8.351**	0.187	**8.464**	0.304	**9.261**	0.552	**3.593**	0.128
13	**3.056**	0.112	**2.090**	0.097	**2.186**	0.099	**9.754**	0.624	**5.955**	0.308	**7.878**	0.485	**9.628**	0.431	**13.263**	0.402	**3.810**	0.244
14	**2.899**	0.127	**2.687**	0.110	**3.801**	0.311	**15.297**	0.588	**10.306**	0.285	**15.004**	0.705	**2.207**	0.090	**7.607**	0.590	**8.365**	0.263
15	**3.139**	0.087	**4.160**	0.087	**5.469**	0.194	**14.049**	0.534	**9.153**	0.256	**20.013**	1.589	**3.099**	0.148	**17.143**	0.739	**11.366**	0.595
LoD	0.084		0.080		0.081		0.462		0.152		0.211		0.273		0.273		0.273	
LoQ	0.230		0.221		0.185		0.985		0.432		0.421		0.466		0.466		0.466	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 52: Vanadium concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**1.011**	0.019	**0.655**	0.012	**0.337**	0.013	**0.426**	0.021	0.063	0.004	**0.194**	0.009	**0.284**	0.016	**1.184**	0.037	**0.930**	0.073
-3	**0.919**	0.033	**0.590**	0.021	**0.344**	0.027	**0.476**	0.018	**0.069**	0.003	**0.290**	0.008	**0.475**	0.034	**1.198**	0.075	**1.160**	0.063
-2	**0.593**	0.024	**0.519**	0.029	**0.275**	0.013	**0.501**	0.038	**0.120**	0.005	**0.294**	0.005	**0.642**	0.011	**1.272**	0.052	**0.987**	0.096
-1	**0.478**	0.008	**0.470**	0.022	**0.298**	0.013	**0.520**	0.028	**0.170**	0.010	**0.358**	0.016	**0.579**	0.037	**0.934**	0.055	**0.953**	0.049
0	**0.289**	0.014	**1.692**	0.064	**0.610**	0.035	**0.404**	0.027	**0.684**	0.018	**1.969**	0.069	**0.518**	0.015	**0.744**	0.033	**0.381**	0.030
1	0.128	0.004	**1.527**	0.044	**1.006**	0.056	**1.144**	0.091	**3.600**	0.078	**5.997**	0.271	**1.137**	0.057	**0.826**	0.048	**0.547**	0.033
2	**0.293**	0.007	**2.521**	0.093	**1.734**	0.086	**2.333**	0.082	**6.061**	0.176	**7.790**	0.469	**2.137**	0.134	**1.934**	0.077	**1.826**	0.080
3	**0.370**	0.020	**3.839**	0.144	**2.181**	0.071	**2.581**	0.176	**5.394**	0.122	**7.154**	0.278	**2.751**	0.170	**4.533**	0.206	**2.825**	0.066
4	0.039	<LoD	**5.668**	0.240	**2.716**	0.129	**3.246**	0.226	**7.172**	0.277	**10.037**	0.094	**5.024**	0.150	**7.883**	0.511	**4.902**	0.181
5	**0.388**	0.151	**6.536**	0.297	**3.502**	0.043	**4.370**	0.189	**6.614**	0.316	**9.826**	0.373	**4.663**	0.436	**8.376**	0.402	**5.151**	0.274
6	**0.819**	0.037	**8.750**	0.453	**4.111**	0.217	**6.084**	0.209	**3.437**	0.105	**5.782**	0.363	**7.680**	0.394	**12.679**	0.161	**6.118**	0.200
7	**0.827**	0.028	**11.316**	0.401	**5.561**	0.072	**8.298**	0.401	**4.470**	0.128	**4.913**	0.255	**6.971**	0.254	**14.580**	1.055	**7.250**	0.401
8	**1.471**	0.056	**7.688**	0.496	**3.759**	0.189	**7.072**	0.128	**4.021**	0.110	**4.605**	0.142	**no sample***		**2.972**	0.132	**6.442**	0.330
9	**2.354**	0.072	**8.624**	0.112	**4.916**	0.221	**7.894**	0.123	**3.815**	0.151	**4.981**	0.184	**10.544**	0.607	**10.177**	0.739	**6.228**	0.225
10	**3.106**	0.082	**9.894**	0.316	**4.931**	0.138	**6.925**	0.328	**3.759**	0.134	**5.159**	0.261	**7.470**	0.448	**6.360**	0.263	**7.520**	0.185
11	**4.210**	0.240	**9.203**	0.136	**4.905**	0.145	**7.249**	0.344	**3.990**	0.033	**5.412**	0.250	**7.529**	0.412	**8.737**	0.170	**8.624**	0.322
12	**4.948**	0.198	**7.526**	0.252	**4.548**	0.210	**6.750**	0.401	**3.950**	0.081	**6.205**	0.242	**6.938**	0.347	**5.880**	0.198	**5.906**	0.204
13	**5.274**	0.177	**6.260**	0.131	**4.304**	0.155	**7.732**	0.389	**4.734**	0.189	**5.755**	0.299	**6.822**	0.269	**7.963**	0.304	**5.894**	0.310
14	**4.356**	0.120	**4.974**	0.115	**4.720**	0.105	**8.125**	0.359	**6.212**	0.158	**7.742**	0.196	**2.681**	0.058	**4.453**	0.309	**5.876**	0.158
15	**3.958**	0.153	**4.815**	0.115	**6.648**	0.105	**7.895**	0.279	**5.862**	0.153	**9.311**	0.576	**3.229**	0.113	**9.394**	0.261	**6.471**	0.398
LoD	0.079		0.146		0.065		0.051		0.024		0.035		0.030		0.030		0.030	
LoQ	0.218		0.410		0.176		0.146		0.068		0.098		0.070		0.070		0.070	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 53: Zink concentrations across the SWI of the sediment cores of sampling site 2. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**21.60**	1.07	**29.38**	0.99	**45.81**	0.66	**3.42**	0.32	**5.14**	0.45	**5.64**	0.50	**8.65**	0.21	**9.37**	0.88	**4.29**	0.34
-3	**27.18**	1.48	**41.84**	1.76	**37.91**	0.69	**7.39**	0.35	**8.90**	0.51	**5.74**	0.39	**4.25**	0.15	**11.52**	0.60	**6.22**	0.28
-2	**17.32**	0.47	**27.29**	0.63	**13.12**	0.73	**24.01**	1.07	**16.19**	1.00	**8.41**	0.29	**5.10**	0.36	**21.76**	1.17	**6.28**	0.61
-1	**33.65**	2.70	**24.33**	0.77	**15.47**	0.91	**27.83**	0.90	**17.57**	1.00	**19.14**	0.62	**16.36**	0.32	**15.35**	1.00	**13.77**	0.73
0	**52.12**	2.87	**8.20**	0.54	**7.93**	0.63	**28.24**	0.80	**13.13**	0.59	**25.86**	0.80	**7.90**	0.35	**31.04**	1.28	**17.23**	0.72
1	**8.65**	0.32	**3.33**	0.27	**5.08**	0.49	**16.79**	0.55	**9.85**	0.27	**24.42**	1.14	**9.72**	0.86	**21.53**	0.90	**38.61**	2.05
2	**13.38**	0.51	**12.77**	0.28	**11.10**	0.43	**8.98**	0.77	**10.32**	0.95	**5.70**	0.44	**17.38**	0.80	**10.89**	0.63	**25.27**	1.34
3	**47.58**	1.97	**24.20**	0.74	**10.88**	1.04	**11.03**	0.39	**12.98**	0.79	**5.87**	0.36	**10.38**	0.29	**13.38**	0.85	**12.04**	0.51
4	**20.75**	2.64	**37.66**	1.25	**6.67**	0.21	**6.63**	0.47	**8.93**	0.67	**9.88**	0.98	**8.16**	0.34	**10.15**	0.57	**12.33**	0.66
5	**59.34**	14.00	**14.89**	0.44	**10.18**	0.20	**13.51**	0.62	**5.79**	0.44	**7.10**	0.40	**7.43**	0.33	**10.04**	0.93	**7.40**	0.60
6	**6.56**	0.17	**7.86**	0.18	**11.67**	0.24	**8.02**	0.39	**5.01**	0.21	**5.40**	0.31	**3.51**	0.24	**13.55**	0.86	**14.88**	0.82
7	**6.82**	0.32	**15.57**	0.35	**11.13**	0.99	**27.29**	0.57	**4.11**	0.32	**6.41**	0.44	**4.01**	0.34	**15.80**	0.99	**5.74**	0.35
8	**8.84**	0.40	**7.00**	0.52	**12.89**	0.45	**9.33**	0.34	**4.26**	0.25	**9.38**	0.70	**no sample***		**13.60**	0.52	**15.53**	0.64
9	**12.28**	0.31	**21.98**	0.34	**16.50**	0.27	**10.65**	0.55	**6.49**	0.37	**8.79**	0.20	**6.13**	0.32	**12.56**	0.45	**15.78**	0.72
10	**5.78**	0.14	**29.81**	0.35	**14.74**	1.09	**10.98**	0.59	**6.68**	0.20	**7.75**	0.29	**6.49**	0.32	**9.26**	0.47	**13.68**	0.23
11	**9.72**	0.55	**16.75**	0.49	**16.02**	0.72	**18.57**	0.81	**12.39**	0.51	**4.88**	0.14	**5.27**	0.36	**15.32**	0.85	**14.06**	0.51
12	**19.31**	0.44	**35.37**	1.25	**12.44**	0.57	**13.59**	0.54	**4.74**	0.34	**4.97**	0.22	**12.40**	0.30	**7.77**	0.21	**37.99**	1.94
13	**19.95**	0.82	**14.10**	0.18	**18.83**	1.00	**10.39**	0.28	**5.17**	0.35	**11.71**	0.44	**6.80**	0.39	**46.80**	1.98	**33.50**	1.71
14	**34.82**	1.27	**19.38**	0.37	**14.49**	0.72	**22.02**	0.76	**10.23**	0.31	**11.70**	0.52	**3.88**	0.29	**5.79**	0.46	**11.76**	0.62
15	**5.87**	0.22	**23.18**	0.60	0.10	<LoD	**29.28**	1.01	**9.46**	0.36	**9.12**	0.24	**5.26**	0.15	**23.73**	1.06	**16.60**	0.27
LoD	0.16		0.24		0.21		0.12		0.09		0.09		0.09		0.09		0.09	
LoQ	0.45		0.67		0.56		0.31		0.23		0.24		0.24		0.24		0.24	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 54: Phosphate concentrations across the SWI of the sediment cores of sampling site 2. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
4	0.01	0.01	0.05	0.05	0.10	0.41	0.05	0.05	0.38
3	0.14	0.06	0.10	0.10	0.05	0.11	0.25	0.25	0.53
2	0.01	0.04	0.35	0.15	0.25	0.25	0.60	0.60	0.73
1	0.09	0.19	0.45	0.00	0.40	0.40	0.10	0.15	0.43
0	0.14	0.29	0.55	0.40	0.15	0.15	0.05	0.25	0.05
1	0.09	0.31	1.90	1.40	3.15	1.40	0.30	0.30	0.95
2	0.01	4.45	1.05	1.40	3.40	1.40	0.20	0.20	3.35
3	0.01	5.65	2.05	5.10	3.65	3.65	2.75	2.75	5.90
4	missing**	8.15	4.10	4.05	5.25	4.05	6.45	4.45	11.70
5	missing**	3.00	3.90	4.15	2.40	2.40	6.90	6.90	11.75
6	0.14	5.60	5.30	2.90	2.35	0.80	4.75	4.75	15.80
7	0.24	5.10	7.15	2.35	2.55	2.35	6.30	6.30	22.10
8	1.04	4.15	5.85	2.40	3.75	2.40	missing*	10.75	21.00
9	1.94	7.80	6.60	3.65	2.30	2.30	10.75	4.25	27.55
10	2.64	8.95	7.65	2.80	3.45	2.80	10.70	10.70	16.35
11	3.74	5.05	7.60	4.10	2.65	2.65	12.74	12.74	36.50
12	2.24	2.35	8.85	6.90	7.30	3.45	8.29	7.60	17.95
13	2.94	7.90	7.45	7.60	13.55	7.60	8.39	8.39	24.10
14	missing**	7.60	8.80	7.20	7.30	7.20	19.89	13.90	19.89
15	missing**	6.30	14.80	9.15	22.35	5.95	17.19	17.19	21.50
*** insufficient sample volume**									
**** handling error**									

Table A3. 55: Sulfate concentrations across the SWI of the sediment cores of sampling site 2. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
-4	924.15	519.35	439.55	795.80	676.95	311.90	242.95	377.85	616.60
-3	420.15	299.55	388.50	881.75	246.00	419.80	368.30	441.60	477.20
-2	914.65	705.30	561.75	713.70	340.10	600.50	1087.20	240.45	434.75
-1	300.90	301.65	431.25	895.60	276.95	444.50	917.50	684.60	781.35
0	344.75	806.90	419.75	833.50	336.15	275.00	841.30	354.45	422.70
1	329.00	361.10	550.55	806.05	179.80	330.80	920.90	296.00	363.60
2	443.05	880.70	427.95	729.55	198.50	387.90	813.05	562.60	425.90
3	428.70	844.30	558.55	735.35	462.75	302.45	721.80	389.20	459.90
4	missing**	796.45	503.40	740.10	282.60	326.75	627.60	246.30	450.30
5	missing**	345.40	306.35	752.70	207.05	177.45	582.85	376.00	344.70
6	944.50	346.40	341.65	176.75	236.70	233.20	580.15	205.50	415.00
7	266.00	249.95	352.30	443.30	238.35	193.50	633.70	227.35	470.75
8	257.60	261.50	587.35	338.85	194.25	233.90	missing*	277.00	448.65
9	273.10	238.70	418.65	300.20	270.50	137.55	565.85	304.90	154.60
10	245.05	271.00	468.15	559.25	141.55	182.90	524.40	241.90	256.95
11	256.45	135.85	410.60	212.45	151.25	118.45	477.20	214.20	238.35
12	326.10	180.35	394.35	171.10	228.75	197.35	131.70	249.80	245.25
13	387.25	441.15	255.90	449.05	151.60	302.00	306.15	105.10	189.00
14	missing**	383.20	256.85	280.15	114.45	102.90	360.90	113.35	215.50
15	missing**	198.20	284.40	154.20	110.50	187.20	386.05	181.75	164.75
*** insufficient sample volume**									
**** handling error**									

Table A3. 56: Ammonium concentrations across the SWI of the sediment cores of sampling site 2. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
-4	0.82	3.09	7.22	1.82	1.27	0.84	3.36	2.63	2.83
-3	0.29	4.36	6.00	1.51	3.15	0.65	3.67	2.71	2.13
-2	0.36	3.95	5.88	2.11	3.08	1.06	2.11	4.08	3.99
-1	3.50	5.04	5.77	2.46	2.76	0.88	1.57	3.18	1.90
0	3.37	6.45	7.50	3.48	4.66	1.05	1.72	3.34	1.47
1	4.62	8.47	7.33	4.85	6.63	3.68	4.21	6.83	5.56
2	5.85	12.75	8.10	6.26	7.39	5.32	7.69	8.31	8.76
3	5.72	13.97	9.89	7.47	9.55	7.21	10.88	11.79	9.39
4		15.22	10.15	7.75	10.54	8.26	13.88	13.56	12.12
5		12.81	12.05	7.29	10.21	9.77	15.36	14.37	13.13
6	7.27	13.55	12.87	6.45	11.44	9.97	17.88	17.92	14.76
7	7.15	15.28	13.49	7.76	11.44	11.29	18.18	21.56	16.31
8	7.37	16.12	9.99	8.68	13.23	12.19	missing*	17.59	17.93
9	8.59	15.28	11.81	10.24	11.86	13.62	21.37	18.21	19.46
10	9.16	23.94	13.26	13.10	14.24	14.69	22.61	21.32	19.64
11	9.47	15.72	14.03	13.11	19.85	15.78	24.15	20.26	18.52
12	9.36	16.22	13.78	12.20	16.42	17.20	16.88	22.36	18.40
13	10.23	23.50	16.96	18.76	17.82	10.78	28.01	19.53	21.78
14		24.01	17.77	15.63	21.52	19.94	24.42	26.86	22.01
15		20.83	19.22	15.64	19.99	20.90	25.23	25.09	24.06
*** insufficient sample volume**									
**** handling error**									

AIII.IX.II.III Concentrations in suction-based pore water samples of sampling site 3

Table A3. 57: Carbon concentrations across the SWI of the sediment cores of sampling site 3 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in mg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	180	4	**143**	3	61	5	**67**	1	**46**	1	**18**	0	**203**	6	**382**	20	**224**	24
-3	**380**	4	**119**	5	51	6	**69**	2	**28**	1	**16**	0	**283**	17	**385**	29	**223**	12
-2	**488**	4	**89**	3	61	8	**21**	1	**21**	1	**17**	0	**334**	15	**499**	15	**237**	21
-1	**353**	4	**90**	2	46	6	**65**	2	**16**	1	**18**	1	**330**	11	**488**	18	**196**	15
0	**586**	4	**80**	2	71	5	**50**	2	**44**	2	**23**	1	**327**	20	**414**	17	**205**	15
1	**559**	2	**24**	1	70	8	**81**	1	**22**	1	**22**	1	**460**	18	**91**	2	**286**	5
2	**364**	3	**101**	3	74	4	**58**	2	**22**	1	**25**	1	**632**	33	**477**	22	**273**	13
3	**347**	5	**92**	1	82	5	**72**	2	**31**	1	**27**	1	**660**	23	**366**	13	**280**	15
4	**282**	4	**44**	2	76	6	**74**	1	**30**	1	**29**	1	**658**	23	**256**	8	**284**	8
5	**393**	2	**129**	2	107	9	**70**	2	**28**	1	**31**	1	**687**	22	**153**	5	**319**	22
6	**344**	2	**117**	3	106	3	**64**	2	**28**	1	**30**	1	**705**	16	**121**	6	**292**	20
7	**451**	2	**111**	3	72	4	**59**	2	**26**	0	**29**	1	**616**	28	**87**	3	**304**	4
8	**428**	1	**124**	2	**no sample***		**53**	2	**no sample***		**32**	1	**408**	17	**74**	0	**237**	8
9	**409**	3	**73**	1	26	7	**56**	1	**29**	1	**33**	1	**368**	7	**63**	1	**221**	10
10	**420**	2	**112**	3	33	3	**54**	1	**29**	1	**35**	1	**384**	13	**63**	4	**212**	9
11	**518**	2	**125**	3	14	6	**47**	3	**30**	1	**35**	1	**361**	13	**61**	4	**197**	8
12	**437**	3	**124**	2	10	7	**38**	2	**no sample***		**42**	1	**270**	8	**48**	2	**221**	18
13	**515**	3	**44**	1	10	50	**30**	2	**no sample***		**47**	1	**361**	8	**50**	1	**186**	8
14	**485**	6	**no sample***		15	27	**16**	19	**no sample***		**50**	2	**294**	5	**51**	2	**202**	20
15	**449**	4	**no sample***		10	9	**no sample***		**no sample***		**no sample***		**192**	10	**56**	3	**128**	2
LoD	79.42		8.93		79.42		2.15		4.55		3.85		15.25		15.25		2.96	
LoQ	204.11		22.33		204.11		5.79		11.46		10.14		39.21		39.21		7.99	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 58: Phosphorous concentrations across the SWI of the sediment cores of sampling site 3 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**454**	14	**559**	25	**1024**	7	**929**	28	**136**	10	**729**	44	**457**	39	**1326**	78	**1630**	57
-3	**457**	9	**347**	6	**840**	30	**988**	35	**116**	6	**748**	33	**635**	26	**1564**	71	**1591**	108
-2	**475**	11	**549**	15	**1037**	66	**828**	30	**88**	5	**774**	31	**797**	46	**1638**	69	**1559**	60
-1	**400**	9	**461**	10	**1010**	63	**861**	19	**74**	4	**781**	52	**667**	47	**1596**	103	**1313**	34
0	**1505**	87	**415**	17	**1670**	99	**638**	29	**75**	4	**1891**	74	**695**	40	**1220**	48	**1412**	44
1	**3292**	100	**1374**	84	**2933**	229	**1208**	38	**178**	10	**1836**	99	**947**	66	**1967**	65	**3832**	124
2	**4345**	181	**2364**	106	**6888**	634	**1104**	76	**138**	13	**1960**	48	**2351**	97	**4118**	181	**5429**	342
3	**4510**	118	**4581**	136	**11611**	792	**2317**	108	**246**	16	**3179**	47	**4764**	395	**4326**	224	**8299**	306
4	**5352**	368	**7051**	176	**13490**	1295	**2856**	147	**222**	14	**3171**	120	**6337**	427	**4649**	209	**9629**	521
5	**6117**	175	**8726**	280	**10035**	923	**3486**	85	**168**	12	**3517**	200	**7124**	313	**4055**	221	**9023**	352
6	**7534**	297	**8504**	455	**15130**	443	**3428**	94	**95**	7	**4500**	287	**7438**	299	**4802**	151	**8858**	664
7	**7653**	150	**7839**	388	**10206**	571	**4138**	81	**106**	6	**5344**	229	**6910**	347	**5751**	253	**10682**	499
8	**8370**	269	**6123**	280	**no sample***		**5675**	178	**no sample***		**6594**	311	**5334**	139	**3990**	246	**6725**	338
9	**7313**	346	**7732**	116	**6751**	157	**6584**	273	**266**	17	**6743**	174	**4326**	210	**4298**	135	**7952**	416
10	**7996**	559	**7884**	121	**8226**	417	**7668**	448	**417**	21	**6736**	273	**4430**	181	**5533**	350	**8139**	348
11	**9534**	614	**9193**	319	**8428**	237	**7618**	108	**616**	37	**6722**	248	**5912**	216	**6699**	401	**9310**	540
12	**6144**	218	**8948**	283	**2473**	140	**5829**	151	**no sample***		**6871**	156	**5496**	127	**5461**	141	**8733**	490
13	**12886**	658	**10887**	319	**3112**	168	**5894**	427	**no sample***		**9478**	482	**6654**	464	**5296**	426	**8873**	584
14	**8104**	450	**no sample***		**4430**	274	**4254**	3836	**no sample***		**12969**	192	**6521**	431	**7651**	298	**8914**	320
15	**9235**	455	**no sample***		**6321**	210	**no sample***		**no sample***		**no sample***		**7055**	267	**5938**	332	**8216**	339
LoD	5.11		3.74		5.11		4.99		1.45		5.16		0.79		0.79		0.19	
LoQ	13.38		10.34		13.38		14.50		3.91		14.43		2.15		2.15		0.48	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 59: Sulfur concentrations across the SWI of the sediment cores of sampling site 3 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in mg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**327**	13	**553**	33	**471**	14	**634**	18	**586**	23	**376**	13	**140**	10	**331**	25	**413**	21
-3	**365**	11	**363**	9	**379**	26	**653**	25	**500**	27	**358**	10	**199**	7	**342**	17	**395**	16
-2	**364**	11	**574**	19	**475**	43	**517**	19	**451**	21	**347**	5	**255**	15	**354**	9	**374**	12
-1	**264**	11	**494**	16	**476**	39	**585**	18	**413**	22	**347**	19	**197**	10	**341**	18	**329**	11
0	**403**	18	**296**	13	**488**	35	**433**	23	**348**	20	**330**	5	**209**	16	**332**	14	**361**	27
1	**336**	10	**311**	13	**448**	32	**613**	22	**332**	15	**318**	16	**239**	14	**326**	18	**500**	43
2	**261**	8	**303**	12	**384**	33	**478**	37	**329**	17	**311**	6	**367**	14	**297**	16	**490**	20
3	**239**	8	**389**	13	**334**	21	**360**	13	**319**	13	**300**	10	**345**	21	**288**	16	**450**	30
4	**205**	11	**416**	8	**263**	24	**302**	14	**335**	11	**299**	8	**331**	10	**276**	14	**415**	20
5	**171**	6	**408**	11	**141**	13	**272**	6	**348**	16	**289**	12	**327**	23	**252**	9	**440**	20
6	**155**	6	**355**	14	**191**	7	**264**	8	**337**	18	**281**	12	**321**	13	**279**	10	**454**	22
7	**130**	6	**324**	18	**114**	6	**228**	6	**331**	11	**283**	10	**308**	9	**284**	10	**439**	10
8	**121**	4	**303**	8	**no sample***		**260**	8	**no sample***		**126**	6	**294**	10	**290**	10	**337**	4
9	**124**	5	**293**	9	**120**	2	**241**	8	**320**	14	**130**	4	**297**	23	**295**	9	**330**	37
10	**116**	5	**275**	2	**96**	5	**235**	12	**310**	13	**133**	5	**291**	10	**301**	14	**308**	21
11	**104**	7	**270**	9	**75**	2	**226**	3	**292**	12	**133**	2	**297**	17	**300**	19	**305**	16
12	**90**	3	**263**	11	**50**	2	**204**	7	**no sample***		**219**	4	**240**	10	**299**	10	**278**	11
13	**98**	7	**264**	7	**48**	2	**159**	7	**no sample***		**196**	8	**273**	19	**296**	15	**271**	21
14	**93**	5	**no sample***		**49**	3	**72**	70	**no sample***		**192**	2	**251**	7	**290**	9	**292**	24
15	**87**	4	**no sample***		**44**	2	**no sample***		**no sample***		**no sample***		**264**	4	**285**	5	**267**	10
LoD	0.20		0.28		0.20		0.51		0.71		0.27		1.02		1.02		1.06	
LoQ	0.53		0.74		0.53		1.32		2.01		0.76		2.78		2.78		2.87	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 60: Manganese concentrations across the SWI of the sediment cores of sampling site 3 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**154**	3	**104**	6	**104**	3	**92**	3	**410**	6	**349**	13	**8**	0	**735**	6	**36**	1
-3	**187**	7	**59**	2	**93**	3	**90**	4	**530**	6	**419**	13	**12**	1	**1118**	33	**47**	2
-2	**202**	2	**68**	3	**58**	2	**69**	3	**53**	2	**757**	19	**22**	0	**1548**	16	**68**	2
-1	**291**	8	**81**	3	**49**	1	**72**	2	**49**	2	**770**	27	**31**	1	**1966**	32	**316**	5
0	**2256**	53	**427**	10	**727**	29	**294**	21	**415**	5	**1356**	29	**62**	1	**923**	25	**59**	1
1	**4858**	148	**1166**	30	**1709**	35	**986**	48	**1427**	18	**1123**	59	**371**	2	**988**	20	**1689**	26
2	**3393**	54	**1439**	40	**2355**	99	**822**	49	**1693**	15	**998**	30	**1108**	22	**1309**	22	**2239**	41
3	**2014**	65	**1497**	43	**2429**	167	**1212**	65	**2008**	14	**983**	25	**1367**	32	**1388**	29	**2582**	30
4	**1700**	68	**1536**	52	**1712**	92	**1136**	19	**1367**	12	**962**	29	**1502**	14	**1511**	29	**2667**	38
5	**1386**	32	**1436**	78	**716**	21	**1067**	30	**875**	8	**940**	16	**1431**	25	**1422**	27	**2545**	51
6	**1308**	57	**1113**	40	**1260**	44	**1058**	27	**898**	9	**994**	26	**1495**	31	**1699**	39	**2441**	38
7	**1059**	19	**810**	13	**698**	13	**896**	24	**1210**	14	**1091**	10	**1457**	26	**1780**	42	**2378**	19
8	**925**	42	**768**	21	**no sample***		**1182**	28	**no sample***		**398**	7	**1242**	31	**1614**	25	**1602**	35
9	**783**	27	**789**	16	**500**	9	**1110**	36	**1247**	8	**416**	10	**928**	26	**1610**	51	**1518**	30
10	**820**	27	**733**	20	**424**	16	**1061**	47	**1241**	15	**417**	10	**875**	11	**1561**	23	**1431**	13
11	**804**	14	**727**	20	**511**	20	**1042**	38	**1237**	20	**429**	12	**1035**	22	**1577**	35	**1379**	28
12	**399**	8	**596**	28	**120**	2	**701**	35	**no sample***		**525**	15	**825**	10	**1587**	20	**1248**	28
13	**626**	20	**661**	22	**114**	5	**546**	52	**no sample***		**582**	55	**996**	9	**1683**	35	**1223**	29
14	**404**	12	**no sample***		**122**	4	**18**	11	**no sample***		**86**	9	**900**	9	**1450**	18	**1231**	22
15	**477**	14	**no sample***		**172**	6	**no sample***		**no sample***		**no sample***		**924**	10	**1612**	28	**1149**	14
LoD	1.31		1.98		1.31		3.24		2.93		1.05		0.81		0.81		2.41	
LoQ	3.61		5.62		3.61		8.36		8.26		2.82		2.17		2.17		6.22	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 61: Iron concentrations across the SWI of the sediment cores of sampling site 3 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**39**	1	**15**	1	**74**	2	**40**	0	**60**	1	**42**	2	**26**	0	**58**	1	**139**	4
-3	**14**	1	**8**	0	**59**	6	**46**	0	**48**	1	**34**	1	**30**	1	**85**	2	**131**	3
-2	**10**	0	**10**	0	**63**	2	**42**	0	**40**	1	**63**	2	**39**	1	**103**	1	**129**	4
-1	**11**	0	**40**	2	**64**	2	**38**	1	**36**	1	**63**	2	**32**	1	**135**	2	**306**	8
0	**1194**	28	**72**	1	**122**	5	**179**	8	**2012**	28	**1327**	35	**39**	0	**75**	2	**100**	2
1	**5558**	121	**2932**	69	**1261**	36	**2840**	111	**12188**	370	**2347**	140	**793**	10	**2954**	68	**9444**	279
2	**7700**	134	**4844**	96	**2337**	87	**2038**	109	**8920**	287	**964**	38	**4341**	84	**9313**	337	**20159**	985
3	**7437**	322	**6761**	103	**2521**	231	**3374**	154	**12191**	202	**1772**	57	**9097**	287	**12248**	296	**25399**	996
4	**7793**	419	**7180**	174	**2371**	183	**4247**	120	**9802**	140	**1754**	66	**11050**	214	**11944**	360	**22586**	564
5	**7122**	279	**6734**	152	**488**	16	**4380**	72	**5363**	168	**89**	2	**8943**	93	**8465**	468	**12107**	273
6	**7030**	366	**6217**	142	**553**	19	**1466**	18	**288**	3	**1207**	26	**7615**	201	**7339**	251	**11278**	666
7	**5144**	163	**4678**	156	**794**	16	**612**	11	**308**	6	**3409**	53	**5856**	165	**7691**	159	**9111**	598
8	**3555**	207	**55**	3	**no sample***		**86**	2	**no sample***		**378**	8	**3184**	99	**1080**	8	**1355**	31
9	**153**	4	**692**	20	**23**	1	**71**	2	**2983**	77	**363**	9	**703**	14	**1653**	42	**351**	4
10	**466**	17	**698**	16	**34**	1	**81**	2	**3377**	146	**328**	10	**152**	2	**2450**	66	**138**	2
11	**836**	24	**1222**	39	**115**	4	**101**	1	**3052**	64	**308**	9	**188**	3	**2305**	64	**140**	2
12	**95**	3	**65**	1	**8**	0	**36**	1	**no sample***		**19**	1	**70**	1	**68**	2	**139**	3
13	**390**	13	**236**	3	**8**	0	**19**	2	**no sample***		**55**	5	**102**	2	**445**	12	**151**	4
14	**22**	0	**no sample***		**9**	0	**19**	20	**no sample***		**106**	11	**114**	1	**70**	1	**153**	5
15	**69**	2	**no sample***		**215**	6	**no sample***		**no sample***		**no sample***		**96**	2	**634**	11	**146**	2
LoD	1.40		2.54		1.40		0.00		1.43		0.81		0.00		1.27		1.45	
LoQ	3.12		6.51		3.12		0.00		3.44		1.18		0.00		3.18		3.16	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 62: Arsenic concentrations across the SWI of the sediment cores of sampling site 3 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**3.607**	0.062	**2.824**	0.088	**5.082**	0.228	**3.858**	0.069	**5.415**	0.418	**3.307**	0.059	**1.452**	0.130	**5.962**	0.473	**5.322**	0.157
-3	**3.455**	0.063	**1.924**	0.059	**4.152**	0.272	**4.188**	0.071	**4.999**	0.299	**3.746**	0.117	**2.043**	0.096	**7.878**	0.410	**5.316**	0.339
-2	**3.527**	0.153	**2.822**	0.066	**5.050**	0.385	**3.699**	0.134	**3.427**	0.240	**6.641**	0.165	**2.557**	0.143	**9.217**	0.440	**5.065**	0.163
-1	**2.755**	0.090	**2.543**	0.119	**5.041**	0.287	**4.057**	0.061	**3.005**	0.146	**6.851**	0.132	**2.158**	0.171	**8.566**	0.588	**4.524**	0.240
0	**7.748**	0.378	**2.649**	0.128	**7.292**	0.500	**4.401**	0.175	**3.491**	0.142	**12.192**	0.359	**2.338**	0.104	**5.000**	0.298	**4.704**	0.267
1	**13.129**	0.270	**5.390**	0.255	**7.974**	0.703	**6.583**	0.158	**6.186**	0.356	**8.191**	0.120	**2.641**	0.235	**4.087**	0.206	**7.809**	0.417
2	**8.604**	0.264	**5.606**	0.124	**8.378**	0.533	**4.681**	0.250	**5.305**	0.428	**7.055**	0.256	**3.550**	0.156	**4.965**	0.177	**7.362**	0.173
3	**6.778**	0.306	**5.544**	0.116	**6.998**	0.362	**5.123**	0.158	**4.604**	0.281	**5.120**	0.207	**4.501**	0.131	**3.682**	0.174	**6.227**	0.295
4	**5.658**	0.137	**5.416**	0.080	**4.747**	0.386	**3.563**	0.113	**3.606**	0.219	**5.216**	0.192	**3.860**	0.108	**3.088**	0.090	**4.353**	0.193
5	**4.969**	0.141	**5.417**	0.115	**8.384**	0.996	**2.756**	0.079	**3.068**	0.207	**4.532**	0.230	**2.752**	0.083	**2.024**	0.157	**3.964**	0.228
6	**4.240**	0.152	**5.016**	0.122	**3.738**	0.078	**2.342**	0.069	**3.617**	0.242	**4.965**	0.101	**2.186**	0.108	**1.898**	0.050	**4.218**	0.227
7	**3.153**	0.135	**3.927**	0.181	**2.312**	0.122	**1.917**	0.062	**3.403**	0.224	**5.723**	0.066	**1.867**	0.115	**1.754**	0.098	**4.596**	0.102
8	**2.545**	0.091	**3.123**	0.058	**no sample***		**2.069**	0.032	**no sample***		**3.698**	0.161	**2.062**	0.107	**1.595**	0.111	**3.244**	0.062
9	**2.188**	0.074	**3.063**	0.059	**2.415**	0.132	**1.808**	0.094	**2.725**	0.194	**3.323**	0.217	**2.974**	0.198	**1.532**	0.127	**2.806**	0.257
10	**1.993**	0.077	**2.908**	0.057	**2.116**	0.113	**1.827**	0.083	**2.278**	0.152	**2.969**	0.218	**3.608**	0.154	**1.836**	0.074	**2.354**	0.142
11	**1.917**	0.106	**2.795**	0.023	**1.809**	0.097	**1.722**	0.035	**2.369**	0.132	**2.700**	0.153	**2.238**	0.122	**1.573**	0.101	**3.406**	0.160
12	**1.707**	0.076	**2.748**	0.074	**1.379**	0.053	**1.539**	0.087	**no sample***		**2.586**	0.099	**1.200**	0.045	**1.264**	0.072	**2.901**	0.230
13	**2.052**	0.109	**3.039**	0.079	**1.441**	0.078	**1.224**	0.041	**no sample***		**2.606**	0.098	**1.398**	0.072	**1.257**	0.070	**2.305**	0.226
14	**1.800**	0.174	**no sample***		**1.711**	0.149	**0.854**	0.457	**no sample***		**2.480**	0.075	**1.240**	0.107	**1.416**	0.110	**2.253**	0.124
15	**1.839**	0.039	**no sample***		**1.871**	0.055	**no sample***		**no sample***		**no sample***		**1.149**	0.098	**1.223**	0.069	**1.977**	0.029
LoD	0.030		0.040		0.030		0.037		0.026		0.020		0.080		0.080		0.074	
LoQ	0.062		0.097		0.062		0.090		0.065		0.038		0.175		0.175		0.186	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 63: Antimony concentrations across the SWI of the sediment cores of sampling site 3 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.388**	0.014	**0.331**	0.005	**0.591**	0.026	**0.438**	0.023	**0.469**	0.029	**0.267**	0.023	0.042	<LoD	**0.242**	0.040	0.747	0.027
-3	**0.389**	0.021	**0.209**	0.005	**0.472**	0.027	**0.420**	0.012	**0.398**	0.023	**0.244**	0.020	0.128	0.030	**0.249**	0.034	0.742	0.043
-2	**0.375**	0.018	**0.326**	0.022	**0.570**	0.056	**0.387**	0.023	**0.392**	0.032	**0.225**	0.016	**0.236**	0.052	**0.246**	0.042	0.704	0.041
-1	**0.296**	0.015	**0.274**	0.007	**0.547**	0.032	**0.427**	0.027	**0.347**	0.020	**0.242**	0.014	0.171	0.059	**0.257**	0.035	0.620	0.040
0	**0.385**	0.027	**0.180**	0.017	**0.531**	0.040	**0.868**	0.081	**0.283**	0.021	**0.155**	0.011	0.175	0.025	**0.239**	0.025	0.635	0.032
1	**0.222**	0.013	**0.116**	0.005	**0.539**	0.041	**0.437**	0.032	**0.141**	0.012	**0.156**	0.012	**0.241**	0.026	0.201	0.018	**1.048**	0.095
2	**0.140**	0.013	0.084	0.007	**0.363**	0.028	**0.292**	0.023	**0.108**	0.009	0.118	0.019	**0.647**	0.032	0.139	0.015	**0.876**	0.044
3	**0.113**	0.013	**0.123**	0.012	**0.218**	0.021	**0.090**	0.008	**0.117**	0.017	0.098	0.010	**0.542**	0.072	0.131	0.022	0.640	0.067
4	**0.106**	0.005	**0.125**	0.006	**0.193**	0.019	**0.079**	0.005	**0.154**	0.019	0.099	0.018	**0.484**	0.039	0.124	0.024	0.563	0.057
5	**0.092**	0.005	**0.155**	0.007	**0.249**	0.018	**0.073**	0.007	**0.215**	0.023	**0.860**	0.047	**0.475**	0.033	0.042	<LoD	0.556	0.054
6	**0.101**	0.007	**0.111**	0.009	**0.158**	0.012	**0.056**	0.006	**0.145**	0.016	0.103	0.012	**0.453**	0.040	0.138	0.027	0.614	0.022
7	**0.088**	0.007	**0.100**	0.004	**0.093**	0.003	**0.043**	0.006	**0.121**	0.009	0.106	0.014	**0.449**	0.034	0.153	0.041	0.553	0.044
8	**0.070**	0.006	**0.106**	0.008	**no sample***		**0.055**	0.003	**no sample***		0.130	0.020	**0.392**	0.031	0.109	0.035	0.315	0.027
9	**0.080**	0.007	**0.102**	0.008	**0.105**	0.010	**0.073**	0.004	**0.095**	0.008	0.130	0.013	**0.426**	0.013	0.110	0.022	0.150	<LoD
10	**0.078**	0.009	**0.116**	0.011	**0.091**	0.008	**0.064**	0.006	**0.097**	0.010	0.124	0.018	**0.385**	0.059	0.140	0.024	0.150	<LoD
11	**0.070**	0.003	0.085	0.006	**0.091**	0.006	**0.062**	0.007	**0.104**	0.009	0.137	0.019	**0.293**	0.026	0.111	0.034	0.150	<LoD
12	**0.073**	0.004	**0.111**	0.014	**0.081**	0.008	**0.075**	0.006	**no sample***		0.125	0.006	0.149	0.025	0.042	<LoD	0.150	<LoD
13	**0.105**	0.013	**0.087**	0.010	**0.068**	0.007	**0.047**	0.007	**no sample***		0.140	0.014	0.194	0.012	0.042	<LoD	0.150	<LoD
14	**0.095**	0.012	**no sample***		**0.074**	0.009	0.027	0.032	**no sample***		**0.156**	0.020	0.175	0.025	0.042	<LoD	0.150	<LoD
15	**0.086**	0.008	**no sample***		**0.101**	0.006	**no sample***		**no sample***		**no sample***		0.146	0.024	0.086	0.026	0.150	<LoD
LoD	0.007		0.034		0.007		0.013		0.029		0.056		0.084		0.084		0.299	
LoQ	0.019		0.085		0.019		0.034		0.055		0.151		0.221		0.221		0.786	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 64: Cadmium concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.106**	0.008	**0.106**	0.009	**0.265**	0.022	**0.074**	0.004	**0.159**	0.010	**0.111**	0.006	**0.032**	0.006	**0.128**	0.008	**0.201**	0.025
-3	**0.119**	0.013	**0.099**	0.009	**0.290**	0.009	**0.168**	0.014	**0.147**	0.011	**0.164**	0.008	**0.069**	0.008	**0.232**	0.009	**0.309**	0.034
-2	**0.124**	0.007	**0.144**	0.011	**0.320**	0.025	**0.168**	0.006	**0.134**	0.012	**0.139**	0.010	**0.112**	0.019	**0.011**	0.002	**0.323**	0.011
-1	**0.096**	0.005	**0.123**	0.005	**0.356**	0.034	**0.225**	0.012	**0.157**	0.012	**0.145**	0.013	**0.106**	0.007	**0.024**	0.006	**0.490**	0.039
0	**0.076**	0.004	**0.108**	0.006	**0.810**	0.062	**0.297**	0.019	**0.128**	0.012	**0.020**	0.002	**0.131**	0.012	**0.017**	0.001	**0.254**	0.014
1	**0.013**	0.003	**0.060**	0.007	**0.531**	0.034	**0.284**	0.015	**0.089**	0.008	**0.017**	0.003	**0.186**	0.024	**0.033**	0.004	**0.630**	0.029
2	0.002	<LoD	**0.020**	0.002	**0.238**	0.008	**0.101**	0.008	**0.031**	0.004	**0.010**	0.002	**0.093**	0.016	0.004	0.002	**0.439**	0.017
3	0.002	<LoD	0.009	0.002	**0.093**	0.008	**0.032**	0.005	**0.016**	0.003	**0.010**	0.001	**0.024**	0.007	0.001	<LoD	**0.189**	0.022
4	0.002	<LoD	**0.016**	0.003	**2.111**	0.199	**0.016**	0.002	0.013	0.003	**0.012**	0.003	**0.009**	0.002	0.001	<LoD	**0.055**	0.010
5	0.002	<LoD	**0.180**	0.013	**0.054**	0.008	**0.016**	0.002	**0.340**	0.023	**0.007**	0.003	0.007	0.002	0.001	<LoD	**0.028**	0.007
6	**0.014**	0.002	**0.017**	0.003	**0.013**	0.004	0.006	0.002	0.006	0.002	**0.012**	0.002	0.001	<LoD	0.005	0.004	**0.016**	0.005
7	**0.031**	0.003	**0.015**	0.002	0.010	0.001	**0.007**	0.002	**0.016**	0.003	**0.011**	0.002	0.005	0.003	0.005	0.002	**0.015**	0.005
8	**0.017**	0.004	0.009	0.003	**no sample***		**0.011**	0.001	**no sample***		**0.027**	0.005	0.003	0.002	0.001	<LoD	0.008	0.004
9	0.002	<LoD	0.010	0.001	**0.016**	0.002	**0.012**	0.001	0.010	0.001	**0.024**	0.003	0.004	0.003	0.001	<LoD	0.009	0.002
10	0.005	0.002	0.011	0.003	0.006	0.002	**0.015**	0.003	0.011	0.003	**0.029**	0.003	0.004	0.003	0.001	<LoD	0.006	0.002
11	**0.013**	0.001	**0.014**	0.002	0.008	0.001	**0.016**	0.001	**0.074**	0.008	**0.024**	0.005	**0.027**	0.007	0.004	0.002	**0.049**	0.007
12	0.002	<LoD	0.011	0.001	0.001	<LoD	**0.027**	0.003	**no sample***		**0.008**	0.002	0.001	<LoD	0.001	<LoD	0.007	0.003
13	**0.030**	0.003	**0.018**	0.001	0.001	<LoD	**0.008**	0.001	**no sample***		**0.011**	0.004	0.001	<LoD	0.001	<LoD	0.009	0.004
14	0.005	0.002	**no sample***		0.001	<LoD	**0.008**	0.008	**no sample***		**0.016**	0.005	0.007	0.003	0.003	0.001	0.007	0.005
15	0.011	0.003	**no sample***		0.006	0.002	**no sample***		**no sample***		**no sample***		0.006	0.003	0.005	0.002	0.006	0.006
LoD	0.005		0.005		0.005		0.003		0.005		0.002		0.003		0.003		0.004	
LoQ	0.011		0.011		0.011		0.007		0.013		0.005		0.008		0.008		0.010	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 65: Chromium concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	0.772	0.063	0.258	0.062	0.614	0.024	0.218	0.033	0.136	0.033	0.378	0.022	0.127	<LoD	0.308	0.051	0.183	0.045
-3	**0.940**	0.049	0.077	<LoD	0.403	0.048	**0.708**	0.064	0.101	0.031	0.366	0.082	0.127	<LoD	0.127	<LoD	0.068	<LoD
-2	0.467	0.009	**0.497**	0.020	0.446	0.037	**0.536**	0.058	0.087	0.037	**0.471**	0.034	0.127	<LoD	0.127	<LoD	0.149	0.040
-1	0.415	0.026	0.372	0.031	0.459	0.030	0.212	0.023	0.089	0.021	**0.484**	0.046	0.127	<LoD	0.329	0.026	0.068	<LoD
0	0.531	0.045	0.268	0.052	0.500	0.037	**5.233**	0.489	0.118	0.026	**0.545**	0.032	0.127	<LoD	0.127	<LoD	0.264	0.029
1	0.461	0.039	0.248	0.056	0.568	0.044	0.146	0.026	0.165	0.041	**0.563**	0.025	0.127	<LoD	0.127	<LoD	**0.358**	0.041
2	0.473	0.039	0.258	0.046	0.816	0.032	0.197	0.027	0.134	0.020	**0.957**	0.067	0.127	<LoD	0.297	0.030	**0.449**	0.039
3	0.497	0.039	**0.386**	0.034	**1.171**	0.080	0.210	0.021	0.187	0.013	**0.978**	0.056	0.349	0.048	**1.947**	0.084	**0.688**	0.051
4	**0.919**	0.048	**0.755**	0.049	**1.267**	0.112	**0.324**	0.063	**33.415**	2.473	**1.226**	0.096	0.472	0.049	0.374	0.038	**0.814**	0.058
5	0.731	0.056	**0.878**	0.061	**2.820**	0.261	**0.746**	0.057	**0.199**	0.021	**0.809**	0.030	**0.638**	0.038	0.343	0.053	**2.825**	0.554
6	**0.922**	0.097	**0.792**	0.050	**1.578**	0.102	**0.737**	0.060	0.165	0.018	**0.887**	0.061	**0.586**	0.066	0.427	0.013	**0.692**	0.084
7	**1.084**	0.054	**0.735**	0.073	**0.992**	0.089	**0.368**	0.021	**5.428**	0.422	**0.960**	0.033	**0.662**	0.088	**3.953**	0.233	**0.895**	0.079
8	**1.066**	0.062	**0.672**	0.012	**no sample***		**0.485**	0.051	**no sample***		**1.532**	0.085	0.552	0.048	0.285	0.044	**0.567**	0.066
9	**0.972**	0.052	**1.823**	0.090	**0.886**	0.055	**0.590**	0.073	**0.204**	0.050	**1.524**	0.119	0.475	0.032	0.353	0.047	**0.701**	0.056
10	**0.926**	0.082	**1.258**	0.115	**0.871**	0.016	**0.712**	0.075	**0.263**	0.043	**1.540**	0.112	**0.573**	0.035	0.498	0.066	**1.435**	1.313
11	**1.058**	0.053	**1.028**	0.025	**1.075**	0.087	**0.737**	0.032	**0.466**	0.060	**1.511**	0.049	**0.651**	0.073	**1.117**	0.057	**1.160**	0.084
12	**17.843**	0.640	**1.804**	0.075	0.488	0.036	**0.928**	0.094	**no sample***		**1.103**	0.065	0.536	0.048	**0.645**	0.084	**0.865**	0.088
13	**1.315**	0.048	**0.857**	0.025	0.608	0.055	**0.547**	0.044	**no sample***		**2.153**	0.099	**0.648**	0.064	**0.613**	0.037	**1.082**	0.088
14	**0.860**	0.036	**no sample***		0.671	0.067	**4.924**	4.433	**no sample***		**1.862**	0.033	**0.704**	0.034	0.555	0.066	**1.090**	0.130
15	**0.988**	0.038	**no sample***		**1.345**	0.106	**no sample***		**no sample***		**no sample***		**1.069**	0.063	**0.580**	0.054	**0.863**	0.019
LoD	0.399		0.154		0.399		0.094		0.072		0.287		0.254		0.254		0.135	
LoQ	0.848		0.381		0.848		0.247		0.188		0.446		0.560		0.560		0.342	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 66: Cobalt concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.356**	0.040	**0.315**	0.023	**0.463**	0.037	0.303	0.012	**0.599**	0.052	**0.466**	0.046	**0.080**	0.006	**0.505**	0.076	**0.512**	0.050
-3	**0.400**	0.022	**0.207**	0.016	**0.477**	0.039	**0.436**	0.016	**0.740**	0.061	**0.638**	0.019	**0.101**	0.014	**0.869**	0.092	**0.520**	0.071
-2	**0.451**	0.041	**0.317**	0.031	**0.514**	0.027	**0.402**	0.025	**0.284**	0.044	**1.188**	0.083	**0.167**	0.018	**1.105**	0.086	**0.549**	0.065
-1	**0.489**	0.025	**0.313**	0.016	**0.515**	0.009	**0.469**	0.018	**0.272**	0.034	**1.235**	0.085	**0.142**	0.014	**1.397**	0.120	**0.938**	0.038
0	**3.101**	0.190	**0.726**	0.045	**1.534**	0.064	**1.466**	0.145	**0.766**	0.071	**4.338**	0.223	**0.158**	0.020	**0.823**	0.048	**0.471**	0.051
1	**4.132**	0.167	**1.184**	0.069	**3.434**	0.216	**2.993**	0.140	**1.314**	0.093	**3.426**	0.188	**0.411**	0.019	**0.624**	0.023	**3.010**	0.161
2	**1.982**	0.049	**1.143**	0.090	**2.758**	0.211	**1.766**	0.147	**1.161**	0.129	**2.006**	0.089	**0.902**	0.080	**0.590**	0.055	**2.816**	0.083
3	**0.969**	0.036	**1.043**	0.067	**2.541**	0.165	**1.270**	0.112	**0.831**	0.061	**1.027**	0.072	**0.632**	0.038	**0.402**	0.039	**2.001**	0.105
4	**0.712**	0.048	**0.943**	0.059	**1.548**	0.128	**0.803**	0.064	**0.805**	0.079	**1.001**	0.042	**0.452**	0.039	**0.287**	0.008	**1.050**	0.053
5	**0.625**	0.048	**0.729**	0.027	**0.772**	0.056	**0.451**	0.032	**0.299**	0.017	**0.693**	0.048	**0.354**	0.029	**0.211**	0.024	**0.895**	0.090
6	**0.641**	0.021	**0.606**	0.031	**0.998**	0.071	**0.363**	0.021	**0.308**	0.010	**0.666**	0.056	**0.264**	0.028	**0.211**	0.030	**0.712**	0.045
7	**0.554**	0.024	**0.428**	0.018	**0.604**	0.048	**0.343**	0.034	**0.383**	0.030	**0.602**	0.051	**0.267**	0.044	**0.235**	0.027	**0.661**	0.068
8	**0.536**	0.028	**0.467**	0.025	**no sample***		**0.449**	0.019	**no sample***		**0.364**	0.038	**0.242**	0.035	**0.193**	0.032	**0.518**	0.035
9	**0.470**	0.025	**0.480**	0.034	**0.612**	0.027	**0.433**	0.035	**0.322**	0.032	**0.360**	0.022	**0.228**	0.029	**0.197**	0.022	**0.503**	0.036
10	**0.465**	0.036	**0.444**	0.033	**0.562**	0.041	**0.465**	0.021	**0.304**	0.025	**0.402**	0.068	**0.226**	0.028	**0.239**	0.025	**0.511**	0.052
11	**0.481**	0.035	**0.420**	0.022	**0.535**	0.032	**0.429**	0.021	**0.318**	0.047	**0.397**	0.048	**0.269**	0.050	**0.259**	0.029	**0.536**	0.039
12	**0.615**	0.032	**0.455**	0.028	**0.395**	0.029	**0.443**	0.035	**no sample***		**0.771**	0.052	**0.207**	0.030	**0.247**	0.024	**0.477**	0.054
13	**0.542**	0.015	**0.511**	0.028	**0.443**	0.042	**0.379**	0.022	**no sample***		**0.803**	0.049	**0.234**	0.032	**0.210**	0.013	**0.485**	0.056
14	**0.458**	0.038	**no sample***		**0.492**	0.034	0.254	0.224	**no sample***		**0.882**	0.050	**0.225**	0.024	**0.238**	0.033	**0.539**	0.027
15	**0.459**	0.053	**no sample***		**0.517**	0.042	**no sample***		**no sample***		**no sample***		**0.230**	0.027	**0.208**	0.036	**0.482**	0.025
LoD	0.006		0.010		0.006		0.127		0.005		0.016		0.003		0.003		0.020	
LoQ	0.014		0.024		0.014		0.329		0.012		0.036		0.009		0.009		0.054	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 67: Copper concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**2.02**	0.13	**2.03**	0.10	**4.94**	0.22	**4.22**	0.13	**3.49**	0.03	**2.44**	0.12	**1.08**	0.05	**2.92**	0.06	**6.27**	0.19
-3	**3.26**	0.16	**2.15**	0.06	**3.74**	0.14	**5.15**	0.12	**3.45**	0.11	**2.68**	0.09	**1.91**	0.08	**2.80**	0.06	**7.32**	0.43
-2	**4.43**	0.02	**3.11**	0.14	**5.00**	0.35	**4.60**	0.23	**4.82**	0.23	**1.77**	0.05	**2.82**	0.12	**1.21**	0.06	**6.99**	0.16
-1	**3.38**	0.14	**2.82**	0.11	**4.50**	0.21	**4.52**	0.17	**3.67**	0.21	**1.76**	0.08	**2.45**	0.02	**1.26**	0.05	**5.37**	0.10
0	**1.12**	0.07	**1.15**	0.02	**2.01**	0.15	1.55	0.15	**2.02**	0.06	**0.94**	0.05	**2.41**	0.16	**1.60**	0.08	**6.06**	0.17
1	0.67	0.07	0.24	<LoD	0.58	0.06	1.20	0.11	0.15	<LoD	**0.82**	0.05	**2.25**	0.14	0.49	0.01	**1.15**	0.07
2	0.26	<LoD	0.24	<LoD	0.13	<LoD	0.11	<LoD	0.15	<LoD	**0.74**	0.02	0.47	0.04	0.20	<LoD	**0.95**	0.07
3	0.26	<LoD	0.24	<LoD	0.13	<LoD	0.11	<LoD	0.15	<LoD	0.56	0.03	0.20	<LoD	0.20	<LoD	0.56	0.08
4	0.26	<LoD	0.60	0.04	**4.25**	0.36	0.11	<LoD	1.20	0.06	**0.66**	0.04	0.20	<LoD	0.20	<LoD	0.59	0.06
5	0.26	<LoD	1.06	0.04	**17.49**	0.90	0.11	<LoD	0.15	<LoD	0.52	0.02	0.20	<LoD	0.20	<LoD	0.60	0.05
6	**1.82**	0.05	0.24	<LoD	0.13	<LoD	0.11	<LoD	0.74	0.05	**0.65**	0.05	0.20	<LoD	0.20	<LoD	**1.13**	0.14
7	0.26	<LoD	0.24	<LoD	0.13	<LoD	0.11	<LoD	0.00	0.00	**0.62**	0.03	0.20	<LoD	0.58	0.06	0.65	0.03
8	0.26	<LoD	0.24	<LoD	**no sample***		0.11	<LoD	**no sample***		**1.04**	0.01	0.20	<LoD	0.20	<LoD	0.53	0.07
9	0.26	<LoD	0.24	<LoD	0.64	0.04	0.11	<LoD	1.19	0.01	**0.69**	0.04	0.44	0.05	**0.95**	0.05	0.20	<LoD
10	0.26	<LoD	0.54	0.02	0.13	<LoD	0.11	<LoD	0.15	<LoD	**0.88**	0.05	0.45	0.06	0.20	<LoD	0.20	<LoD
11	0.59	0.11	0.65	0.05	0.13	<LoD	0.11	<LoD	0.00	0.00	0.54	0.03	0.20	<LoD	0.20	<LoD	0.20	<LoD
12	**3.01**	0.13	0.76	0.04	0.13	<LoD	**19.71**	0.83	**no sample***		0.53	0.03	0.20	<LoD	0.20	<LoD	0.44	0.11
13	0.26	<LoD	0.24	<LoD	0.13	<LoD	0.11	<LoD	**no sample***		**0.69**	0.08	0.20	<LoD	0.20	<LoD	0.20	<LoD
14	0.26	<LoD	**no sample***		0.13	<LoD	**5.48**	4.98	**no sample***		0.07	<LoD	0.20	<LoD	0.20	<LoD	0.20	<LoD
15	0.26	<LoD	**no sample***		**1.41**	0.14	**no sample***		**no sample***		**no sample***		0.20	<LoD	0.20	<LoD	0.20	<LoD
LoD	0.51		0.47		0.51		0.64		0.59		0.28		0.39		0.39		0.40	
LoQ	1.10		1.14		1.10		1.63		1.28		0.61		0.90		0.90		0.95	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 68: Lead concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.254**	0.011	**0.099**	0.009	**0.169**	0.008	**0.858**	0.015	**0.126**	0.004	**0.120**	0.007	0.013	0.001	0.014	0.003	**0.033**	0.006
-3	**0.084**	0.005	**0.129**	0.008	**0.136**	0.010	**0.075**	0.002	**0.057**	0.006	**0.074**	0.004	**0.019**	0.005	**0.025**	0.004	**0.032**	0.005
-2	**0.099**	0.006	**0.089**	0.006	**0.122**	0.005	**0.122**	0.005	**0.090**	0.004	**0.087**	0.011	**0.023**	0.005	**0.039**	0.007	**0.058**	0.007
-1	**0.235**	0.017	**0.462**	0.011	**0.129**	0.013	**0.046**	0.002	**0.042**	0.002	**0.053**	0.003	**0.021**	0.007	0.007	0.002	**0.052**	0.005
0	**0.081**	0.007	**0.117**	0.007	**0.067**	0.007	**0.045**	0.004	**0.041**	0.002	**0.062**	0.004	**0.023**	0.002	0.003	<LoD	**0.077**	0.012
1	**0.078**	0.006	**0.147**	0.004	0.001	<LoD	**0.026**	0.003	**0.058**	0.006	**0.050**	0.008	0.012	0.003	0.003	<LoD	0.020	0.004
2	**0.065**	0.003	**0.066**	0.006	0.013	0.004	**0.035**	0.003	**0.040**	0.003	**0.088**	0.006	0.009	0.003	**0.017**	0.006	0.020	0.004
3	**0.081**	0.003	**0.189**	0.015	**0.053**	0.003	**0.025**	0.002	**0.065**	0.009	**0.090**	0.009	0.009	0.004	**0.020**	0.004	0.019	0.005
4	**0.037**	0.005	**0.175**	0.013	**0.061**	0.006	**0.022**	0.002	**0.069**	0.005	**0.396**	0.017	0.003	<LoD	0.003	<LoD	0.021	0.004
5	**0.034**	0.003	**0.531**	0.015	**2.081**	0.086	**0.085**	0.003	**0.033**	0.002	**0.085**	0.007	0.011	0.002	0.008	0.003	**0.028**	0.006
6	**0.544**	0.033	**0.120**	0.010	**0.074**	0.005	**0.050**	0.001	**0.042**	0.003	**0.162**	0.015	0.003	<LoD	0.003	<LoD	**0.062**	0.007
7	**0.141**	0.011	**0.128**	0.008	**0.052**	0.005	**0.037**	0.003	**0.689**	0.039	**0.082**	0.007	**0.023**	0.011	**0.024**	0.005	**0.031**	0.005
8	**0.141**	0.011	**0.098**	0.009	**no sample***		**0.019**	0.002	**no sample***		**0.217**	0.009	0.013	0.003	0.012	0.004	0.016	0.003
9	**0.158**	0.012	**0.057**	0.004	**0.088**	0.009	**0.037**	0.004	**0.178**	0.005	**0.208**	0.016	**0.019**	0.004	**0.031**	0.005	0.019	0.004
10	**0.067**	0.004	**0.285**	0.018	**0.045**	0.005	**0.034**	0.002	**0.151**	0.009	**0.526**	0.025	**0.019**	0.003	**0.036**	0.008	0.021	0.006
11	**0.126**	0.012	**0.271**	0.011	**0.164**	0.012	**0.041**	0.002	**0.190**	0.012	**0.142**	0.007	**0.024**	0.010	**0.039**	0.008	**0.041**	0.002
12	**0.226**	0.007	**0.201**	0.011	**0.076**	0.006	**0.635**	0.017	**no sample***		**0.132**	0.006	0.013	0.005	**0.028**	0.006	**0.034**	0.008
13	**0.115**	0.007	**0.055**	0.007	**0.044**	0.006	**0.038**	0.005	**no sample***		**0.276**	0.022	0.010	0.006	**0.057**	0.003	**0.037**	0.004
14	**0.038**	0.005	**no sample***		**0.029**	0.003	**0.108**	0.101	**no sample***		**0.029**	0.021	**0.015**	0.004	**0.018**	0.008	**0.042**	0.004
15	**0.065**	0.005	**no sample***		**0.970**	0.036	**no sample***		**no sample***		**no sample***		**0.015**	0.003	**0.051**	0.006	**0.027**	0.002
LoD	0.010		0.009		0.010		0.006		0.006		0.007		0.006		0.006		0.008	
LoQ	0.027		0.023		0.027		0.016		0.015		0.017		0.014		0.014		0.022	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 69: Molybdenum concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**8.404**	0.058	**6.716**	0.339	**11.743**	0.556	**8.104**	0.220	**8.946**	0.745	**4.710**	0.156	**2.672**	0.209	**7.001**	0.469	**8.614**	0.069
-3	**8.886**	0.161	**4.518**	0.191	**9.315**	0.703	**8.082**	0.280	**7.327**	0.396	**4.746**	0.190	**3.794**	0.197	**7.330**	0.363	**8.234**	0.497
-2	**8.848**	0.293	**7.560**	0.438	**11.351**	0.874	**6.948**	0.476	**6.720**	0.423	**4.778**	0.129	**4.732**	0.238	**7.470**	0.363	**7.943**	0.295
-1	**6.640**	0.193	**6.315**	0.135	**11.236**	0.730	**7.534**	0.267	**5.935**	0.332	**4.980**	0.167	**3.770**	0.234	**6.986**	0.431	**6.518**	0.168
0	**10.009**	0.407	**3.821**	0.185	**11.014**	0.677	**5.474**	0.526	**4.877**	0.254	**4.080**	0.136	**4.090**	0.197	**6.526**	0.288	**7.248**	0.238
1	**7.593**	0.205	**3.416**	0.228	**9.095**	0.786	**7.957**	0.427	**3.476**	0.230	**3.138**	0.115	**4.862**	0.301	**5.372**	0.127	**8.142**	0.405
2	**5.154**	0.094	**2.757**	0.067	**5.499**	0.424	**5.123**	0.408	**2.897**	0.242	**2.240**	0.028	**7.145**	0.280	**4.152**	0.153	**6.192**	0.154
3	**4.264**	0.181	**2.350**	0.030	**2.872**	0.169	**2.011**	0.106	**2.092**	0.146	**1.285**	0.063	**4.746**	0.203	**2.551**	0.111	**3.433**	0.131
4	**2.800**	0.084	**1.415**	0.021	**1.121**	0.082	**1.305**	0.060	**3.890**	0.222	**1.296**	0.038	**3.650**	0.100	**1.404**	0.043	**2.245**	0.143
5	**1.383**	0.056	**0.771**	0.026	**20.326**	2.038	**1.077**	0.062	**4.180**	0.387	**1.278**	0.050	**2.856**	0.116	**1.541**	0.067	**2.473**	0.164
6	**0.532**	0.016	**0.581**	0.024	**0.388**	0.028	**0.709**	0.027	**3.153**	0.249	**1.647**	0.037	**2.628**	0.078	**1.551**	0.099	**4.617**	0.269
7	**0.236**	0.022	**0.672**	0.038	0.159	0.011	**0.400**	0.012	**2.498**	0.195	**2.007**	0.073	**2.889**	0.141	**1.238**	0.072	**4.470**	0.107
8	0.191	0.009	**0.360**	0.012	**no sample***		**0.471**	0.016	**no sample***		**0.888**	0.072	**3.387**	0.154	**1.836**	0.066	**3.266**	0.071
9	**0.218**	0.020	**0.245**	0.024	0.178	0.012	**0.338**	0.024	**1.634**	0.145	**0.698**	0.046	**4.632**	0.258	**1.978**	0.121	**2.582**	0.213
10	0.207	0.009	**0.372**	0.028	0.125	0.010	**0.230**	0.013	**1.444**	0.078	**0.616**	0.021	**4.534**	0.189	**1.938**	0.073	**3.120**	0.171
11	0.143	0.006	**0.245**	0.013	0.130	0.005	**0.297**	0.016	**1.141**	0.064	**0.475**	0.045	**2.854**	0.126	**1.274**	0.054	**3.900**	0.180
12	0.171	0.011	0.167	0.025	0.101	0.005	**0.220**	0.018	**no sample***		**0.245**	0.012	**1.277**	0.051	**1.020**	0.068	**3.286**	0.197
13	0.183	0.016	**0.190**	0.013	0.094	0.011	**0.104**	0.004	**no sample***		**0.184**	0.010	**1.705**	0.095	**1.627**	0.107	**3.194**	0.243
14	0.123	0.005	**no sample***		0.118	0.010	0.066	0.059	**no sample***		**0.187**	0.020	**1.421**	0.131	**1.451**	0.068	**3.124**	0.145
15	0.157	0.010	**no sample***		0.208	0.014	**no sample***		**no sample***		**no sample***		**1.091**	0.052	**1.726**	0.102	**2.550**	0.069
LoD	0.076		0.062		0.076		0.031		0.089		0.051		0.089		0.089		0.072	
LoQ	0.217		0.170		0.217		0.090		0.244		0.148		0.247		0.247		0.216	
* insufficient sample volume for ICP-MS measurement																		

Table A70: Nickel concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**3.52**	0.05	**3.27**	0.24	**3.23**	0.15	**2.89**	0.12	**5.49**	0.12	**3.22**	0.14	2.21	<LoD	4.87	0.30	**83.48**	5.83
-3	**4.25**	0.21	**2.17**	0.08	**2.85**	0.07	**3.57**	0.17	**6.74**	0.12	**4.13**	0.24	2.21	<LoD	6.71	0.16	18.68	0.60
-2	**4.87**	0.19	**3.93**	0.25	**3.64**	0.16	**5.37**	0.39	**6.39**	0.31	**4.73**	0.19	4.66	0.15	6.89	0.38	18.30	1.42
-1	**4.09**	0.08	**2.87**	0.08	**4.29**	0.22	**7.62**	0.68	**6.82**	0.21	**4.76**	0.20	2.21	<LoD	7.77	0.25	15.38	2.18
0	**6.79**	0.17	**2.24**	0.12	**4.48**	0.17	**10.72**	1.10	**6.68**	0.12	**4.73**	0.20	2.21	<LoD	8.45	0.80	12.81	0.92
1	**4.93**	0.06	**1.94**	0.05	**3.57**	0.16	**9.27**	1.10	**5.12**	0.11	**4.36**	0.22	2.21	<LoD	6.72	0.53	6.06	<LoD
2	**3.33**	0.15	**1.73**	0.11	**2.66**	0.15	**5.35**	0.37	**4.82**	0.28	**3.42**	0.18	4.43	0.29	5.46	0.23	6.06	<LoD
3	**2.40**	0.20	**2.30**	0.08	**2.32**	0.17	**3.82**	0.20	**4.26**	0.28	**2.39**	0.10	2.21	<LoD	5.03	0.71	6.06	<LoD
4	**1.89**	0.12	**2.06**	0.15	**1.56**	0.06	**4.45**	0.41	**20.63**	0.30	**2.48**	0.12	2.21	<LoD	2.21	<LoD	6.06	<LoD
5	**1.56**	0.07	**2.12**	0.18	**1.39**	0.07	**3.30**	0.15	**3.15**	0.25	**1.68**	0.08	2.21	<LoD	2.21	<LoD	6.06	<LoD
6	**1.68**	0.10	**1.47**	0.08	**1.40**	0.14	**2.56**	0.16	**1.55**	0.08	**1.97**	0.06	2.21	<LoD	2.21	<LoD	6.06	<LoD
7	**1.10**	0.08	1.07	0.10	**3.12**	0.19	**2.54**	0.13	**4.70**	0.10	**1.71**	0.08	2.21	<LoD	2.21	<LoD	6.06	<LoD
8	**0.87**	0.05	0.96	0.04	**no sample***		**3.07**	0.28	**no sample***		**0.82**	0.03	2.21	<LoD	2.21	<LoD	6.06	<LoD
9	0.76	0.06	**1.36**	0.07	**2.44**	0.14	**3.55**	0.50	**1.80**	0.13	**0.71**	0.06	2.21	<LoD	2.21	<LoD	6.06	<LoD
10	0.71	0.06	**1.38**	0.09	0.40	0.07	**4.94**	0.77	**1.47**	0.10	**0.83**	0.07	2.21	<LoD	2.21	<LoD	6.06	<LoD
11	**0.95**	0.04	1.05	0.04	0.67	0.04	**9.04**	1.70	**10.73**	0.22	**0.69**	0.06	2.21	<LoD	5.94	1.73	6.06	<LoD
12	**8.14**	0.19	**1.26**	0.06	0.09	<LoD	**28.52**	0.72	**no sample***		**1.11**	0.08	2.21	<LoD	2.21	<LoD	20.19	3.13
13	**0.89**	0.09	0.78	0.06	0.09	<LoD	**7.55**	0.30	**no sample***		**1.47**	0.07	2.21	<LoD	2.21	<LoD	6.06	<LoD
14	**0.88**	0.07	**no sample***		0.09	<LoD	**73.29**	72.49	**no sample***		0.16	0.25	2.21	<LoD	2.21	<LoD	6.06	<LoD
15	0.85	0.04	**no sample***		0.62	0.02	**no sample***		**no sample***		**no sample***		2.21	<LoD	2.21	<LoD	6.06	<LoD
LoD	0.38		0.46		0.38		1.28		0.50		0.10		4.42		4.42		12.12	
LoQ	0.86		1.16		0.86		2.14		1.42		0.24		10.07		10.07		34.19	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 71: Selenium concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	1.032	0.132	0.869	0.154	1.105	0.113	0.517	0.064	0.666	0.105	0.397	0.039	0.624	0.215	0.620	0.158	0.784	0.245
-3	0.871	0.114	0.738	0.128	1.049	0.146	0.481	0.071	0.644	0.134	0.405	0.080	0.681	0.101	0.633	0.223	0.919	0.149
-2	1.034	0.135	0.985	0.096	0.965	0.080	0.498	0.165	0.579	0.107	0.607	0.052	0.665	0.220	0.680	0.113	1.220	0.221
-1	0.923	0.042	0.988	0.150	1.002	0.134	0.373	0.098	0.594	0.130	0.607	0.055	0.759	0.078	0.747	0.195	0.917	0.214
0	1.194	0.140	0.791	0.110	1.131	0.079	0.389	0.097	0.753	0.116	**0.762**	0.058	0.809	0.137	0.638	0.143	1.343	0.197
1	0.988	0.103	0.831	0.188	1.123	0.103	0.511	0.082	0.592	0.111	**0.785**	0.084	0.866	0.208	0.721	0.262	1.260	0.152
2	1.090	0.099	0.896	0.139	**1.306**	0.088	0.355	0.048	0.783	0.198	**0.785**	0.097	1.099	0.136	1.009	0.145	1.310	0.105
3	0.984	0.132	1.044	0.122	**1.311**	0.215	0.357	0.051	0.672	0.081	**0.685**	0.132	**1.175**	0.213	0.962	0.081	1.349	0.178
4	0.942	0.107	**1.285**	0.131	1.214	0.142	0.331	0.093	0.648	0.126	**0.787**	0.093	**1.157**	0.074	0.834	0.065	0.996	0.230
5	0.959	0.168	**1.298**	0.176	**1.447**	0.178	0.306	0.082	0.636	0.043	**0.805**	0.056	**1.325**	0.343	0.897	0.427	1.098	0.151
6	0.999	0.100	1.048	0.024	1.244	0.112	0.070	<LoD	0.742	0.161	**0.811**	0.073	**1.250**	0.208	1.082	0.141	**2.438**	0.663
7	0.955	0.121	1.003	0.048	1.058	0.260	0.296	0.020	0.733	0.067	**0.817**	0.086	1.115	0.242	0.695	0.273	**1.581**	0.126
8	1.002	0.105	1.017	0.147	**no sample***		0.306	0.098	**no sample***		**0.916**	0.076	0.986	0.170	0.772	0.157	**1.657**	0.182
9	0.975	0.177	1.052	0.159	0.903	0.064	0.423	0.054	0.695	0.084	**0.905**	0.053	1.013	0.189	0.942	0.203	**1.427**	0.290
10	0.987	0.161	0.970	0.100	0.862	0.108	0.322	0.054	0.668	0.092	**0.788**	0.060	0.909	0.157	0.770	0.185	1.110	0.276
11	0.912	0.170	1.030	0.064	0.904	0.103	0.310	0.136	0.651	0.135	**0.915**	0.088	0.964	0.080	0.766	0.119	1.181	0.456
12	0.980	0.116	0.972	0.112	0.841	0.095	0.339	0.109	**no sample***		**0.871**	0.044	0.913	0.133	0.750	0.137	1.206	0.169
13	1.029	0.105	1.093	0.117	0.803	0.085	0.322	0.123	**no sample***		**0.987**	0.084	0.786	0.210	0.802	0.137	1.161	0.227
14	1.030	0.165	**no sample***		0.777	0.097	0.070	<LoD	**no sample***		**1.020**	0.117	0.956	0.268	1.018	0.116	1.343	0.190
15	0.978	0.066	**no sample***		0.706	0.075	**no sample***		**no sample***		**no sample***		0.811	0.177	0.869	0.192	1.292	0.305
LoD	0.696		0.609		0.696		0.267		0.526		0.385		0.576		0.576		0.539	
LoQ	1.295		1.267		1.295		0.562		1.157		0.621		1.123		1.123		1.424	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 72: Silver concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.210**	0.005	**0.006**	0.001	**0.095**	0.008	**0.022**	0.002	**0.052**	0.003	**0.048**	0.004	**0.030**	0.001	**0.033**	0.006	**0.063**	0.005
-3	**0.125**	0.010	**0.011**	0.002	**0.062**	0.006	0.015	0.001	**0.042**	0.001	**0.031**	0.003	**0.031**	0.005	**0.021**	0.004	**0.042**	0.006
-2	**0.138**	0.006	**0.016**	0.003	**0.077**	0.008	**0.022**	0.001	**0.055**	0.003	**0.025**	0.003	**0.035**	0.002	0.006	0.001	**0.034**	0.003
-1	**0.102**	0.006	**0.026**	0.002	**0.045**	0.006	0.014	0.004	**0.050**	0.005	**0.022**	0.003	**0.025**	0.003	**0.008**	0.003	**0.077**	0.009
0	**0.094**	0.006	**0.012**	0.002	**0.026**	0.003	**0.022**	0.002	**0.029**	0.003	**0.012**	0.002	**0.018**	0.002	0.005	0.001	**0.025**	0.003
1	**0.086**	0.004	**0.009**	0.002	**0.027**	0.005	**0.022**	0.001	**0.063**	0.003	**0.009**	0.001	**0.035**	0.003	0.005	0.001	**0.013**	0.003
2	**0.146**	0.003	**0.006**	0.002	**0.034**	0.002	0.008	0.002	0.012	0.002	**0.005**	0.002	0.004	0.001	0.004	0.001	**0.010**	0.002
3	**0.070**	0.005	**0.027**	0.003	**0.029**	0.004	0.008	0.002	0.012	0.001	**0.006**	0.001	0.005	0.002	0.005	0.002	0.008	0.003
4	**0.068**	0.006	**0.016**	0.002	**0.036**	0.003	0.008	0.001	0.001	<LoD	**0.006**	0.001	0.005	0.002	0.004	0.002	0.008	0.004
5	**0.052**	0.002	**0.042**	0.004	**0.076**	0.008	0.011	0.001	0.017	0.003	**0.010**	0.001	0.006	0.002	0.003	0.001	0.005	0.001
6	**0.056**	0.005	**0.011**	0.003	**0.014**	0.002	0.007	0.001	0.001	<LoD	**0.005**	0.001	0.004	0.002	**0.007**	0.002	0.005	0.003
7	**0.051**	0.005	**0.009**	0.001	**0.014**	0.001	0.006	0.001	**0.033**	0.003	**0.006**	0.001	**0.006**	0.002	**0.010**	0.002	**0.009**	0.002
8	**0.060**	0.004	**0.011**	0.002	**no sample***		0.008	0.002	**no sample***		**0.054**	0.005	0.005	0.002	0.003	0.001	0.002	<LoD
9	**0.049**	0.003	**0.012**	0.002	**0.015**	0.002	0.007	0.001	0.008	0.002	**0.027**	0.002	**0.007**	0.002	0.005	0.001	0.007	0.003
10	**0.047**	0.006	**0.023**	0.003	**0.010**	0.001	**0.024**	0.003	0.008	0.002	**0.010**	0.001	**0.008**	0.001	**0.007**	0.002	0.008	0.003
11	**0.050**	0.004	**0.016**	0.002	**0.011**	0.002	0.015	0.002	0.010	0.002	**0.012**	0.002	**0.009**	0.001	**0.008**	0.003	**0.010**	0.003
12	**0.011**	0.001	**0.026**	0.003	**0.011**	0.002	**0.038**	0.003	**no sample***		**0.007**	0.001	**0.007**	0.002	**0.007**	0.002	**0.009**	0.001
13	**0.005**	0.002	**0.007**	0.001	**0.007**	0.001	0.010	0.001	**no sample***		**0.016**	0.002	**0.009**	0.002	**0.007**	0.002	0.009	0.005
14	**0.004**	0.001	**no sample***		**0.005**	0.001	0.012	0.013	**no sample***		**0.010**	0.001	**0.007**	0.001	**0.008**	0.002	0.008	0.002
15	**0.012**	0.001	**no sample***		**0.123**	0.005	**no sample***		**no sample***		**no sample***		**0.006**	0.002	**0.013**	0.003	0.004	0.002
LoD	0.001		0.002		0.001		0.005		0.008		0.002		0.003		0.003		0.004	
LoQ	0.003		0.004		0.003		0.015		0.023		0.005		0.006		0.006		0.009	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 73: Tin concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**1.454**	0.099	**0.424**	0.039	**0.417**	0.065	**0.495**	0.021	**0.450**	0.094	**0.319**	0.037	0.043	<LoD	0.179	0.016	0.306	0.053
-3	**0.858**	0.065	0.215	0.036	0.096	0.039	**0.182**	0.045	**0.265**	0.044	**0.062**	0.006	0.043	<LoD	**4.415**	0.537	0.234	0.079
-2	**0.721**	0.070	0.320	0.066	0.151	0.061	**0.162**	0.017	**0.261**	0.067	**0.103**	0.012	0.043	<LoD	0.043	<LoD	0.218	0.070
-1	**0.393**	0.034	0.303	0.042	0.163	0.075	**0.121**	0.028	**0.194**	0.022	**0.088**	0.011	0.043	<LoD	0.043	<LoD	0.238	0.120
0	0.041	<LoD	0.063	<LoD	0.102	0.105	**0.146**	0.019	**0.210**	0.039	**0.086**	0.021	0.043	<LoD	0.043	<LoD	0.224	0.074
1	0.041	<LoD	0.063	<LoD	0.011	<LoD	**0.291**	0.032	**0.902**	0.087	**0.085**	0.010	0.043	<LoD	0.043	<LoD	0.210	0.081
2	0.041	<LoD	0.063	<LoD	0.101	0.047	**0.201**	0.057	0.143	0.045	**0.066**	0.028	0.043	<LoD	0.087	0.067	0.279	0.050
3	0.041	<LoD	0.063	<LoD	0.145	0.071	**0.178**	0.017	0.133	0.032	**0.110**	0.042	0.043	<LoD	0.043	<LoD	0.221	0.068
4	0.041	<LoD	0.256	0.026	**65.075**	6.255	**0.193**	0.029	**0.157**	0.022	**0.094**	0.014	0.043	<LoD	0.043	<LoD	0.254	0.040
5	0.092	0.092	**5.079**	0.131	**1.400**	0.231	**0.244**	0.058	**11.424**	0.762	**0.156**	0.040	0.158	0.140	0.043	<LoD	0.183	0.035
6	**0.245**	0.046	0.311	0.031	0.160	0.071	**0.107**	0.020	0.098	0.063	**0.140**	0.058	0.088	0.076	0.140	0.081	0.148	0.057
7	**1.118**	0.161	0.284	0.071	0.135	0.097	**0.212**	0.043	**0.241**	0.096	**0.151**	0.035	0.125	0.137	0.118	0.088	0.240	0.095
8	**0.503**	0.105	0.129	0.065	**no sample***		**0.357**	0.108	**no sample***		**0.808**	0.146	0.088	0.045	0.043	<LoD	0.067	<LoD
9	0.041	<LoD	0.164	0.023	0.011	<LoD	**0.327**	0.025	0.134	0.049	**0.743**	0.113	0.159	0.089	0.043	<LoD	0.170	0.080
10	0.089	0.093	0.280	0.070	0.011	<LoD	**0.490**	0.056	**0.249**	0.095	**0.860**	0.134	0.093	0.076	0.043	<LoD	0.195	0.101
11	**0.290**	0.029	0.272	0.048	0.011	<LoD	**0.451**	0.100	**2.720**	0.110	**0.780**	0.093	**0.606**	0.064	0.043	<LoD	**1.249**	0.160
12	0.041	<LoD	0.257	0.136	0.011	<LoD	**0.504**	0.067	**no sample***		**0.151**	0.065	0.043	<LoD	0.043	<LoD	0.210	0.079
13	**0.847**	0.075	**0.496**	0.083	0.011	<LoD	**0.188**	0.051	**no sample***		**0.147**	0.042	0.043	<LoD	0.119	0.066	0.231	0.050
14	0.041	<LoD	**no sample***		0.011	<LoD	0.067	0.015	**no sample***		**0.340**	0.094	0.162	0.089	0.043	<LoD	0.318	0.100
15	**0.290**	0.053	**no sample***		0.103	0.081	**no sample***		**no sample***		**no sample***		0.138	0.061	0.096	0.053	0.157	0.112
LoD	0.083		0.125		0.083		0.033		0.071		0.027		0.086		0.086		0.134	
LoQ	0.222		0.357		0.222		0.087		0.156		0.054		0.218		0.218		0.346	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 74: Titanium concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.334**	0.024	0.332	<LoD	**0.411**	0.034	0.163	<LoD	0.296	0.107	0.053	<LoD	0.076	<LoD	0.076	<LoD	0.192	<LoD
-3	**0.302**	0.031	0.332	<LoD	**0.339**	0.026	0.163	<LoD	0.266	0.063	0.053	<LoD	0.076	<LoD	0.076	<LoD	0.192	<LoD
-2	**0.280**	0.024	0.332	<LoD	**0.346**	0.026	0.163	<LoD	0.228	0.069	0.053	<LoD	0.076	<LoD	0.076	<LoD	0.192	<LoD
-1	**0.284**	0.008	0.776	0.040	**0.378**	0.032	0.163	<LoD	0.028	<LoD	0.053	<LoD	0.076	<LoD	0.076	<LoD	0.192	<LoD
0	**0.413**	0.032	0.332	<LoD	**0.393**	0.039	0.163	<LoD	0.419	0.069	0.053	<LoD	0.076	<LoD	0.076	<LoD	0.192	<LoD
1	**0.368**	0.031	0.332	<LoD	**0.654**	0.030	0.163	<LoD	**0.702**	0.062	0.053	<LoD	0.076	<LoD	0.193	0.042	0.192	<LoD
2	**0.400**	0.039	0.332	<LoD	**1.544**	0.051	0.163	<LoD	0.413	0.029	0.053	<LoD	0.076	<LoD	0.284	0.055	0.720	0.076
3	**0.516**	0.065	1.131	0.034	**3.135**	0.173	0.163	<LoD	0.557	0.100	0.398	0.036	**0.385**	0.083	**0.397**	0.058	**1.568**	0.165
4	**0.717**	0.020	**2.079**	0.078	**4.249**	0.326	0.163	<LoD	0.543	0.055	0.454	0.023	**0.605**	0.052	**0.557**	0.075	**2.119**	0.171
5	**1.204**	0.054	**3.143**	0.087	**4.863**	0.467	**0.645**	0.120	0.442	0.099	0.770	0.036	**0.901**	0.108	**0.638**	0.077	**1.002**	0.084
6	**2.089**	0.036	**2.875**	0.113	**3.623**	0.160	0.163	<LoD	0.401	0.055	**0.958**	0.070	**0.860**	0.079	**1.075**	0.060	**1.327**	0.088
7	**2.481**	0.167	**3.240**	0.148	**2.785**	0.155	**0.491**	0.048	0.573	0.102	**1.106**	0.038	**1.022**	0.033	**1.610**	0.109	**2.499**	0.108
8	**3.307**	0.164	1.571	0.046	**no sample***		**1.433**	0.101	**no sample***		**3.924**	0.335	**2.628**	0.151	**0.439**	0.066	0.584	0.062
9	**1.603**	0.056	**2.461**	0.137	**1.310**	0.089	**1.725**	0.201	**0.609**	0.049	**3.795**	0.259	**1.124**	0.129	**0.582**	0.026	**1.077**	0.209
10	**1.926**	0.105	**2.524**	0.169	**2.003**	0.066	**2.260**	0.225	**0.929**	0.094	**3.831**	0.282	**1.360**	0.060	**1.097**	0.057	**1.689**	0.083
11	**2.507**	0.119	**3.195**	0.155	**2.732**	0.141	**2.252**	0.139	**1.526**	0.181	**3.699**	0.257	**1.848**	0.190	**1.850**	0.081	**2.673**	0.206
12	**1.011**	0.027	**2.258**	0.121	**0.721**	0.087	**0.894**	0.065	**no sample***		**1.294**	0.087	**1.456**	0.118	**1.067**	0.126	**2.624**	0.225
13	**3.277**	0.123	**2.749**	0.028	**0.782**	0.077	**0.963**	0.043	**no sample***		**2.414**	0.131	**1.617**	0.174	**1.145**	0.057	**2.825**	0.299
14	**1.417**	0.067	**no sample***		**1.152**	0.100	**0.835**	1.263	**no sample***		**4.727**	0.165	**1.883**	0.183	**1.193**	0.090	**3.021**	0.183
15	**1.978**	0.068	**no sample***		**2.077**	0.136	**no sample***		**no sample***		**no sample***		**2.152**	0.092	**1.317**	0.056	**2.911**	0.173
LoD	0.099		0.665		0.099		0.363		0.213		0.328		0.151		0.151		0.384	
LoQ	0.265		1.674		0.265		0.450		0.578		0.845		0.368		0.368		0.950	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 75: Vanadium concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**1.440**	0.049	**1.780**	0.089	**3.208**	0.041	**1.997**	0.025	**2.550**	0.195	**1.595**	0.104	**1.047**	0.094	**1.651**	0.134	**4.715**	0.152
-3	**1.671**	0.049	**1.102**	0.021	**2.985**	0.075	**3.017**	0.078	**2.517**	0.167	**1.852**	0.093	**1.609**	0.113	**1.493**	0.117	**5.105**	0.340
-2	**1.780**	0.026	**1.787**	0.058	**3.598**	0.208	**2.651**	0.175	**2.388**	0.147	**1.813**	0.090	**2.136**	0.188	**1.366**	0.043	**5.186**	0.212
-1	**1.467**	0.035	**1.566**	0.047	**3.643**	0.194	**3.032**	0.088	**2.037**	0.154	**1.857**	0.144	**1.761**	0.141	**2.438**	0.165	**5.034**	0.111
0	**1.576**	0.088	**1.216**	0.057	**4.348**	0.282	**2.823**	0.209	**1.459**	0.065	**1.615**	0.085	**1.959**	0.167	**3.068**	0.183	**4.498**	0.187
1	**1.292**	0.018	**1.014**	0.063	**3.638**	0.246	**2.546**	0.123	**1.403**	0.091	**0.991**	0.071	**1.999**	0.170	**1.752**	0.075	**4.699**	0.134
2	**1.316**	0.028	**1.067**	0.052	**4.296**	0.267	**1.342**	0.103	**0.967**	0.084	**0.887**	0.037	**1.133**	0.056	**1.075**	0.036	**2.762**	0.110
3	**1.437**	0.048	**1.839**	0.074	**4.883**	0.254	**1.630**	0.090	**1.097**	0.094	**1.202**	0.054	**1.300**	0.094	**1.133**	0.070	**2.815**	0.128
4	**1.886**	0.059	**3.159**	0.039	**4.911**	0.346	**1.821**	0.074	**1.064**	0.073	**1.196**	0.047	**1.541**	0.076	**1.204**	0.087	**3.054**	0.082
5	**2.653**	0.035	**4.318**	0.137	**9.397**	0.849	**1.847**	0.075	**0.916**	0.070	**1.448**	0.079	**1.809**	0.151	**1.150**	0.047	**2.708**	0.102
6	**3.623**	0.115	**3.863**	0.120	**5.554**	0.256	**1.777**	0.078	**0.991**	0.081	**1.290**	0.065	**1.769**	0.083	**1.457**	0.101	**2.510**	0.160
7	**3.186**	0.095	**3.208**	0.142	**3.590**	0.171	**2.056**	0.075	**0.966**	0.065	**1.207**	0.042	**1.704**	0.063	**1.631**	0.084	**3.177**	0.146
8	**3.288**	0.107	**2.856**	0.071	**no sample***		**2.711**	0.075	**no sample***		**5.648**	0.386	**1.377**	0.093	**1.052**	0.059	**2.099**	0.031
9	**2.703**	0.065	**3.372**	0.086	**3.714**	0.156	**2.606**	0.158	**0.834**	0.065	**5.060**	0.300	**1.146**	0.095	**1.216**	0.068	**2.633**	0.090
10	**2.811**	0.096	**2.936**	0.071	**3.415**	0.182	**2.633**	0.109	**1.006**	0.062	**4.626**	0.295	**1.213**	0.048	**1.405**	0.082	**2.680**	0.064
11	**3.022**	0.169	**2.991**	0.121	**3.468**	0.150	**2.439**	0.047	**1.348**	0.086	**4.486**	0.219	**1.559**	0.099	**1.669**	0.113	**2.914**	0.088
12	**2.507**	0.084	**2.905**	0.083	**2.067**	0.133	**2.380**	0.153	**no sample***		**2.882**	0.129	**1.397**	0.088	**1.453**	0.079	**2.766**	0.064
13	**3.715**	0.147	**3.217**	0.096	**2.218**	0.151	**2.155**	0.080	**no sample***		**3.299**	0.188	**1.544**	0.118	**1.364**	0.058	**2.740**	0.092
14	**2.700**	0.152	**no sample***		**2.277**	0.172	**1.350**	1.206	**no sample***		**4.294**	0.191	**1.463**	0.058	**1.556**	0.099	**2.750**	0.180
15	**2.871**	0.103	**no sample***		**2.286**	0.156	**no sample***		**no sample***		**no sample***		**1.569**	0.049	**1.364**	0.035	**2.479**	0.056
LoD	0.066		0.014		0.066		0.078		0.228		0.009		0.012		0.012		0.013	
LoQ	0.189		0.038		0.189		0.120		0.622		0.023		0.030		0.030		0.035	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 76: Zink concentrations across the SWI of the sediment cores of sampling site 3. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**126.18**	3.42	**11.57**	0.69	**14.33**	0.59	**203.85**	4.35	**10.30**	0.28	**19.04**	0.56	**8.75**	0.20	**6.50**	0.23	**9.84**	0.20
-3	**84.71**	1.98	**48.91**	1.85	**15.54**	1.43	**11.75**	0.37	**24.02**	0.32	**16.17**	0.47	**9.80**	0.50	**18.51**	0.52	**11.48**	0.86
-2	**29.21**	0.55	**36.48**	1.64	**11.43**	0.83	**40.35**	1.39	**11.20**	0.21	**39.55**	1.20	**30.09**	1.17	**11.79**	0.29	**35.70**	0.38
-1	**34.50**	0.76	**208.20**	7.65	**22.53**	0.88	**22.29**	0.67	**10.59**	0.68	**30.80**	1.07	**31.42**	0.83	**15.09**	0.39	**32.84**	1.35
0	**15.60**	0.74	**231.22**	5.84	**52.36**	3.09	**64.62**	4.03	**48.32**	1.05	**45.91**	1.48	**27.44**	0.49	**11.48**	0.34	**26.77**	0.83
1	**5.63**	0.14	**109.00**	2.70	**32.05**	0.64	**95.59**	4.45	**42.40**	1.15	**29.87**	2.01	**38.63**	0.95	**8.32**	0.50	**46.74**	1.54
2	**6.80**	0.25	**23.28**	0.94	**14.63**	1.22	**26.09**	1.21	**8.79**	0.47	**25.48**	1.37	**6.82**	0.40	**5.74**	0.27	**49.27**	1.05
3	**7.07**	0.42	**26.68**	0.71	**14.58**	1.10	**38.20**	1.87	**16.32**	0.74	**11.15**	0.31	**13.55**	0.55	**12.63**	0.63	**43.09**	0.85
4	**12.10**	0.84	**44.61**	1.64	**9.00**	0.47	**29.84**	1.00	**11.59**	0.50	**11.32**	0.50	**8.80**	0.77	**3.85**	0.30	**33.42**	1.28
5	**9.46**	0.28	**42.68**	2.09	**135.47**	5.39	**56.64**	2.02	**15.54**	0.24	**15.57**	0.61	**9.32**	0.32	**3.69**	0.50	**9.24**	0.30
6	**11.72**	0.94	**23.17**	0.88	**24.68**	0.68	**26.54**	0.98	**14.23**	0.48	**38.33**	0.85	**7.89**	0.79	**3.38**	0.16	**10.30**	0.42
7	**11.46**	0.24	**19.99**	0.57	**8.46**	0.41	**20.89**	0.85	**87.75**	2.30	**14.92**	0.84	**11.52**	0.80	**8.30**	0.42	**18.38**	0.75
8	**9.29**	0.62	**27.83**	0.77	**no sample***		**7.66**	0.22	**no sample***		**20.36**	0.40	**6.33**	0.60	**3.79**	0.12	**2.98**	0.24
9	**10.21**	0.67	**33.42**	0.60	**32.16**	0.77	**10.66**	0.44	**15.68**	0.39	**15.38**	0.83	**5.80**	0.18	**7.45**	0.26	**7.30**	0.69
10	**10.11**	0.47	**64.03**	1.80	**9.31**	0.29	**13.82**	0.66	**17.72**	0.33	**48.10**	2.05	**17.65**	0.51	**12.32**	0.49	**56.54**	1.64
11	**12.46**	0.57	**54.92**	2.58	**16.67**	0.58	**57.65**	1.75	**20.03**	0.70	**12.30**	0.51	**9.66**	0.45	**10.32**	0.55	**8.36**	0.30
12	**23.12**	0.15	**72.49**	3.31	**10.64**	0.26	**134.73**	6.37	**no sample***		**46.90**	0.66	**6.26**	0.54	**11.93**	0.43	**8.56**	0.37
13	**14.23**	0.67	**37.71**	1.08	**5.84**	0.29	**43.64**	3.35	**no sample***		**23.50**	0.90	**5.47**	0.16	**18.30**	1.02	**20.18**	0.60
14	**7.14**	0.34	**no sample***		**1.88**	0.14	**1.48**	1.20	**no sample***		**1.83**	0.36	**12.69**	0.47	**8.65**	0.51	**11.11**	0.75
15	**6.64**	0.28	**no sample***		**34.65**	1.38	**no sample***		**no sample***		**no sample***		**7.71**	0.47	**12.56**	0.64	**7.89**	0.80
LoD	0.08		0.30		0.08		0.15		0.16		0.10		0.27		0.27		0.09	
LoQ	0.20		0.80		0.20		0.39		0.40		0.27		0.47		0.47		0.24	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 77: Phosphate concentrations across the SWI of the sediment cores of sampling site 3. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
4	0.95	0.70	0.00	0.00	0.30	0.95	0.65	2.01	3404.10
3	0.85	0.25	0.85	0.20	0.05	0.85	0.65	1.71	0.90
2	0.80	0.30	0.65	0.15	0.10	0.80	0.75	0.86	0.75
1	0.60	0.20	0.85	0.05	0.15	0.60	0.90	0.19	0.90
0	0.80	0.40	0.10	0.30	1.25	0.80	1.40	0.44	1.40
1	0.75	0.65	2.05	1.50	1.50	0.75	0.90	0.06	0.90
2	0.75	2.45	5.25	1.45	2.85	0.75	1.26	0.09	1.26
3	0.30	1.80	3.40	2.25	3.30	0.30	3.31	0.06	3.31
4	0.20	3.30	9.70	5.50	3.90	0.20	2.96	2.96	5.35
5	0.05	10.30	15.45	11.20	10.55	0.05	2.31	2.31	5.15
6	0.45	8.30	12.40	8.35	5.95	0.45	3.01	0.84	5.00
7	0.25	6.55	8.85	12.45	11.00	0.25	4.76	3.45	4.76
8	0.45	10.75	missing*	12.30	missing*	0.45	2.96	2.96	4.94
9	2.45	11.40	5.95	10.40	6.65	2.45	12.46	3.95	12.46
10	3.20	5.20	7.60	16.95	6.85	3.20	5.56	5.56	7.39
11	7.40	15.95	14.35	47.80	17.20	7.40	4.66	4.66	9.30
12	9.35	26.65	10.35	14.30	missing*	9.35	9.56	7.99	13.75
13	12.40	6.65	8.10	2.40	missing*	12.04	14.76	5.19	14.76
14	20.00	missing*	7.80	14.75	missing*	20.00	15.06	8.09	15.06
15	26.60	missing*	10.45	missing*	missing*	6.85	13.16	10.27	13.16
*** insufficient sample volume**									
**** handling error**									

Table A3. 78: Sulfate concentrations across the SWI of the sediment cores of sampling site 3. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
4	955.00	1089.45	695.80	457.15	564.75	633.40	0.00	156.20	562.20
3	360.80	927.00	803.30	975.10	760.10	736.90	720.35	382.75	357.65
2	697.70	819.45	404.20	735.50	646.60	693.40	759.15	481.55	406.95
1	785.75	519.90	651.75	626.95	782.00	732.15	602.60	798.15	596.40
0	546.25	632.40	781.45	810.25	800.85	621.20	681.95	1074.70	906.35
1	592.05	421.70	1124.45	877.30	800.15	775.30	573.65	638.05	415.35
2	396.70	870.20	841.85	417.75	656.75	746.30	740.90	657.55	713.20
3	534.65	380.95	341.50	600.10	564.25	516.95	775.80	545.45	954.70
4	670.00	353.45	489.75	716.45	450.80	573.55	900.10	1140.30	470.00
5	665.65	515.10	659.20	786.90	640.85	1109.60	571.00	1102.85	552.70
6	412.05	604.05	409.35	643.40	893.65	528.65	496.45	841.80	536.95
7	405.70	461.30	279.75	553.75	733.30	897.70	349.50	886.30	599.85
8	392.85	605.55	missing*	570.95	missing*	733.85	517.50	1123.85	344.10
9	521.40	618.95	286.70	523.50	738.95	483.50	574.00	842.90	1085.85
10	535.35	294.85	270.55	528.25	519.45	329.40	801.40	951.20	487.55
11	479.70	676.70	408.45	623.05	606.45	512.80	747.15	828.20	382.45
12	358.80	713.80	516.95	449.20	missing*	433.65	886.70	888.35	824.90
13	79.10	266.15	349.45	376.05	missing*	542.40	630.75	708.35	1115.20
14	463.15	missing*	280.40	457.10	missing*	545.95	684.50	778.85	1074.10
15	missing*	missing*	238.15	379.60	missing*	241.30	654.80	781.20	1069.90
*** insufficient sample volume**									
**** handling error**									

Table A3. 79: Ammonium concentrations across the SWI of the sediment cores of sampling site 3. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
4	1.84	0.63	1.36	0.58	0.90	2.18	0.50	0.89	0.00
3	1.73	0.68	0.46	0.67	0.91	2.36	0.00	0.41	0.05
2	1.48	0.37	0.87	0.26	0.14	2.26	0.00	1.62	0.00
1	1.01	0.63	1.27	0.65	3.74	1.62	0.00	0.52	0.04
0	0.34	0.65	1.28	0.67	3.37	1.28	0.00	1.83	0.00
1	1.60	1.25	1.95	2.10	3.67	4.12	0.86	1.04	0.84
2	2.82	1.80	4.48	2.18	3.42	5.23	0.00	0.42	0.64
3	5.36	2.13	6.22	2.06	3.53	6.22	0.00	0.20	1.83
4	5.45	2.99	7.19	2.82	4.89	4.86	0.65	0.09	2.42
5	5.90	3.70	8.41	3.94	0.64	3.79	1.06	0.21	2.31
6	6.00	3.61	9.25	5.25	0.61	4.02	1.45	1.43	2.29
7	6.40	4.59	9.18	6.03	0.90	6.30	0.99	0.41	2.73
8	6.44	4.28	missing*	5.58	missing*	7.05	1.11	0.36	2.33
9	6.99	4.61	9.58	6.09	1.77	7.45	0.63	0.26	2.50
10	7.92	4.83	10.45	6.54	0.01	8.52	0.76	0.60	2.35
11	8.06	5.03	10.25	9.96	1.12	10.38	1.25	0.80	2.45
12	8.18	5.00	10.27	9.25	missing*	10.65	1.42	1.05	2.52
13	8.72	5.15	11.35	7.98	missing*	12.37	1.46	1.19	2.47
14	10.83	missing*	11.09	8.96	missing*	15.56	1.59	1.04	2.18
15	12.53	missing*	12.77	missing*	missing*	17.33	1.67	1.34	2.07
*** insufficient sample volume**									
**** handling error**									

AIII.IX.II.IV Concentrations in suction-based pore water samples of sampling site 4

Table A3. 80: Carbon concentrations across the SWI of the sediment cores of sampling site 4 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in mg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**709**	13	**795**	0	173	8	**251**	1	**118**	5	**154**	9	**166**	12	**91**	3	**251**	9
-3	**606**	20	**530**	2	**245**	7	**11**	<LoD	**166**	7	**189**	9	**211**	13	**173**	10	**310**	10
-2	**500**	16	**438**	3	139	3	**319**	1	**134**	4	**180**	7	**186**	5	**166**	10	**277**	12
-1	**570**	14	**293**	5	**953**	5	**193**	0	**210**	6	**186**	3	**154**	5	**217**	10	**327**	25
0	**847**	17	**423**	4	**1106**	2	**280**	1	**193**	6	**247**	7	**181**	5	**201**	4	**438**	16
1	**832**	14	**491**	2	**1167**	1	**706**	1	**164**	6	**313**	16	**283**	15	**190**	9	**547**	7
2	**859**	15	**517**	2	**1006**	2	**243**	1	**202**	5	**329**	10	**387**	24	**208**	8	**674**	9
3	**1366**	4	**347**	2	**1205**	3	**1034**	2	**143**	5	**368**	14	**276**	11	**207**	8	**679**	18
4	**2066**	3	**1264**	4	**1221**	6	**259**	1	**848**	4	**333**	14	**344**	9	**310**	8	**665**	14
5	**2081**	9	**431**	3	**1059**	6	**597**	2	**1397**	5	**333**	21	**420**	18	**550**	47	**435**	12
6	**1459**	6	**1271**	7	**2740**	4	**1249**	3	**1245**	4	**369**	29	**333**	12	**460**	25	**442**	18
7	**1588**	5	**1062**	1	**2921**	6	**1351**	3	**1075**	4	**386**	18	**534**	28	**534**	33	**364**	8
8	**no sample***		**1388**	1	**2765**	4	**1429**	2	**940**	4	**332**	5	**377**	18	**648**	25	**334**	13
9	**1409**	4	**1798**	2	**2951**	4	**911**	4	**967**	3	**349**	18	**531**	20	**805**	32	**346**	19
10	**1324**	8	**1809**	1	**2129**	4	**1563**	2	**897**	4	**415**	15	**520**	18	**946**	47	**376**	13
11	**1347**	5	**2016**	2	**2997**	6	**1603**	2	**792**	3	**437**	16	**493**	19	**730**	13	**275**	15
12	**847**	6	**2404**	2	**2136**	8	**1652**	2	**775**	2	**363**	16	**452**	20	**634**	18	**286**	21
13	**1143**	8	**2137**	3	**2127**	5	**1360**	4	**no sample***		**395**	12	**436**	14	**543**	14	**261**	20
14	**944**	6	**980**		**2159**	3	**1264**	3	**no sample***		**400**	13	**279**	11	**314**	13	**262**	10
15	**1151**	5	**1438**	2	**1649**	5	**1222**	5	**no sample***		**388**	16	**no sample***		**354**	16	**216**	8
LoD	79.42		8.93		79.42		2.15		4.55		3.85		6.04		6.04		2.96	
LoQ	204.11		22.33		204.11		5.79		11.46		10.14		14.59		14.59		7.99	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 81: Phosphorous concentrations across the SWI of the sediment cores of sampling site 4 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**1264**	20	**188**	7	**909**	42	**563**	28	**1038**	81	**1040**	78	**518**	37	**498**	24	**1665**	46
-3	**1359**	71	**200**	4	**749**	24	**978**	34	**1053**	66	**1332**	70	**325**	25	**399**	20	**2205**	41
-2	**1962**	73	**1149**	45	**700**	13	**430**	37	**1229**	75	**1112**	71	**201**	8	**953**	26	**2883**	130
-1	**3151**	214	**1932**	43	**823**	35	**1846**	78	**1232**	75	**1734**	104	**249**	14	**1265**	42	**3721**	103
0	**5004**	216	**3498**	247	**3746**	120	**2156**	125	**1580**	109	**3455**	58	**648**	33	**2389**	124	**8832**	255
1	**5196**	224	**5713**	175	**5576**	300	**4030**	90	**3088**	216	**4664**	27	**1246**	73	**4020**	223	**10185**	368
2	**5665**	164	**6748**	158	**6679**	363	**3999**	247	**4764**	280	**4950**	143	**2650**	170	**5027**	255	**13465**	305
3	**6079**	278	**7471**	404	**11255**	571	**6842**	306	**5787**	398	**5336**	223	**1954**	125	**5181**	162	**12378**	459
4	**5657**	69	**6077**	165	**9836**	411	**6430**	427	**6225**	219	**5673**	280	**2836**	125	**5030**	346	**14808**	595
5	**5165**	330	**5882**	253	**8625**	484	**6300**	468	**6202**	410	**6017**	170	**2998**	147	**4579**	264	**11782**	645
6	**4291**	93	**5503**	236	**8358**	241	**4524**	159	**6342**	361	**6709**	382	**2977**	143	**5974**	272	**12781**	439
7	**4236**	354	**6048**	249	**7310**	530	**4883**	223	**6314**	344	**6634**	229	**5612**	399	**4883**	384	**11071**	356
8	**no sample***		**5495**	172	**6108**	284	**6226**	419	**6646**	362	**3842**	197	**3483**	145	**5218**	214	**8511**	430
9	**5388**	178	**8470**	254	**5580**	237	**6051**	590	**6379**	401	**4802**	137	**7023**	234	**5293**	318	**9064**	452
10	**5400**	60	**7900**	199	**6107**	136	**5996**	268	**6536**	501	**7605**	276	**8095**	299	**5378**	384	**9120**	490
11	**4723**	148	**7667**	202	**4887**	222	**5931**	155	**6623**	400	**10184**	431	**7384**	463	**5756**	251	**9360**	318
12	**4580**	132	**7235**	85	**4235**	145	**5545**	240	**6596**	212	**6828**	349	**8243**	311	**6013**	258	**9815**	810
13	**4076**	115	**6618**	169	**4029**	117	**5245**	160	**no sample***		**6796**	283	**8874**	174	**6270**	205	**10803**	758
14	**4091**	79	0		**6529**	147	**696**	128	**no sample***		**7100**	332	**6788**	233	**6731**	358	**10571**	270
15	**4143**	83	**6705**	92	**17469**	77	**6106**	276	**no sample***		**7524**	322	**no sample***		**6581**	339	**8719**	449
LoD	5.11		3.74		5.11		4.99		1.45		5.16		0.29		0.29		0.19	
LoQ	13.38		10.34		13.38		14.50		3.91		14.43		0.61		0.61		0.48	

Table A3. 82: Sulfur concentrations across the SWI of the sediment cores of sampling site 4 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in mg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**305**	6	**150**	4	**560**	33	**173**	7	**179**	9	**127**	6	**83**	4	**141**	7	**168**	5
-3	**267**	12	**134**	7	**536**	26	**252**	12	**172**	10	**155**	6	**78**	4	**114**	8	**159**	3
-2	**229**	6	**250**	13	**492**	14	**92**	7	**192**	9	**116**	6	**88**	5	**216**	15	**130**	5
-1	**182**	6	**167**	5	**468**	28	**266**	8	**183**	8	**141**	2	**52**	2	**201**	5	**118**	3
0	**248**	5	**173**	11	**431**	14	**200**	5	**163**	7	**133**	3	**65**	3	**221**	7	**132**	4
1	**227**	3	**140**	5	**368**	22	**265**	9	**153**	8	**125**	3	**55**	3	**205**	6	**124**	6
2	**217**	7	**142**	4	**266**	18	**155**	10	**146**	6	**129**	2	**93**	5	**173**	7	**148**	4
3	**228**	7	**158**	8	**265**	14	**222**	11	**142**	7	**126**	4	**41**	1	**140**	3	**117**	3
4	**223**	7	**148**	4	**224**	12	**201**	13	**142**	6	**125**	4	**43**	1	**112**	4	**127**	5
5	**236**	15	**176**	7	**258**	12	**193**	15	**140**	7	**126**	1	**53**	1	**92**	4	**94**	4
6	**218**	3	**184**	3	**238**	5	**142**	3	**148**	7	**130**	10	**42**	2	**106**	2	**91**	7
7	**220**	20	**205**	9	**213**	12	**149**	5	**148**	6	**128**	4	**103**	5	**85**	6	**76**	4
8	**no sample***		**203**	5	**187**	8	**180**	13	**155**	6	**309**	14	**60**	1	**84**	3	**74**	4
9	**303**	6	**337**	8	**185**	7	**171**	13	**156**	7	**287**	8	**128**	2	**85**	2	**79**	6
10	**328**	6	**333**	6	**219**	5	**153**	5	**164**	7	**254**	5	**143**	6	**86**	5	**77**	4
11	**313**	8	**321**	5	**190**	6	**147**	4	**164**	6	**234**	6	**125**	3	**85**	4	**69**	2
12	**295**	7	**310**	4	**173**	3	**143**	5	**168**	5	**137**	6	**131**	3	**87**	5	**70**	4
13	**278**	6	**305**	5	**173**	3	**139**	5	**no sample***		**135**	6	**129**	4	**86**	1	**68**	6
14	**273**	3	0		**282**	5	**13**	3	**no sample***		**138**	6	**100**	3	**87**	5	**68**	3
15	**265**	5	**255**	3	**555**	1	**140**	5	**no sample***		**140**	5	**no sample***		**86**	2	**75**	2
LoD	0.20		0.28		0.20		0.51		0.71		0.27		0.28		0.28		1.06	
LoQ	0.53		0.74		0.53		1.32		2.01		0.76		0.77		0.77		2.87	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 83: Manganese concentrations across the SWI of the sediment cores of sampling site 4 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**521**	12	**7**	0	**12**	1	**71**	2	**142**	1	**152**	3	**26**	1	**110**	3	**401**	3
-3	**547**	21	**9**	0	**13**	0	**194**	7	**166**	2	**187**	4	**22**	1	**171**	3	**570**	11
-2	**584**	9	**124**	4	**13**	0	**95**	2	**209**	4	**156**	3	**70**	2	**536**	13	**636**	11
-1	**578**	20	**259**	8	**133**	6	**303**	10	**216**	3	**222**	5	**152**	4	**828**	22	**726**	12
0	**839**	21	**382**	5	**644**	23	**292**	9	**242**	3	**285**	6	**259**	3	**1021**	23	**871**	13
1	**790**	17	**419**	12	**910**	41	**387**	12	**297**	6	**322**	12	**195**	6	**996**	13	**680**	45
2	**708**	18	**425**	8	**644**	11	**256**	8	**337**	5	**353**	13	**320**	7	**901**	25	**931**	36
3	**720**	21	**440**	10	**931**	50	**429**	12	**355**	5	**349**	5	**146**	5	**702**	18	**563**	240
4	**646**	13	**433**	12	**838**	45	**358**	12	**358**	4	**363**	10	**162**	5	**602**	14	**713**	84
5	**618**	13	**464**	5	**1124**	29	**354**	10	**366**	4	**380**	3	**177**	2	**512**	5	**635**	10
6	**571**	7	**469**	28	**803**	25	**303**	6	**379**	5	**376**	6	**158**	5	**532**	6	**585**	11
7	**555**	15	**514**	2	**590**	16	**284**	8	**408**	4	**390**	11	**404**	12	**440**	7	**523**	6
8	**no sample***		**448**	6	**513**	16	**295**	16	**416**	8	**976**	36	**228**	6	**491**	13	**372**	5
9	**894**	12	**800**	8	**516**	8	**241**	4	**425**	4	**1041**	28	**518**	11	**464**	9	**392**	7
10	**969**	12	**755**	9	**654**	12	**232**	13	**424**	4	**1016**	17	**555**	14	**474**	7	**371**	5
11	**940**	8	**777**	8	**523**	16	**266**	9	**428**	5	**1047**	38	**499**	9	**469**	15	**393**	6
12	**980**	21	**753**	8	**469**	11	**276**	13	**439**	4	**447**	19	**481**	8	**440**	8	**397**	9
13	**981**	18	**779**	8	**490**	9	**276**	8	**no sample***		**470**	24	**488**	17	**442**	15	**397**	7
14	**957**	16	0		**948**	10	**21**	4	**no sample***		**475**	21	**361**	9	**427**	11	**387**	5
15	**915**	17	**686**	3	**2039**	3	**104**	95	**no sample***		**478**	15	**no sample***		**400**	8	**339**	12
LoD	1.31		1.98		1.31		3.24		2.93		1.05		0.41		0.41		2.41	
LoQ	3.61		5.62		3.61		8.36		8.26		2.82		1.08		1.08		6.22	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 84: Iron concentrations across the SWI of the sediment cores of sampling site 4 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**65**	2	**8**	0	**45**	1	**267**	2	**49**	1	**42**	1	**92**	3	**36**	1	**91**	1
-3	**66**	3	**17**	0	**36**	2	**58**	1	**44**	0	**51**	2	**59**	1	**26**	0	**88**	1
-2	**125**	2	**33**	1	**38**	2	**23**	0	**51**	1	**49**	1	**32**	2	**56**	2	**94**	2
-1	**249**	8	**96**	1	**77**	4	**105**	1	**64**	1	**106**	3	**55**	2	**79**	2	**126**	2
0	**372**	11	**309**	9	**942**	32	**142**	2	**72**	1	**372**	9	**126**	2	**131**	4	**7535**	290
1	**435**	12	**530**	11	**3171**	123	**206**	7	**389**	5	**433**	14	**497**	7	**364**	5	**2758**	220
2	**383**	11	**364**	3	**1231**	43	**163**	4	**532**	11	**319**	11	**621**	10	**810**	21	**1015**	46
3	**253**	8	**305**	6	**1269**	76	**264**	5	**640**	10	**289**	4	**550**	11	**836**	26	**692**	298
4	**224**	4	**251**	5	**788**	45	**202**	10	**664**	7	**294**	10	**1366**	32	**805**	22	**943**	117
5	**226**	4	**221**	5	**161**	3	**199**	5	**611**	10	**310**	3	**1201**	11	**603**	7	**815**	9
6	**186**	2	**168**	3	**484**	17	**168**	3	**540**	9	**344**	4	**170**	5	**507**	10	**746**	9
7	**182**	4	**163**	3	**277**	6	**140**	1	**600**	10	**384**	11	**467**	9	**366**	7	**695**	7
8	**no sample***		**131**	2	**193**	6	**154**	5	**627**	9	**71**	2	**297**	4	**374**	9	**190**	3
9	**326**	6	**218**	0	**188**	2	**129**	4	**628**	12	**314**	9	**661**	8	**384**	9	**209**	5
10	**244**	3	**224**	3	**224**	4	**132**	3	**627**	4	**1119**	19	**589**	12	**391**	8	**197**	5
11	**221**	2	**187**	1	**175**	5	**155**	2	**520**	10	**1896**	53	**427**	7	**377**	17	**232**	3
12	**227**	4	**190**	0	**152**	4	**139**	2	**467**	1	**300**	13	**364**	6	**326**	5	**287**	9
13	**214**	4	**212**	1	**142**	2	**136**	1	**no sample***		**298**	16	**387**	7	**342**	8	**391**	4
14	**217**	3	0		**256**	3	**21**	5	**no sample***		**271**	9	**299**	5	**364**	11	**386**	5
15	**217**	4	**434**	1	**1182**	4	**53**	50	**no sample***		**239**	7	**no sample***		**227**	4	**315**	7
LoD	0.00		2.54		1.40		0.00		1.43		0.81		2.19		2.19		1.45	
LoQ	0.00		6.51		3.12		0.00		3.44		1.18		5.56		5.56		3.16	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 85: Arsenic concentrations across the SWI of the sediment cores of sampling site 4 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**8.596**	0.212	**1.718**	0.090	**5.527**	0.318	**3.282**	0.145	**3.532**	0.251	**2.792**	0.235	**1.311**	0.061	**3.042**	0.225	**5.875**	0.111
-3	**10.124**	0.240	**1.759**	0.064	**5.303**	0.157	**6.064**	0.112	**3.555**	0.216	**3.463**	0.135	**1.343**	0.104	**2.959**	0.130	**6.525**	0.168
-2	**15.342**	0.331	**6.399**	0.331	**5.077**	0.271	**2.751**	0.201	**4.298**	0.258	**2.866**	0.167	**1.856**	0.072	**6.742**	0.231	**6.186**	0.205
-1	**17.572**	0.541	**9.361**	0.247	**5.496**	0.346	**7.601**	0.211	**4.244**	0.257	**3.623**	0.055	**1.992**	0.121	**7.089**	0.315	**7.150**	0.135
0	**25.608**	0.620	**14.759**	0.590	**14.437**	0.865	**5.370**	0.168	**3.918**	0.309	**3.147**	0.060	**2.935**	0.158	**8.237**	0.408	**8.555**	0.293
1	**17.546**	0.519	**11.980**	0.255	**17.347**	0.806	**6.353**	0.331	**3.781**	0.209	**3.168**	0.120	**2.241**	0.176	**7.028**	0.232	**5.884**	0.269
2	**10.814**	0.543	**8.303**	0.157	**12.870**	0.649	**4.140**	0.168	**4.037**	0.271	**3.094**	0.083	**3.760**	0.211	**5.617**	0.310	**7.015**	0.088
3	**8.339**	0.238	**6.613**	0.146	**11.034**	0.449	**6.507**	0.201	**4.055**	0.274	**3.367**	0.049	**1.600**	0.097	**5.072**	0.146	**5.779**	0.197
4	**7.156**	0.350	**5.097**	0.127	**8.087**	0.454	**6.131**	0.269	**4.212**	0.224	**3.675**	0.144	**1.726**	0.082	**4.460**	0.283	**5.909**	0.288
5	**6.566**	0.133	**4.882**	0.145	**2.522**	0.100	**5.584**	0.190	**4.162**	0.277	**4.276**	0.222	**1.985**	0.122	**3.793**	0.201	**4.352**	0.188
6	**5.689**	0.154	**4.580**	0.086	**6.595**	0.288	**4.061**	0.112	**4.316**	0.289	**4.466**	0.249	**1.292**	0.076	**4.336**	0.178	**4.185**	0.291
7	**5.264**	0.312	**4.334**	0.164	**4.776**	0.293	**4.224**	0.120	**4.502**	0.367	**4.140**	0.210	**3.043**	0.170	**3.410**	0.203	**3.596**	0.184
8	**no sample***		**3.659**	0.100	**3.703**	0.189	**4.449**	0.149	**4.516**	0.256	**4.467**	0.128	**1.605**	0.062	**3.328**	0.170	**3.396**	0.232
9	**6.330**	0.170	**5.807**	0.120	**3.384**	0.101	**3.494**	0.143	**4.264**	0.282	**3.410**	0.175	**3.517**	0.122	**3.219**	0.186	**3.449**	0.253
10	**6.392**	0.077	**5.352**	0.066	**3.850**	0.101	**3.002**	0.115	**3.866**	0.272	**3.393**	0.068	**3.758**	0.143	**3.114**	0.150	**3.570**	0.227
11	**5.728**	0.134	**5.063**	0.093	**3.138**	0.140	**2.823**	0.060	**3.295**	0.192	**2.957**	0.086	**3.351**	0.061	**3.033**	0.162	**3.076**	0.182
12	**5.189**	0.128	**4.476**	0.084	**2.868**	0.159	**2.561**	0.056	**2.975**	0.166	**2.727**	0.119	**3.500**	0.150	**2.901**	0.173	**3.083**	0.134
13	**4.754**	0.046	**4.511**	0.073	**2.605**	0.066	**2.379**	0.111	**no sample***		**2.587**	0.132	**3.420**	0.064	**2.671**	0.146	**2.896**	0.266
14	**4.440**	0.105	0.000		**4.307**	0.076	**0.539**	0.116	**no sample***		**2.446**	0.123	**2.348**	0.061	**2.602**	0.138	**2.863**	0.129
15	**4.048**	0.070	**4.658**	0.058	**9.703**	0.064	**2.267**	0.052	**no sample***		**2.421**	0.077	**no sample***		**2.610**	0.110	**2.141**	0.108
LoD	0.030		0.040		0.030		0.037		0.026		0.020		0.067		0.067		0.074	
LoQ	0.062		0.097		0.062		0.090		0.065		0.038		0.179		0.179		0.186	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 86: Antimony concentrations across the SWI of the sediment cores of sampling site 4 and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.422**	0.016	**0.197**	0.007	**0.702**	0.029	**0.280**	0.019	**0.292**	0.014	0.150	0.012	0.217	0.043	0.353	0.056	0.256	0.015
-3	**0.310**	0.001	**0.171**	0.010	**0.675**	0.034	**0.346**	0.017	**0.250**	0.019	**0.173**	0.016	0.182	0.020	0.200	0.023	0.189	0.022
-2	**0.205**	0.012	**0.296**	0.027	**0.680**	0.025	**0.110**	0.006	**0.281**	0.019	0.110	0.015	0.188	0.027	**0.460**	0.050	0.065	<LoD
-1	**0.148**	0.012	**0.171**	0.015	**0.589**	0.056	**0.279**	0.021	**0.245**	0.019	0.098	0.005	0.086	<LoD	0.358	0.030	0.065	<LoD
0	**0.204**	0.012	**0.195**	0.012	**0.540**	0.028	**0.113**	0.009	**0.146**	0.012	0.099	0.010	0.086	<LoD	0.420	0.023	0.164	0.033
1	**0.184**	0.013	**0.206**	0.012	**0.421**	0.026	**0.134**	0.009	**0.108**	0.010	0.104	0.019	0.086	<LoD	**0.502**	0.023	0.195	0.031
2	**0.166**	0.017	**0.181**	0.014	**0.329**	0.024	**0.092**	0.009	**0.246**	0.022	0.109	0.013	0.086	<LoD	**0.506**	0.036	**0.341**	0.022
3	**0.125**	0.006	**0.181**	0.012	**0.350**	0.020	**0.149**	0.012	**0.155**	0.003	0.115	0.010	0.086	<LoD	**0.469**	0.031	0.276	0.032
4	**0.110**	0.016	**0.148**	0.006	**0.286**	0.013	**0.131**	0.010	**0.167**	0.014	0.120	0.017	0.086	<LoD	0.426	0.040	0.290	0.027
5	**0.102**	0.007	**0.122**	0.007	**0.094**	0.006	**0.132**	0.012	**0.158**	0.019	0.140	0.011	0.086	<LoD	0.351	0.042	0.208	0.039
6	**0.101**	0.007	**0.109**	0.010	**0.201**	0.017	**0.079**	0.005	**0.161**	0.016	**0.164**	0.024	0.086	<LoD	0.347	0.027	0.194	0.014
7	**0.089**	0.006	**0.103**	0.011	**0.146**	0.007	**0.080**	0.007	**0.156**	0.015	**0.160**	0.018	0.246	0.008	0.266	0.023	0.165	0.021
8	**no sample***		**0.087**	0.009	**0.113**	0.010	**0.094**	0.003	**0.173**	0.018	0.133	0.021	0.086	<LoD	0.276	0.021	0.065	<LoD
9	**0.161**	0.009	**0.142**	0.007	**0.109**	0.011	**0.086**	0.009	**0.167**	0.013	0.123	0.014	0.366	0.025	0.269	0.016	0.065	<LoD
10	**0.143**	0.004	**0.152**	0.017	**0.141**	0.014	**0.072**	0.007	**0.156**	0.017	0.150	0.018	0.393	0.033	0.273	0.035	0.065	<LoD
11	**0.144**	0.007	**0.146**	0.011	**0.121**	0.008	**0.068**	0.009	**0.149**	0.014	**0.155**	0.011	0.367	0.036	0.274	0.023	0.065	<LoD
12	**0.153**	0.004	**0.119**	0.004	**0.104**	0.004	**0.067**	0.005	**0.160**	0.012	0.137	0.026	0.316	0.027	0.259	0.025	0.065	<LoD
13	**0.139**	0.004	**0.171**	0.012	**0.093**	0.008	**0.069**	0.007	**no sample***		0.146	0.015	0.337	0.009	0.249	0.011	0.065	<LoD
14	**0.118**	0.004	0.000		**0.173**	0.011	0.007	<LoD	**no sample***		**0.155**	0.019	0.238	0.037	0.246	0.034	0.065	<LoD
15	**0.137**	0.005	**0.104**	0.009	**0.480**	0.004	**0.072**	0.008	**no sample***		**0.160**	0.019	**no sample***		0.275	0.028	0.065	<LoD
LoD	0.007		0.034		0.007		0.013		0.029		0.056		0.171		0.171		0.131	
LoQ	0.019		0.085		0.019		0.034		0.055		0.151		0.452		0.452		0.316	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 87: Cadmium concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.126**	0.005	**0.028**	0.003	**0.127**	0.006	**0.034**	0.006	**0.023**	0.001	**0.016**	0.002	**0.019**	0.002	**0.053**	0.010	**0.131**	0.024
-3	**0.022**	0.005	**0.030**	0.002	**0.126**	0.008	**0.037**	0.003	**0.022**	0.004	**0.016**	0.002	**0.060**	0.004	**0.142**	0.012	**0.126**	0.017
-2	0.005	0.002	**0.112**	0.007	**0.197**	0.010	**0.010**	0.002	**0.037**	0.003	**0.014**	0.001	**0.059**	0.004	**0.159**	0.019	**0.062**	0.004
-1	0.009	0.003	**0.050**	0.004	**0.184**	0.017	**0.044**	0.003	**0.022**	0.002	**0.020**	0.003	**0.035**	0.004	**0.076**	0.008	**0.027**	0.006
0	**0.018**	0.002	**0.051**	0.002	**0.094**	0.010	**0.027**	0.003	**0.020**	0.003	**0.016**	0.002	**0.028**	0.004	**0.026**	0.006	**0.030**	0.006
1	**0.021**	0.005	**0.049**	0.004	**0.048**	0.005	**0.025**	0.002	**0.031**	0.004	**0.023**	0.003	**0.015**	0.002	**0.024**	0.004	**0.034**	0.006
2	**0.017**	0.002	**0.053**	0.003	**0.050**	0.005	**0.023**	0.004	**7.172**	9.138	**0.023**	0.006	**0.016**	0.004	**0.043**	0.006	**0.065**	0.006
3	**0.019**	0.003	**0.041**	0.004	**0.060**	0.006	**0.037**	0.003	**0.057**	0.007	**0.020**	0.001	0.005	0.001	**0.037**	0.006	**0.067**	0.003
4	**0.016**	0.005	**0.040**	0.005	**0.046**	0.007	**0.031**	0.002	**0.037**	0.002	**0.022**	0.002	0.009	0.003	**0.031**	0.004	**0.077**	0.008
5	**0.022**	0.006	**0.037**	0.002	0.009	0.003	**0.033**	0.001	**0.036**	0.005	**0.021**	0.004	**0.011**	0.004	**0.029**	0.007	**0.051**	0.002
6	**0.022**	0.002	**0.029**	0.002	**0.039**	0.003	**0.017**	0.001	**0.030**	0.001	**0.025**	0.003	**0.011**	0.001	**0.031**	0.004	**0.054**	0.005
7	**0.018**	0.003	**0.034**	0.002	**0.028**	0.002	**0.018**	0.002	**0.032**	0.003	**0.028**	0.004	**0.032**	0.003	**0.026**	0.002	**0.047**	0.010
8	**no sample***		**0.030**	0.003	**0.024**	0.002	**0.027**	0.001	**0.031**	0.002	**0.015**	0.001	**0.016**	0.003	**0.028**	0.005	**0.031**	0.006
9	**0.034**	0.004	**0.045**	0.004	**0.023**	0.002	**0.022**	0.002	**0.032**	0.004	**0.013**	0.003	**0.039**	0.006	**0.026**	0.002	**0.032**	0.013
10	**0.023**	0.002	**0.064**	0.003	**0.024**	0.004	**0.021**	0.002	**0.033**	0.004	**0.014**	0.002	**0.041**	0.004	**0.025**	0.003	**0.032**	0.005
11	**0.022**	0.003	**0.050**	0.005	**0.020**	0.003	**0.023**	0.001	**0.033**	0.002	**0.057**	0.005	**0.035**	0.006	**0.041**	0.002	**0.029**	0.002
12	**0.030**	0.001	**0.045**	0.001	**0.018**	0.003	**0.020**	0.002	**0.035**	0.004	**0.035**	0.004	**0.040**	0.005	**0.027**	0.010	**0.034**	0.005
13	**0.024**	0.003	**0.054**	0.003	**0.015**	0.003	**0.020**	0.004	**no sample***		**0.029**	0.003	**0.047**	0.003	**0.032**	0.006	**0.037**	0.007
14	**0.027**	0.002	0.000		**0.031**	0.001	0.001	<LoD	**no sample***		**0.030**	0.005	**0.031**	0.005	**0.033**	0.003	**0.039**	0.005
15	**0.028**	0.001	**0.066**	0.003	**0.122**	0.003	**0.029**	0.003	**no sample***		**0.028**	0.002	**no sample***		**0.035**	0.004	**0.037**	0.008
LoD	0.005		0.005		0.005		0.003		0.005		0.002		0.005		0.005		0.004	
LoQ	0.011		0.011		0.011		0.007		0.013		0.005		0.010		0.010		0.010	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 88: Chromium concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

Sediment core 1							Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	0.559	0.034	0.077	<LoD	**0.874**	0.066	0.047	<LoD	0.103	<LoD	**0.466**	0.039	0.238	<LoD	0.238	<LoD	0.166	0.017
-3	0.437	0.017	0.158	0.012	0.471	0.032	0.154	0.030	0.103	<LoD	**0.687**	0.038	0.238	<LoD	0.238	<LoD	0.218	0.044
-2	0.472	0.029	0.346	0.024	0.434	0.054	0.047	<LoD	0.103	<LoD	**0.578**	0.047	0.238	<LoD	0.827	0.068	0.215	0.023
-1	0.650	0.084	0.335	0.027	0.512	0.017	0.193	0.047	0.103	<LoD	**0.622**	0.033	0.238	<LoD	0.751	0.056	**0.426**	0.050
0	**1.186**	0.018	**0.822**	0.053	**1.374**	0.073	**1.940**	0.116	0.103	<LoD	**0.942**	0.051	0.238	<LoD	0.768	0.049	**0.924**	0.035
1	**1.273**	0.091	**1.271**	0.060	**1.759**	0.041	**0.453**	0.047	0.442	0.054	**1.205**	0.084	0.238	<LoD	**1.347**	0.089	**1.215**	0.050
2	**26.460**	3.512	**1.179**	0.043	**1.681**	0.050	**0.441**	0.037	**0.767**	0.082	**2.160**	0.081	0.637	0.078	**1.802**	0.139	**2.007**	0.042
3	**0.978**	0.063	**1.144**	0.059	**2.228**	0.060	**0.753**	0.071	**0.717**	0.063	**1.156**	0.056	0.238	<LoD	**1.659**	0.136	**1.931**	0.057
4	**0.919**	0.062	**0.819**	0.070	**1.666**	0.090	**0.773**	0.061	**0.839**	0.070	**1.225**	0.074	0.238	<LoD	**1.564**	0.087	**2.174**	0.106
5	**0.895**	0.037	**0.824**	0.075	**1.128**	0.075	**0.675**	0.048	**0.888**	0.029	**1.249**	0.099	0.551	0.018	**1.397**	0.104	**1.678**	0.098
6	0.817	0.054	**0.617**	0.033	**9.229**	4.030	**0.466**	0.048	**0.851**	0.064	**1.461**	0.069	0.521	0.038	**1.582**	0.152	**1.775**	0.131
7	**1.031**	0.084	**0.676**	0.007	**1.489**	0.102	**0.497**	0.036	**0.914**	0.058	**1.516**	0.036	1.066	0.079	**1.299**	0.096	**1.623**	0.058
8	**no sample***		**0.523**	0.037	**0.968**	0.022	**0.628**	0.054	**0.993**	0.074	**0.890**	0.052	0.670	0.059	**1.314**	0.067	**1.141**	0.063
9	**1.617**	0.068	**0.842**	0.040	**0.966**	0.025	**0.533**	0.049	**0.949**	0.094	**1.078**	0.066	**1.363**	0.116	**1.285**	0.094	**1.275**	0.097
10	**1.557**	0.057	**1.733**	0.044	**1.177**	0.029	**0.534**	0.048	**1.901**	0.135	**98.998**	2.497	**1.545**	0.087	**1.307**	0.116	**1.285**	0.122
11	**1.686**	0.085	**0.863**	0.028	**0.930**	0.075	**1.243**	0.109	**0.819**	0.071	**2.578**	0.141	**1.396**	0.094	**1.395**	0.036	**1.211**	0.024
12	**1.565**	0.032	**0.875**	0.023	**0.894**	0.044	**0.482**	0.045	**0.787**	0.064	**1.830**	0.074	**1.570**	0.030	**1.440**	0.125	**1.271**	0.107
13	**1.465**	0.046	**1.185**	0.031	**0.888**	0.022	**0.445**	0.030	**no sample***		**1.985**	0.155	**1.702**	0.040	**1.469**	0.111	**1.464**	0.129
14	**1.455**	0.049	0.000		**1.614**	0.055	0.047	<LoD	**no sample***		**1.860**	0.036	**1.313**	0.082	**2.140**	0.183	**1.568**	0.084
15	**1.574**	0.067	**1.014**	0.051	**4.458**	0.063	**0.571**	0.056	**no sample***		**1.956**	0.086	**no sample***		**1.620**	0.137	**1.142**	0.056
LoD	0.399		0.154		0.399		0.094		0.206		0.287		0.476		0.476		0.135	
LoQ	0.848		0.381		0.848		0.247		0.578		0.446		1.089		1.089		0.342	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 89: Cobalt concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.534**	0.045	**0.111**	0.010	**0.466**	0.022	0.151	0.023	**0.158**	0.036	**0.162**	0.009	**0.113**	0.013	**0.252**	0.012	**0.623**	0.014
-3	**0.498**	0.038	**0.102**	0.013	**0.415**	0.029	0.258	0.025	**0.175**	0.017	**0.205**	0.009	**0.121**	0.008	**0.349**	0.027	**0.776**	0.032
-2	**0.435**	0.017	**0.273**	0.022	**0.373**	0.028	0.064	<LoD	**0.238**	0.029	**0.162**	0.017	**0.205**	0.028	**1.059**	0.047	**0.693**	0.034
-1	**0.395**	0.022	**0.271**	0.023	**0.487**	0.021	0.318	0.022	**0.207**	0.010	**0.196**	0.019	**0.205**	0.023	**1.225**	0.083	**0.685**	0.039
0	**0.549**	0.022	**0.447**	0.038	**0.923**	0.030	0.237	0.023	**0.190**	0.027	**0.235**	0.022	**0.463**	0.037	**1.297**	0.080	**0.752**	0.044
1	**0.543**	0.023	**0.527**	0.031	**1.041**	0.021	0.231	0.014	**0.195**	0.027	**0.254**	0.024	**0.384**	0.010	**0.833**	0.035	**0.762**	0.061
2	**0.608**	0.044	**0.493**	0.049	**0.882**	0.047	0.154	0.024	**0.217**	0.031	**0.247**	0.019	**0.429**	0.034	**0.608**	0.055	**0.984**	0.075
3	**0.375**	0.031	**0.362**	0.035	**0.986**	0.028	0.272	0.030	**0.249**	0.020	**0.246**	0.025	**0.138**	0.017	**0.532**	0.007	**0.825**	0.065
4	**0.319**	0.022	**0.264**	0.026	**0.747**	0.037	0.236	0.011	**0.249**	0.010	**0.262**	0.023	**0.151**	0.018	**0.487**	0.061	**0.937**	0.036
5	**0.304**	0.024	**0.284**	0.028	**0.739**	0.049	0.233	0.020	**0.273**	0.041	**0.276**	0.018	**0.199**	0.026	**0.407**	0.052	**0.779**	0.018
6	**0.249**	0.021	**0.222**	0.026	**1.159**	0.042	0.190	0.013	**0.278**	0.059	**0.303**	0.015	**0.144**	0.016	**0.494**	0.030	**0.755**	0.038
7	**0.289**	0.037	**0.253**	0.019	**0.461**	0.033	0.196	0.020	**0.295**	0.026	**0.338**	0.018	**0.340**	0.029	**0.361**	0.015	**0.661**	0.059
8	**no sample***		**0.227**	0.014	**0.353**	0.031	0.255	0.021	**0.284**	0.043	**0.548**	0.040	**0.195**	0.030	**1.097**	0.053	**0.654**	0.047
9	**0.480**	0.023	**0.361**	0.014	**0.328**	0.016	0.242	0.019	**0.291**	0.049	**0.575**	0.041	**0.443**	0.046	**0.373**	0.036	**0.644**	0.058
10	**0.405**	0.023	**0.415**	0.016	**0.396**	0.034	0.238	0.009	**0.296**	0.028	**1.569**	0.085	**0.531**	0.047	**0.407**	0.062	**0.666**	0.039
11	**0.427**	0.030	**0.441**	0.023	**0.320**	0.013	0.249	0.025	**0.287**	0.032	**0.711**	0.074	**0.506**	0.028	**0.415**	0.028	**0.590**	0.052
12	**0.449**	0.018	**0.373**	0.014	**0.319**	0.020	0.255	0.021	**0.277**	0.006	**0.441**	0.043	**0.583**	0.043	**0.434**	0.047	**0.634**	0.052
13	**0.453**	0.018	**0.490**	0.015	**0.315**	0.015	0.244	0.023	**no sample***		**0.426**	0.015	**0.591**	0.045	**0.439**	0.025	**0.610**	0.045
14	**0.446**	0.017	0.000		**0.647**	0.016	0.064	<LoD	**no sample***		**0.463**	0.034	**0.411**	0.046	**0.463**	0.071	**0.668**	0.031
15	**0.472**	0.013	**0.383**	0.009	**1.338**	0.018	0.281	0.020	**no sample***		**0.451**	0.030	**no sample***		**0.515**	0.050	**0.524**	0.033
LoD	0.006		0.010		0.006		0.127		0.005		0.016		0.010		0.010		0.020	
LoQ	0.014		0.024		0.014		0.329		0.012		0.036		0.025		0.025		0.054	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 90: Copper concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**3.22**	0.08	**1.25**	0.04	**5.29**	0.43	**6.07**	0.26	**2.30**	0.03	**1.37**	0.04	**1.34**	0.07	**4.27**	0.09	**6.82**	0.14
-3	**1.31**	0.09	**1.37**	0.02	**13.82**	4.85	**4.73**	0.18	**2.01**	0.04	**1.89**	0.12	**1.29**	0.07	**4.51**	0.10	**6.59**	0.16
-2	0.26	<LoD	**1.74**	0.06	**5.75**	0.24	**2.84**	0.19	**2.01**	0.04	**5.20**	0.08	**0.96**	0.03	**4.76**	0.25	**3.47**	0.06
-1	0.26	<LoD	1.07	0.04	**5.29**	0.35	**4.20**	0.15	**2.12**	0.04	**0.91**	0.06	0.36	0.04	**2.66**	0.07	**1.09**	0.08
0	0.26	<LoD	0.63	0.02	**10.94**	3.25	**3.17**	0.16	1.01	0.05	0.46	0.03	0.36	0.05	**1.33**	0.04	0.20	<LoD
1	0.26	<LoD	0.61	0.03	0.66	0.09	**2.75**	0.05	0.30	<LoD	**0.85**	0.07	0.10	<LoD	**0.66**	0.05	0.20	<LoD
2	0.89	0.07	0.53	0.02	0.26	<LoD	**2.77**	0.03	**41.09**	0.80	**0.82**	0.03	0.10	<LoD	**0.95**	0.06	0.20	<LoD
3	0.26	<LoD	0.61	0.03	0.26	<LoD	**2.56**	0.14	0.30	<LoD	0.56	0.02	0.10	<LoD	**0.64**	0.02	0.20	<LoD
4	0.26	<LoD	0.60	0.04	0.26	<LoD	**2.79**	0.08	0.30	<LoD	**2.00**	0.08	0.10	<LoD	**0.57**	0.03	0.20	<LoD
5	0.26	<LoD	0.24	<LoD	0.26	<LoD	**2.42**	0.12	0.30	<LoD	**2.83**	0.03	0.10	<LoD	**0.84**	0.03	0.20	<LoD
6	0.26	<LoD	0.63	0.06	0.26	<LoD	**2.14**	0.09	0.30	<LoD	**0.86**	0.04	0.10	<LoD	0.39	0.06	0.20	<LoD
7	0.92	0.06	0.62	0.05	0.26	<LoD	**1.90**	0.11	0.30	<LoD	**1.08**	0.09	0.10	<LoD	0.35	0.03	0.20	<LoD
8	**no sample***		0.24	<LoD	0.26	<LoD	**1.71**	0.13	0.30	<LoD	**0.97**	0.06	0.10	<LoD	0.38	0.04	0.20	<LoD
9	**2.45**	0.07	0.24	<LoD	0.26	<LoD	1.45	0.03	0.93	0.04	0.56	0.04	**0.53**	0.02	0.36	0.02	0.20	<LoD
10	0.38	<LoD	**1.41**	0.03	0.26	<LoD	1.51	0.09	0.96	0.02	**3.13**	0.09	0.10	<LoD	**2.15**	0.06	0.20	<LoD
11	0.38	<LoD	0.24	<LoD	0.26	<LoD	**2.57**	0.10	0.98	0.06	**1.45**	0.05	0.10	<LoD	**11.62**	3.32	0.20	<LoD
12	0.38	<LoD	0.24	<LoD	0.26	<LoD	1.25	0.11	0.90	0.04	**0.66**	0.03	0.46	0.06	**0.93**	0.03	0.20	<LoD
13	0.38	<LoD	**1.34**	0.04	**10.56**	2.19	1.12	0.08	**no sample***		**0.69**	0.06	0.29	0.02	0.41	0.02	0.20	<LoD
14	0.38	<LoD	0.00		0.38	<LoD	**4.18**	3.55	**no sample***		**0.89**	0.07	0.10	<LoD	**0.65**	0.05	0.20	<LoD
15	0.38	<LoD	**1.42**	0.02	0.38	<LoD	0.32	<LoD	**no sample***		**1.02**	0.05	**no sample***		**2.32**	0.08	0.20	<LoD
LoD	0.51		0.47		0.51		0.64		0.59		0.28		0.19		0.19		0.40	
LoQ	1.10		1.14		1.10		1.63		1.28		0.61		0.51		0.51		0.95	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 91: Lead concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.415**	0.017	**0.055**	0.004	**0.641**	0.044	**0.105**	0.012	**0.084**	0.003	**0.104**	0.010	**0.076**	0.005	**0.039**	0.005	**0.059**	0.005
-3	**0.114**	0.008	**0.090**	0.006	**0.492**	0.009	**0.187**	0.008	**0.072**	0.005	**0.104**	0.008	**0.036**	0.007	**0.045**	0.003	**0.072**	0.015
-2	**0.072**	0.009	**0.060**	0.004	**0.099**	0.008	**0.021**	0.001	**0.176**	0.007	**0.262**	0.010	**0.042**	0.004	**0.082**	0.008	**0.058**	0.008
-1	**0.134**	0.013	**0.074**	0.004	**0.107**	0.006	**0.129**	0.006	**0.078**	0.006	**0.035**	0.004	**0.064**	0.003	0.020	0.004	**0.064**	0.008
0	**0.124**	0.010	**0.055**	0.003	**1.846**	0.041	**0.266**	0.007	**0.062**	0.003	**0.064**	0.006	**0.051**	0.012	0.007	<LoD	**0.027**	0.006
1	**0.078**	0.005	**0.182**	0.007	**0.042**	0.004	**0.135**	0.006	**0.107**	0.005	**0.074**	0.003	0.007	<LoD	0.007	<LoD	**0.023**	0.005
2	**0.055**	0.005	**0.050**	0.005	**0.067**	0.006	**0.142**	0.006	**0.760**	0.028	**1.349**	0.039	0.014	0.005	**0.069**	0.005	**0.024**	0.007
3	**0.070**	0.006	**0.128**	0.005	**0.122**	0.009	**0.030**	0.001	**0.065**	0.006	**0.050**	0.004	0.007	<LoD	0.014	0.006	**0.022**	0.012
4	**0.030**	0.005	**0.371**	0.009	**0.073**	0.006	**0.270**	0.010	**0.098**	0.006	**0.236**	0.010	0.007	<LoD	**0.061**	0.007	**0.043**	0.008
5	**0.221**	0.020	**0.217**	0.007	**0.094**	0.007	**0.069**	0.007	**0.163**	0.009	**0.185**	0.012	0.007	<LoD	**0.570**	0.025	**0.028**	0.007
6	**0.326**	0.011	**0.208**	0.016	**0.172**	0.011	**0.033**	0.004	**0.090**	0.007	**0.344**	0.023	**0.048**	0.005	**0.043**	0.003	**0.039**	0.005
7	**0.100**	0.007	**0.182**	0.003	**0.054**	0.003	**0.036**	0.003	**0.149**	0.012	**0.202**	0.008	**0.033**	0.004	**0.053**	0.012	**0.107**	0.006
8	**no sample***		**0.067**	0.006	0.012	0.002	**0.032**	0.002	**0.131**	0.007	**0.162**	0.009	0.007	<LoD	**0.055**	0.005	**0.025**	0.006
9	**1.324**	0.021	**0.111**	0.005	**0.067**	0.006	**0.062**	0.004	**0.053**	0.003	**0.072**	0.010	**0.093**	0.004	**0.062**	0.009	**0.034**	0.004
10	**0.276**	0.006	**0.499**	0.006	**0.082**	0.007	**0.093**	0.005	**0.157**	0.011	**0.307**	0.009	**0.046**	0.008	**0.155**	0.012	**0.025**	0.004
11	**0.387**	0.015	**0.231**	0.004	**0.055**	0.004	**0.109**	0.003	**0.668**	0.018	**0.390**	0.008	**0.061**	0.006	**0.124**	0.005	**0.047**	0.005
12	**0.294**	0.005	**0.327**	0.009	**0.275**	0.014	**0.110**	0.005	**0.217**	0.017	**0.148**	0.011	**0.197**	0.013	**0.069**	0.002	**0.032**	0.007
13	**0.304**	0.010	**0.422**	0.006	**0.984**	0.026	**0.090**	0.003	**no sample***		**0.287**	0.016	**0.142**	0.006	**0.082**	0.007	**0.038**	0.006
14	**0.208**	0.007	0.000		**0.297**	0.005	**0.085**	0.068	**no sample***		**0.365**	0.016	**0.062**	0.007	**0.105**	0.006	**0.023**	0.006
15	**0.394**	0.008	**0.587**	0.007	**4.365**	0.012	**0.026**	0.029	**no sample***		**0.228**	0.020	**no sample***		**0.288**	0.008	**0.050**	0.007
LoD	0.010		0.009		0.010		0.006		0.006		0.007		0.014		0.014		0.008	
LoQ	0.027		0.023		0.027		0.016		0.015		0.017		0.031		0.031		0.022	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 92: Molybdenum concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**5.444**	0.147	**2.614**	0.071	**9.886**	0.540	**3.211**	0.108	**3.379**	0.250	**2.179**	0.066	**1.589**	0.126	**3.207**	0.227	**4.011**	0.100
-3	**4.887**	0.107	**2.442**	0.110	**9.330**	0.280	**4.250**	0.135	**3.102**	0.227	**2.657**	0.153	**1.574**	0.109	**2.407**	0.111	**3.604**	0.091
-2	**4.342**	0.175	**4.860**	0.285	**8.827**	0.475	**1.700**	0.124	**3.684**	0.248	**2.072**	0.087	**1.804**	0.073	**5.098**	0.102	**2.697**	0.116
-1	**3.603**	0.094	**3.335**	0.189	**8.308**	0.640	**4.566**	0.199	**3.338**	0.214	**2.284**	0.110	**1.012**	0.044	**4.757**	0.176	**2.157**	0.088
0	**4.763**	0.143	**3.478**	0.113	**7.996**	0.456	**14.821**	0.000	**2.784**	0.214	**1.698**	0.089	**1.163**	0.070	**4.253**	0.249	**2.137**	0.112
1	**3.657**	0.107	**2.448**	0.051	**7.220**	0.243	**3.585**	0.211	**2.200**	0.133	**1.619**	0.090	**0.857**	0.051	**3.410**	0.143	**1.807**	0.102
2	**3.698**	0.174	**1.948**	0.075	**4.569**	0.288	**1.880**	0.159	**2.036**	0.144	**1.531**	0.055	**1.305**	0.097	**2.431**	0.107	**1.905**	0.060
3	**2.727**	0.075	**1.771**	0.099	**4.570**	0.205	**2.669**	0.182	**1.805**	0.134	**1.417**	0.075	**0.535**	0.036	**1.798**	0.076	**1.410**	0.041
4	**2.411**	0.110	**1.505**	0.057	**2.602**	0.157	**2.310**	0.216	**1.792**	0.108	**1.368**	0.040	**0.500**	0.018	**1.316**	0.106	**1.265**	0.068
5	**2.112**	0.075	**1.469**	0.052	**0.344**	0.020	**2.213**	0.156	**1.710**	0.132	**1.384**	0.065	**0.525**	0.035	**0.942**	0.079	**0.865**	0.050
6	**1.714**	0.059	**1.153**	0.043	**121.304**	4.721	**1.611**	0.034	**1.642**	0.153	**1.323**	0.129	**0.317**	0.034	**0.938**	0.045	**0.769**	0.061
7	**1.367**	0.088	**1.030**	0.069	**7.275**	0.475	**1.465**	0.068	**1.548**	0.142	**1.098**	0.088	**0.844**	0.073	**0.658**	0.059	**0.661**	0.031
8	**no sample***		**0.754**	0.035	**0.741**	0.021	**1.460**	0.072	**1.418**	0.084	**2.392**	0.145	**0.429**	0.027	**0.651**	0.047	**0.577**	0.048
9	**1.397**	0.039	**1.019**	0.033	**0.627**	0.021	**1.095**	0.048	**1.216**	0.065	**1.812**	0.092	**0.954**	0.046	**0.495**	0.024	**0.515**	0.048
10	**1.165**	0.034	**0.891**	0.028	**0.719**	0.036	**0.914**	0.059	**0.962**	0.067	**2.839**	0.092	**0.807**	0.038	**0.409**	0.010	**0.448**	0.029
11	**0.855**	0.014	**0.753**	0.016	**0.525**	0.036	**0.814**	0.028	**0.762**	0.060	**0.530**	0.028	**0.612**	0.048	**0.337**	0.013	**0.378**	0.039
12	**0.780**	0.018	**0.494**	0.017	**0.438**	0.035	**0.641**	0.048	**0.655**	0.030	**0.503**	0.039	**0.536**	0.030	**0.267**	0.016	**0.320**	0.013
13	**0.505**	0.011	**0.408**	0.008	**0.355**	0.032	**0.552**	0.033	**no sample***		**0.384**	0.026	**0.430**	0.022	**0.216**	0.009	**0.272**	0.023
14	**0.443**	0.012	0.000		**0.544**	0.012	0.061	0.022	**no sample***		**0.339**	0.020	0.205	0.014	0.182	0.012	**0.228**	0.008
15	**0.411**	0.005	**0.358**	0.010	**1.352**	0.013	**0.420**	0.017	**no sample***		**0.269**	0.014	**no sample***		0.157	0.017	**0.815**	0.035
LoD	0.076		0.062		0.076		0.031		0.089		0.051		0.073		0.073		0.072	
LoQ	0.217		0.170		0.217		0.090		0.244		0.148		0.213		0.213		0.216	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 93: Nickel concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**7.55**	0.17	**1.39**	0.11	**5.29**	0.06	**3.14**	0.26	**2.66**	0.21	**1.44**	0.05	0.66	<LoD	2.50	0.22	10.23	0.71
-3	**2.37**	0.09	**1.48**	0.06	**5.55**	0.16	**3.77**	0.14	**2.36**	0.16	**2.03**	0.11	0.66	<LoD	**4.35**	0.21	6.67	0.66
-2	**2.21**	0.11	**3.15**	0.16	**5.75**	0.33	**2.33**	0.15	**2.84**	0.08	**1.51**	0.07	1.65	0.12	**15.56**	0.91	2.61	<LoD
-1	**1.39**	0.10	**1.81**	0.10	**7.13**	0.34	**3.45**	0.09	**2.64**	0.13	**1.59**	0.10	2.11	0.19	**17.17**	1.13	2.61	<LoD
0	**1.90**	0.10	**1.71**	0.04	**6.60**	0.48	**3.64**	0.11	**1.96**	0.04	**1.07**	0.10	1.99	0.05	**22.01**	3.01	9.32	1.06
1	**1.31**	0.09	**1.35**	0.05	**3.77**	0.28	1.99	0.12	**1.55**	0.08	**0.99**	0.10	1.82	0.08	**7.98**	0.43	11.86	1.92
2	**12.74**	2.73	1.01	0.06	**1.98**	0.09	1.64	0.06	1.41	0.07	**1.37**	0.08	2.15	0.14	**7.72**	0.70	**160.67**	17.82
3	0.80	0.11	**2.63**	0.09	**2.15**	0.08	1.82	0.15	1.10	0.05	**0.83**	0.05	0.66	<LoD	**6.78**	0.54	**22.73**	7.62
4	0.65	0.10	0.67	0.06	**1.27**	0.12	1.75	0.05	0.94	0.03	**0.88**	0.04	1.41	0.12	**5.97**	0.84	**19.52**	4.98
5	**0.86**	0.05	0.80	0.08	**1.24**	0.03	**2.63**	0.23	0.98	0.03	**0.91**	0.03	1.48	0.11	**4.77**	0.32	13.80	1.30
6	0.64	0.09	0.53	0.07	**5.51**	0.16	**2.46**	0.18	1.06	0.13	**1.20**	0.07	1.46	0.11	**6.25**	0.59	2.61	<LoD
7	0.54	0.06	0.78	0.07	0.67	0.06	**4.35**	0.21	0.92	0.08	**0.80**	0.05	1.87	0.17	**6.43**	0.43	**15.02**	1.87
8	**no sample***		0.23	<LoD	0.19	<LoD	**10.05**	1.97	0.91	0.08	**2.00**	0.07	1.44	0.17	**33.44**	3.90	**35.77**	45.58
9	0.82	0.03	0.23	<LoD	0.19	<LoD	**6.36**	1.08	0.82	0.07	**1.40**	0.07	2.02	0.17	1.84	0.17	12.36	2.53
10	**1.26**	0.07	0.86	0.05	0.54	0.03	**6.90**	0.37	1.33	0.12	**34.36**	1.79	0.66	<LoD	1.54	0.12	2.61	<LoD
11	**0.97**	0.04	0.23	<LoD	0.19	<LoD	**9.24**	0.41	0.79	0.10	**1.80**	0.14	0.66	<LoD	1.40	0.10	2.61	<LoD
12	0.65	0.08	0.23	<LoD	0.19	<LoD	**9.59**	0.39	0.70	0.08	**0.74**	0.07	0.66	<LoD	1.41	0.18	2.61	<LoD
13	0.29	<LoD	0.77	0.05	0.19	<LoD	**11.61**	1.21	**no sample***		**0.95**	0.13	0.66	<LoD	3.15	0.20	2.61	<LoD
14	0.58	0.03	0.00		0.29	<LoD	**59.10**	75.17	**no sample***		**0.84**	0.06	0.66	<LoD	2.08	0.26	2.61	<LoD
15	**0.97**	0.05	0.69	<LoD	0.00	0.00	**4.43**	1.96	**no sample***		**0.85**	0.07	**no sample***		0.66	<LoD	2.61	<LoD
LoD	0.38		0.46		0.38		1.28		0.50		0.10		1.33		1.33		5.22	
LoQ	0.86		1.16		0.86		2.14		1.42		0.24		3.58		3.58		14.93	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 94: Selenium concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	0.910	0.161	0.305	<LoD	1.080	0.208	0.133	<LoD	0.541	0.084	0.429	0.027	0.220	<LoD	0.656	0.078	0.664	0.063
-3	0.977	0.143	0.305	<LoD	1.139	0.051	0.133	<LoD	0.263	<LoD	0.440	0.077	0.220	<LoD	0.581	0.239	0.866	0.154
-2	1.028	0.158	0.756	0.063	1.164	0.176	0.133	<LoD	0.263	<LoD	0.446	0.024	0.459	0.084	0.766	0.146	0.621	0.259
-1	0.890	0.059	0.756	0.133	1.177	0.109	0.351	0.046	0.263	<LoD	0.508	0.064	0.220	<LoD	0.693	0.238	0.675	0.177
0	1.223	0.181	0.984	0.124	**1.608**	0.124	0.329	0.048	0.263	<LoD	0.561	0.070	0.220	<LoD	**0.895**	0.083	0.996	0.150
1	1.149	0.121	1.143	0.215	**1.599**	0.197	0.356	0.073	0.540	0.163	0.617	0.063	0.220	<LoD	**0.989**	0.224	1.170	0.125
2	1.059	0.123	1.061	0.183	**1.485**	0.144	0.358	0.072	0.263	<LoD	**0.778**	0.068	0.220	<LoD	**1.217**	0.187	**1.505**	0.292
3	1.045	0.107	1.081	0.063	**1.728**	0.199	0.420	0.095	0.635	0.122	**0.814**	0.037	0.220	<LoD	**1.066**	0.036	**1.617**	0.211
4	0.964	0.092	0.789	0.143	**1.555**	0.234	0.408	0.104	0.660	0.114	**0.891**	0.077	0.220	<LoD	**1.062**	0.285	**1.649**	0.274
5	0.841	0.108	0.866	0.113	0.995	0.188	0.414	0.080	0.574	0.132	**0.884**	0.152	0.598	0.216	**0.997**	0.233	1.278	0.330
6	0.856	0.104	0.911	0.096	**1.353**	0.180	0.371	0.023	0.624	0.117	**0.857**	0.056	0.220	<LoD	**0.873**	0.091	1.318	0.274
7	0.809	0.107	0.880	0.167	1.212	0.028	0.290	0.038	0.717	0.210	**0.941**	0.149	**0.814**	0.137	**0.817**	0.147	1.258	0.285
8	**no sample***		0.816	0.036	1.076	0.135	0.455	0.048	0.668	0.074	**0.881**	0.154	0.526	0.102	**0.873**	0.204	0.799	0.199
9	**1.680**	0.106	**1.583**	0.143	1.018	0.118	0.294	0.063	0.654	0.092	**0.941**	0.110	**0.870**	0.082	**0.880**	0.217	0.912	0.236
10	**1.717**	0.045	**1.707**	0.095	1.064	0.124	0.295	0.052	0.580	0.122	**0.933**	0.082	**0.941**	0.240	**0.866**	0.127	0.960	0.270
11	**1.747**	0.058	**1.497**	0.141	1.061	0.036	0.383	0.073	0.713	0.101	**0.910**	0.074	**0.961**	0.151	**1.019**	0.141	0.857	0.421
12	**1.765**	0.086	**1.464**	0.065	0.950	0.127	0.370	0.073	0.669	0.059	**1.107**	0.112	**0.935**	0.145	**0.908**	0.089	0.752	0.326
13	**1.805**	0.115	**1.558**	0.063	1.047	0.098	0.374	0.157	**no sample***		**1.082**	0.076	**1.049**	0.163	**0.930**	0.088	0.813	0.153
14	**1.605**	0.232	0.000		**1.899**	0.150	0.133	<LoD	**no sample***		**1.189**	0.138	**0.885**	0.201	**0.931**	0.129	0.781	0.217
15	**1.737**	0.110	**2.185**	0.067	**6.002**	0.058	0.300	0.115	**no sample***		**1.169**	0.084	**no sample***		**0.980**	0.123	0.677	0.207
LoD	0.696		0.609		0.696		0.267		0.526		0.385		0.441		0.441		0.539	
LoQ	1.295		1.267		1.295		0.562		1.157		0.621		0.796		0.796		1.424	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 95: Silver concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**0.098**	0.008	0.004	0.002	**0.051**	0.005	**0.025**	0.003	0.023	0.002	**0.011**	0.001	0.008	0.003	**0.049**	0.007	**0.096**	0.010
-3	**0.073**	0.003	**0.005**	0.001	**0.044**	0.004	**0.025**	0.003	0.014	0.001	**0.016**	0.002	0.003	<LoD	**0.026**	0.006	**0.072**	0.007
-2	**0.075**	0.008	**0.007**	0.002	**0.092**	0.010	0.007	0.001	0.015	0.002	**0.017**	0.001	0.003	<LoD	**0.025**	0.004	**0.051**	0.004
-1	**0.055**	0.004	**0.011**	0.002	**0.062**	0.007	**0.028**	0.003	0.015	0.003	**0.013**	0.002	0.003	<LoD	**0.026**	0.004	**0.020**	0.003
0	**0.068**	0.004	**0.026**	0.002	**0.059**	0.005	0.011	0.001	0.012	0.002	**0.014**	0.002	0.003	<LoD	0.009	0.002	0.006	0.003
1	**0.064**	0.004	**0.037**	0.002	**0.019**	0.003	**0.029**	0.002	0.011	0.003	**0.021**	0.003	0.003	<LoD	0.003	<LoD	0.002	<LoD
2	**0.058**	0.005	**0.036**	0.003	**0.027**	0.003	**0.034**	0.002	**0.028**	0.004	**0.020**	0.001	0.003	<LoD	**0.038**	0.007	0.007	0.003
3	**0.059**	0.009	**0.040**	0.003	**0.063**	0.003	**0.029**	0.003	0.022	0.002	**0.015**	0.003	0.003	<LoD	**0.036**	0.004	**0.022**	0.003
4	**0.050**	0.007	**0.031**	0.003	**0.068**	0.005	**0.034**	0.003	0.022	0.002	**0.015**	0.002	0.003	<LoD	**0.035**	0.006	**0.027**	0.003
5	**0.050**	0.004	**0.033**	0.003	**0.013**	0.002	**0.034**	0.004	0.023	0.001	**0.081**	0.005	0.003	<LoD	**0.041**	0.004	**0.029**	0.006
6	**0.057**	0.004	**0.032**	0.003	**0.059**	0.006	**0.018**	0.001	**0.570**	0.010	**0.010**	0.003	0.003	<LoD	**0.045**	0.004	**0.033**	0.006
7	**0.048**	0.004	**0.025**	0.004	**0.051**	0.005	**0.019**	0.002	0.014	0.002	**0.011**	0.003	0.008	0.002	**0.038**	0.003	**0.019**	0.003
8	**no sample***		**0.017**	0.002	**0.047**	0.006	**0.019**	0.002	0.015	0.004	**0.011**	0.002	0.003	<LoD	**0.027**	0.005	**0.013**	0.004
9	**0.077**	0.005	**0.033**	0.002	**0.044**	0.005	**0.020**	0.003	0.016	0.002	**0.006**	0.001	**0.019**	0.002	**0.026**	0.005	**0.012**	0.001
10	**0.078**	0.002	**0.034**	0.002	**0.045**	0.004	**0.020**	0.002	**0.062**	0.004	**0.009**	0.002	**0.019**	0.003	**0.029**	0.004	0.008	0.002
11	**0.086**	0.002	**0.037**	0.004	**0.060**	0.005	**0.020**	0.003	0.019	0.002	**0.010**	0.002	**0.020**	0.002	**0.037**	0.003	**0.017**	0.003
12	**0.023**	0.002	**0.026**	0.003	**0.034**	0.004	**0.017**	0.002	**0.030**	0.003	**0.014**	0.002	**0.025**	0.002	**0.022**	0.003	**0.012**	0.003
13	**0.019**	0.001	**0.043**	0.002	**0.036**	0.006	**0.023**	0.002	**no sample***		**0.013**	0.002	**0.021**	0.004	**0.020**	0.004	0.008	0.001
14	**0.014**	0.002	0.000		**0.062**	0.003	0.003	<LoD	**no sample***		**0.030**	0.002	**0.016**	0.003	**0.022**	0.002	0.006	0.001
15	**0.033**	0.003	**0.058**	0.001	**0.212**	0.003	**0.033**	0.003	**no sample***		**0.012**	0.001	**no sample***		**0.026**	0.005	0.006	0.002
LoD	0.001		0.002		0.001		0.005		0.008		0.002		0.006		0.006		0.004	
LoQ	0.003		0.004		0.003		0.015		0.023		0.005		0.016		0.016		0.009	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 96: Tin concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**3.621**	0.251	**0.508**	0.076	**2.526**	0.299	**0.914**	0.076	0.465	0.061	**0.189**	0.042	**0.264**	0.083	0.164	0.043	0.328	0.085
-3	**0.631**	0.072	0.302	0.055	**1.554**	0.127	**0.758**	0.056	0.326	0.055	**0.185**	0.057	0.139	0.053	0.088	0.029	0.316	0.103
-2	0.041	<LoD	**0.468**	0.060	**1.077**	0.026	**0.229**	0.038	0.305	0.098	**0.155**	0.036	0.099	0.049	**0.348**	0.064	0.235	0.061
-1	0.113	0.056	**0.363**	0.048	**0.648**	0.085	**0.910**	0.115	0.315	0.101	**0.210**	0.078	0.039	<LoD	**0.264**	0.027	0.238	0.106
0	**0.604**	0.048	**0.788**	0.025	**0.998**	0.080	**0.544**	0.092	0.400	0.051	**0.405**	0.042	0.104	0.046	**0.323**	0.042	**0.686**	0.048
1	**0.765**	0.081	**1.101**	0.099	**0.963**	0.067	**0.785**	0.073	**0.665**	0.077	**0.629**	0.085	0.164	0.045	**0.732**	0.096	**0.900**	0.051
2	**0.688**	0.161	**1.198**	0.095	**1.138**	0.082	**0.671**	0.072	**255.322**	20.820	**0.550**	0.079	**0.368**	0.093	**1.276**	0.139	**1.449**	0.158
3	**0.544**	0.096	**1.039**	0.102	**1.627**	0.148	**1.161**	0.114	**1.656**	0.116	**0.599**	0.088	0.172	0.050	**1.255**	0.186	**1.590**	0.277
4	**0.464**	0.070	**0.876**	0.035	**1.321**	0.145	**0.978**	0.133	**1.038**	0.089	**0.610**	0.166	**0.254**	0.033	**1.113**	0.078	**1.682**	0.231
5	**0.607**	0.100	**0.762**	0.057	0.041	<LoD	**0.954**	0.064	**0.954**	0.067	**0.723**	0.119	**0.307**	0.039	**0.886**	0.150	**1.335**	0.188
6	**0.467**	0.050	**0.694**	0.045	**1.016**	0.089	**0.608**	0.057	**0.918**	0.132	**0.733**	0.133	**0.236**	0.036	**1.137**	0.119	**1.332**	0.126
7	**0.597**	0.115	**0.651**	0.078	**0.856**	0.141	**0.727**	0.095	**0.906**	0.151	**0.801**	0.082	**0.692**	0.129	**0.902**	0.090	**1.200**	0.188
8	**no sample***		**0.646**	0.021	**0.554**	0.030	**0.768**	0.051	**1.098**	0.096	**0.095**	0.071	**0.353**	0.107	**0.875**	0.083	**0.832**	0.081
9	**0.648**	0.067	**1.084**	0.051	**0.454**	0.064	**0.682**	0.048	**0.872**	0.088	**0.101**	0.051	**0.937**	0.153	**0.935**	0.096	**0.869**	0.133
10	**0.555**	0.061	**1.025**	0.052	**0.701**	0.061	**0.607**	0.058	**1.106**	0.135	**0.284**	0.104	**1.181**	0.079	**0.923**	0.219	**0.900**	0.224
11	**0.706**	0.065	**1.034**	0.067	**0.494**	0.039	**0.582**	0.051	**0.923**	0.139	**0.476**	0.071	**0.980**	0.093	**1.110**	0.114	**0.803**	0.163
12	**0.735**	0.049	**1.205**	0.063	**0.369**	0.037	**0.595**	0.039	**0.878**	0.132	**0.984**	0.142	**1.186**	0.132	**0.952**	0.115	**0.953**	0.151
13	**0.880**	0.083	**1.272**	0.096	**0.405**	0.032	**0.656**	0.034	**no sample***		**0.866**	0.119	**1.350**	0.159	**1.007**	0.067	**1.071**	0.141
14	**1.022**	0.084	0.000		**0.717**	0.053	0.074	0.058	**no sample***		**0.789**	0.062	**0.941**	0.111	**1.073**	0.235	**1.227**	0.142
15	**1.033**	0.076	**1.750**	0.052	**1.787**	0.035	**0.652**	0.120	**no sample***		**0.827**	0.092	**no sample***		**1.034**	0.158	**0.841**	0.115
LoD	0.083		0.125		0.083		0.033		0.204		0.027		0.078		0.078		0.134	
LoQ	0.222		0.357		0.222		0.087		0.547		0.054		0.193		0.193		0.346	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 97: Titanium concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	0.259	0.023	0.332	<LoD	**0.504**	0.047	0.181	<LoD	0.107	<LoD	0.164	<LoD	0.129	0.016	0.149	0.028	0.192	<LoD
-3	**0.348**	0.026	0.332	<LoD	**0.304**	0.005	0.181	<LoD	0.107	<LoD	0.164	<LoD	0.062	<LoD	0.126	0.041	0.192	<LoD
-2	**0.356**	0.021	0.332	<LoD	**0.294**	0.020	0.181	<LoD	0.107	<LoD	0.164	<LoD	0.062	<LoD	**0.397**	0.040	0.192	<LoD
-1	**1.054**	0.066	0.332	<LoD	**0.422**	0.023	0.181	<LoD	0.107	<LoD	0.339	0.037	0.062	<LoD	**0.497**	0.021	0.192	<LoD
0	**1.415**	0.106	1.500	0.104	**2.226**	0.060	0.181	<LoD	0.216	0.045	**1.771**	0.050	0.174	0.029	**0.702**	0.082	**2.062**	0.063
1	**1.884**	0.105	**3.568**	0.186	**3.404**	0.142	**1.004**	0.087	**1.565**	0.150	**2.560**	0.079	**0.486**	0.028	**2.131**	0.119	**2.349**	0.189
2	**1.721**	0.064	**3.220**	0.099	**4.067**	0.244	**0.923**	0.075	**2.198**	0.262	**2.541**	0.095	**0.822**	0.103	**4.523**	0.218	**4.851**	0.108
3	**1.545**	0.081	**3.087**	0.184	**5.687**	0.166	**2.062**	0.079	**2.632**	0.176	**2.952**	0.095	**0.417**	0.039	**4.279**	0.176	**5.472**	0.228
4	**1.513**	0.084	**2.489**	0.153	**4.631**	0.150	**2.051**	0.095	**2.903**	0.203	**3.135**	0.179	**0.556**	0.037	**3.747**	0.268	**6.275**	0.254
5	**1.690**	0.079	**3.671**	0.228	**1.790**	0.124	**2.045**	0.202	**3.173**	0.313	**3.420**	0.192	**0.769**	0.073	**2.983**	0.282	**4.754**	0.231
6	**1.400**	0.043	**2.043**	0.154	**3.978**	0.193	**1.179**	0.106	**3.369**	0.269	**3.953**	0.294	**0.755**	0.053	**3.858**	0.169	**4.847**	0.338
7	**1.375**	0.083	**2.129**	0.055	**3.007**	0.234	**1.124**	0.102	**3.532**	0.178	**4.265**	0.252	**2.133**	0.187	**2.828**	0.129	**4.440**	0.240
8	**no sample***		**1.790**	0.073	**2.448**	0.134	**1.505**	0.102	**3.542**	0.347	0.718	0.027	**1.231**	0.064	**3.419**	0.066	**2.238**	0.217
9	**2.400**	0.085	**2.827**	0.101	**2.391**	0.097	**1.329**	0.029	**3.484**	0.298	**0.971**	0.070	**3.244**	0.217	**3.248**	0.139	**2.482**	0.145
10	**2.782**	0.088	**3.458**	0.070	**2.938**	0.044	**1.234**	0.060	**3.443**	0.345	**1.863**	0.148	**3.893**	0.185	**3.500**	0.130	**2.506**	0.159
11	**2.163**	0.076	**3.070**	0.100	**2.200**	0.119	**1.330**	0.060	**2.924**	0.229	**3.366**	0.154	**3.451**	0.142	**3.790**	0.209	**2.450**	0.109
12	**2.615**	0.095	**2.955**	0.127	**1.940**	0.098	**1.224**	0.094	**2.513**	0.231	**4.064**	0.134	**3.906**	0.201	**3.489**	0.241	**2.974**	0.174
13	**2.354**	0.109	**3.192**	0.032	**1.822**	0.097	**1.222**	0.101	**no sample***		**4.152**	0.172	**4.416**	0.165	**3.724**	0.119	**3.639**	0.423
14	**2.172**	0.080	0.000		**2.995**	0.089	0.181	<LoD	**no sample***		**4.164**	0.143	**3.370**	0.092	**4.003**	0.238	**4.072**	0.264
15	**2.272**	0.044	**2.525**	0.077	**7.652**	0.039	**1.463**	0.100	**no sample***		**4.198**	0.193	**no sample***		**3.709**	0.165	**2.994**	0.192
LoD	0.099		0.665		0.099		0.363		0.213		0.328		0.124		0.124		0.384	
LoQ	0.265		1.674		0.265		0.450		0.578		0.845		0.299		0.299		0.950	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 98: Vanadium concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**1.607**	0.050	**0.629**	0.028	**2.063**	0.120	**1.346**	0.056	**1.015**	0.088	**0.838**	0.070	**1.118**	0.070	**1.165**	0.074	**1.170**	0.033
-3	**1.111**	0.076	**0.588**	0.015	**1.932**	0.078	**1.716**	0.066	**1.298**	0.082	**1.089**	0.058	**1.223**	0.074	**0.948**	0.059	**1.097**	0.018
-2	**1.299**	0.068	**1.434**	0.071	**1.818**	0.014	**0.598**	0.043	**1.567**	0.115	**0.830**	0.057	**1.227**	0.093	**1.672**	0.100	**1.039**	0.048
-1	**2.883**	0.135	**1.472**	0.041	**2.278**	0.115	**1.669**	0.071	**1.346**	0.093	**1.134**	0.047	**0.693**	0.022	**1.084**	0.046	**1.967**	0.112
0	**6.759**	0.190	**5.100**	0.295	**7.915**	0.196	**1.629**	0.082	**1.362**	0.110	**3.115**	0.193	**1.237**	0.094	**2.562**	0.068	**4.740**	0.160
1	**7.498**	0.320	**8.577**	0.248	**9.442**	0.193	**3.598**	0.181	**3.470**	0.287	**3.930**	0.087	**1.547**	0.095	**7.472**	0.069	**7.008**	0.194
2	**6.437**	0.185	**8.141**	0.039	**9.084**	0.520	**3.401**	0.302	**5.109**	0.389	**4.144**	0.103	**3.735**	0.252	**9.816**	0.406	**11.058**	0.225
3	**5.197**	0.231	**7.043**	0.234	**12.167**	0.496	**6.102**	0.388	**5.675**	0.435	**4.502**	0.193	**1.772**	0.028	**9.921**	0.296	**9.669**	0.289
4	**4.487**	0.155	**5.028**	0.117	**9.339**	0.295	**5.577**	0.407	**5.901**	0.377	**4.893**	0.283	**2.034**	0.097	**8.378**	0.272	**10.115**	0.406
5	**4.181**	0.127	**4.690**	0.102	**3.148**	0.193	**5.602**	0.364	**6.376**	0.526	**5.176**	0.215	**2.495**	0.081	**6.083**	0.120	**7.389**	0.156
6	**3.282**	0.104	**3.618**	0.143	**6.872**	0.198	**3.868**	0.069	**6.985**	0.482	**5.938**	0.454	**1.857**	0.118	**7.128**	0.140	**7.737**	0.340
7	**3.304**	0.268	**3.499**	0.115	**5.320**	0.328	**3.515**	0.102	**7.220**	0.594	**5.841**	0.322	**4.595**	0.266	**5.214**	0.243	**6.954**	0.134
8	**no sample***		**2.990**	0.072	**4.275**	0.119	**3.947**	0.138	**7.136**	0.518	**1.022**	0.057	**2.632**	0.089	**5.497**	0.328	**6.476**	0.282
9	**4.435**	0.114	**4.819**	0.147	**4.160**	0.116	**3.361**	0.116	**6.440**	0.497	**1.450**	0.076	**6.156**	0.216	**5.559**	0.243	**6.191**	0.304
10	**4.591**	0.096	**4.632**	0.093	**5.017**	0.052	**3.048**	0.149	**5.968**	0.413	**2.420**	0.084	**6.808**	0.352	**5.389**	0.262	**5.956**	0.401
11	**4.458**	0.167	**4.465**	0.088	**3.672**	0.125	**3.102**	0.141	**5.174**	0.372	**2.850**	0.125	**5.367**	0.136	**5.198**	0.217	**5.587**	0.229
12	**4.338**	0.157	**4.341**	0.118	**3.128**	0.051	**2.993**	0.123	**4.532**	0.218	**4.447**	0.236	**5.634**	0.238	**5.126**	0.228	**5.409**	0.310
13	**4.194**	0.140	**4.563**	0.096	**2.737**	0.045	**2.799**	0.120	**no sample***		**4.367**	0.213	**6.107**	0.219	**5.032**	0.190	**5.213**	0.238
14	**4.276**	0.088	0.000		**4.735**	0.113	**0.357**	0.144	**no sample***		**4.296**	0.220	**4.211**	0.210	**4.920**	0.320	**4.884**	0.158
15	**4.368**	0.106	**4.018**	0.066	**10.291**	0.063	**3.256**	0.226	**no sample***		**4.156**	0.228	**no sample***		**5.069**	0.251	**3.455**	0.151
LoD	0.066		0.014		0.066		0.078		0.228		0.009		0.150		0.150		0.013	
LoQ	0.189		0.038		0.189		0.120		0.622		0.023		0.417		0.417		0.035	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 99: Zink concentrations across the SWI of the sediment cores of sampling site 4. Values <LoD were removed from the data set. Values > LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sediment core 1						Sediment core 2						Sediment core 3					
Depth	Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3		Profile 1		Profile 2		Profile 3	
(cm)	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-4	**46.67**	1.08	**7.84**	0.41	**39.26**	0.91	**7.82**	0.28	**5.33**	0.22	**9.00**	0.37	**19.61**	0.89	**49.21**	0.59	**34.62**	0.79
-3	**9.26**	0.22	**8.06**	0.66	**26.95**	1.44	**11.11**	0.65	**7.57**	0.51	**14.89**	0.58	**11.27**	0.61	**34.04**	0.25	**36.63**	0.64
-2	**11.36**	0.27	**10.72**	0.52	**13.81**	0.56	**1.94**	0.12	**18.66**	0.55	**15.14**	0.44	**11.17**	0.59	**48.03**	1.81	**128.48**	2.19
-1	**10.71**	0.71	**9.15**	0.43	**14.97**	0.79	**11.40**	0.34	**12.77**	0.31	**9.13**	0.29	**29.46**	0.22	**47.23**	0.60	**95.28**	1.38
0	**6.31**	0.43	**7.19**	0.43	**27.85**	0.97	**114.29**	3.96	**6.24**	0.38	**6.88**	0.25	**37.08**	0.59	**21.73**	1.07	**11.60**	0.65
1	**5.39**	0.24	**10.81**	0.41	**9.32**	0.49	**14.84**	0.87	**10.02**	0.20	**40.21**	1.26	**13.58**	0.51	**7.46**	0.59	**6.00**	0.67
2	**4.51**	0.11	**7.89**	0.35	**4.52**	0.17	**26.17**	1.36	**12.35**	0.39	**17.52**	0.69	**19.49**	0.84	**80.32**	1.26	**10.63**	0.58
3	**9.60**	0.30	**13.36**	0.46	**24.97**	1.42	**6.52**	0.18	**5.41**	0.07	**12.10**	0.29	**3.32**	0.18	**9.51**	0.11	**9.84**	4.10
4	**9.71**	0.15	**28.88**	0.71	**4.71**	0.32	**22.26**	0.86	**5.34**	0.43	**12.85**	0.54	**15.15**	0.85	**31.61**	1.06	**25.15**	2.67
5	**13.06**	0.60	**25.97**	1.11	**10.96**	0.37	**7.22**	0.29	**13.64**	0.31	**17.09**	0.17	**20.73**	0.42	**32.37**	0.64	**13.58**	0.54
6	**13.92**	0.35	**17.90**	1.06	**968.75**	2.70	**4.72**	0.15	**8.69**	0.47	**21.15**	0.26	**36.81**	1.45	**12.66**	0.53	**25.91**	0.49
7	**13.81**	0.28	**18.37**	0.28	**37.61**	1.44	**6.13**	0.28	**7.81**	0.41	**20.50**	0.93	**19.80**	1.09	**34.28**	0.59	**28.45**	0.91
8	**no sample***		**5.34**	0.31	**3.84**	0.19	**8.51**	0.57	**8.26**	0.55	**36.15**	0.80	**7.76**	0.17	**42.25**	1.32	**15.08**	0.50
9	**387.01**	1.65	**8.22**	0.26	**6.07**	0.15	**5.68**	0.14	**11.74**	0.33	**8.49**	0.52	**26.74**	0.77	**80.65**	3.13	**15.46**	0.43
10	**16.14**	0.40	**51.01**	1.01	**3.72**	0.16	**9.10**	0.81	**28.53**	0.60	**31.66**	0.82	**25.06**	1.09	**70.14**	1.94	**17.11**	0.60
11	**25.06**	0.30	**75.19**	1.13	**6.16**	0.53	**13.33**	0.62	**28.60**	0.71	0.00	0.00	**43.59**	0.54	**89.28**	4.34	**25.94**	0.97
12	**40.12**	0.88	**26.07**	0.49	**8.63**	0.44	**15.27**	0.62	**33.68**	0.52	**17.93**	0.82	**87.08**	1.34	**62.48**	1.41	**44.92**	1.26
13	**25.25**	0.82	**57.53**	0.84	**16.02**	0.26	**11.84**	0.66	**no sample***		**17.37**	0.92	**39.57**	0.43	**73.39**	2.45	**13.06**	0.26
14	**37.54**	0.85	0.00		**19.94**	0.21	0.25	0.14	**no sample***		**26.16**	1.00	**51.84**	1.39	**74.04**	2.22	**15.90**	1.00
15	**26.62**	0.83	**57.62**	0.27	**34.00**	1.59	**1.46**	1.01	**no sample***		**13.58**	0.33	**no sample***		**196.22**	3.16	**15.45**	0.51
LoD	0.08		0.30		0.08		0.15		0.16		0.10		0.18		0.18		0.09	
LoQ	0.20		0.80		0.20		0.39		0.40		0.27		0.49		0.49		0.24	
* insufficient sample volume for ICP-MS measurement																		

Table A3. 100: Phosphate concentrations across the SWI of the sediment cores of sampling site 4. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
-4	0.25	0.30	0.30	0.15	0.25	1.85	1.18	0.94	missing**
-3	0.35	0.20	0.40	0.05	0.05	1.15	0.98	1.04	0.50
-2	1.40	0.90	0.05	0.30	0.55	1.10	1.78	0.64	1.05
-1	3.05	0.80	0.20	0.55	0.20	3.25	1.48	1.14	1.10
0	6.40	2.85	1.45	0.85	0.60	6.05	1.78	2.39	5.85
1	6.40	10.15	2.25	1.60	1.20	4.15	4.93	2.89	11.75
2	11.00	5.05	3.05	3.85	1.90	5.25	5.63	2.79	6.85
3	8.65	4.95	5.25	9.90	6.50	10.65	6.68	6.59	5.15
4	8.80	5.05	6.60	6.55	7.95	12.05	1.88	8.64	4.10
5	8.40	5.90	6.20	4.35	7.70	12.85	1.58	4.29	9.75
6	10.70	4.55	5.95	9.90	4.60	18.85	2.83	12.59	5.30
7	8.10	5.60	6.15	6.30	3.30	11.30	5.28	10.74	8.70
8	missing*	3.85	8.75	8.75	11.75	18.15	7.68	4.39	6.60
9	5.20	5.60	10.25	7.65	11.55	11.60	10.43	10.24	6.10
10	7.50	12.70	3.45	5.65	8.00	15.60	12.93	3.14	8.60
11	9.00	5.95	8.60	9.90	6.15	17.25	4.58	4.29	5.75
12	6.00	4.95	3.10	11.90	8.30	10.95	4.08	4.79	7.95
13	5.10	3.00	7.30	8.00	missing*	12.95	6.98	3.69	8.55
14	8.15	missing*	4.45	10.40	missing*	10.50	1.70	6.30	8.25
15	6.60	missing*	9.35	10.75	missing*	18.40	missing*	5.80	8.95
* insufficient sample volume									
** handling error									

Table A3. 101: Sulfate concentrations across the SWI of the sediment cores of sampling site 4. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
-4	178.75	198.30	418.05	323.10	388.15	384.35	539.90	1008.85	0.00
-3	104.90	220.00	328.20	258.00	193.20	283.35	353.65	539.05	148.75
-2	333.55	288.80	444.40	281.60	372.55	259.70	541.45	491.75	174.25
-1	247.15	133.55	421.40	251.90	299.00	417.35	512.00	451.80	126.10
0	400.90	160.20	264.80	222.55	240.35	324.20	236.75	392.30	280.45
1	270.20	298.40	206.75	225.10	147.70	165.25	359.55	355.20	364.80
2	334.70	151.40	163.70	262.20	132.40	187.55	411.55	195.55	157.05
3	365.35	142.25	162.85	485.40	270.45	306.85	357.30	282.75	121.35
4	480.45	171.85	174.85	335.65	288.15	343.30	28.65	347.65	92.40
5	509.40	240.75	237.00	262.50	243.85	341.75	28.45	181.40	150.15
6	591.80	183.50	441.55	418.50	164.70	434.20	118.35	345.30	105.30
7	572.80	236.15	235.05	270.05	143.55	280.65	184.40	341.65	166.10
8	missing*	223.15	355.45	372.85	365.20	392.85	322.50	155.30	108.25
9	374.40	315.85	434.95	283.80	390.40	270.80	582.60	288.20	103.95
10	696.95	666.85	175.30	218.90	265.55	390.00	556.65	115.50	129.20
11	722.25	309.25	413.75	339.60	216.50	385.90	186.85	135.05	76.35
12	598.25	261.25	193.95	419.90	290.30	281.50	153.90	149.50	115.95
13	545.05	212.55	468.25	310.70	missing*	299.35	197.90	168.05	112.95
14	699.70	missing*	248.55	377.50	missing*	267.90	105.85	210.55	104.60
15	594.60	missing*	365.15	319.95	missing*	394.05	missing*	166.85	150.10
* insufficient sample volume									
** handling error									

Table A3. 102: Ammonium concentrations across the SWI of the sediment cores of sampling site 4. All values in mg/L.

Depth	Sediment core 1			Sediment core 2			Sediment core 3		
(cm)	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3	Profile 1	Profile 2	Profile 3
-4	3.74	1.15	4.26	3.69	5.58	4.22	2.61	0.59	0.00
-3	4.33	1.18	4.88	5.53	5.97	5.61	0.00	2.63	3.06
-2	5.84	1.39	3.67	5.93	6.12	5.16	0.00	2.71	3.84
-1	8.83	4.23	3.85	5.17	7.01	3.85	0.00	3.94	5.24
0	7.08	5.58	6.46	4.27	8.32	5.74	5.75	5.72	6.19
1	7.96	6.16	9.32	5.23	9.00	6.48	0.06	7.47	6.27
2	5.41	5.51	11.79	6.43	8.21	6.05	1.36	8.54	7.05
3	5.75	4.89	11.46	8.15	8.94	5.14	2.63	9.14	7.76
4	6.26	4.36	11.33	7.93	8.76	5.01	4.42	8.92	7.47
5	6.01	4.74	11.33	7.40	9.17	6.05	4.70	8.99	8.16
6	5.41	4.20	10.33	6.58	7.84	7.43	13.73	6.76	6.99
7	5.66	3.96	10.77	6.63	8.88	6.02	13.70	9.80	8.72
8	missing*	3.50	10.11	5.96	8.71	6.43	13.20	9.62	6.38
9	5.11	3.00	9.94	6.00	9.34	7.13	12.16	9.37	7.49
10	2.22	2.82	8.84	6.92	8.85	6.72	12.32	8.72	6.71
11	5.90	2.85	9.45	5.55	9.40	7.09	13.39	8.55	6.24
12	4.98	3.12	8.87	5.54	8.58	6.87	12.79	8.85	6.87
13	5.92	2.96	7.95	5.87	missing*	7.04	13.38	9.31	6.36
14	6.43	missing*	7.07	6.33	missing*	7.14	12.39	10.36	6.64
15	6.80	missing*	9.72	6.19	missing*	7.29	missing*	8.26	5.42
*** insufficient sample volume**									
**** handling error**									

AIII.IV.III Measured concentrations in dialyses-based sediment pore water samples

Table A3. 103: Carbon concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**83**	3														
-14					**69**	4	**149**	8	**115**	4	**140**	9												
-13			**141**	4	**138**	6	**173**	8	**110**	4	**117**	9												
-12	**103**	2	**246**	15	**114**	6	**144**	6	**120**	5	**123**	10												
-11	**93**	3	**182**	3	**120**	5	**185**	10	**120**	5	**122**	6												
-10	**104**	3	**231**	9	**118**	6	**121**	5	**111**	4	**138**	9							**130**	6				
-9	**110**	5	**154**	7	**99**	5	**180**	8	**89**	3	**134**	9							**151**	7				
-8	**83**	3	**215**	19	**101**	5	**120**	6	**106**	5	**124**	10							**107**	5				
-7	**86**	3	**162**	11	**144**	7	**161**	8	**77**	3	**161**	11							**118**	6				
-6	**74**	1	**195**	8	**no sample***		**137**	6	**114**	6	**137**	9					**184**	6	**76**	4			**127**	3
-5	**116**	6	**112**	3	**115**	6	**162**	9	**97**	4	**117**	7	**162**	13	**129**	5	**216**	7	**131**	6			**150**	7
-4	**84**	4	**207**	10	**103**	4	**129**	7	**357**	28	**129**	11	**177**	13	**149**	4	**157**	6	**146**	9	**132**	8	**140**	10
-3	**107**	4	**172**	6	**109**	5	**151**	8	**293**	19	**144**	10	**18**	2	**126**	5	**200**	9	**189**	8	**115**	10	**164**	9
-2	**93**	4	**76**	3	**44**	1	**127**	6	**374**	23	**94**	6	**187**	10	**149**	5	**175**	8	**189**	9	**126**	8	**141**	16
-1	**126**	8	**137**	3	**143**	6	**166**	7	**78**	3	**188**	16	**158**	12	**169**	6	**213**	9	**141**	3	**82**	7	**173**	22
0	**58**	2	**223**	8	**49**	1	**167**	8	**90**	3	**192**	13	**171**	10	**103**	5	**177**	8	**125**	2	**122**	11	**128**	5
1	**181**	4	**169**	4	**157**	7	**199**	9	**102**	4	**308**	20	**22**	1	**45**	2	**258**	21	**179**	6	**140**	8	**228**	14
2	**177**	7	**203**	7	**156**	5	**243**	14	**119**	5	**277**	15	**204**	12	**203**	9	**176**	8	**438**	21	**130**	4	**209**	16
3	**217**	9	**312**	18	**232**	9	**362**	13	**114**	5	**429**	30	**171**	8	**31**	0	**268**	12	**606**	35	**140**	5	**234**	6
4	**224**	8	**318**	8	**267**	15	**386**	20	**182**	9	**432**	23	**no sample***		**262**	11	**217**	21	**613**	26	**186**	12	**330**	14
5	**250**	12	**236**	8	**367**	16	**512**	33	**206**	10	**494**	33	**206**	21	**64**	4	**no sample***		**806**	50	**227**	20	**249**	10
6	**306**	13	**359**	11	**359**	5	**521**	28	**278**	14	**448**	35	**no sample***		**337**	13	**210**	12	**801**	22	**335**	16	**257**	6
7	**215**	4	**321**	17	**440**	19	**490**	25	**252**	13	**576**	36	**215**	2	**310**	20	**238**	16	**1143**	73	**368**	19	**665**	18
8	**296**	12	**336**	14	**429**	19	**613**	22	**310**	8	**352**	24	**309**	4	**403**	20	**227**	21	**497**	26	**524**	20	**739**	33
9	**358**	13	**225**	9	**503**	24	**637**	24	**334**	18	**510**	34	**352**	22	**386**	32	**230**	12	**1534**	87	**608**	43	**963**	20
10	**440**	24	**552**	12	**525**	23	**588**	26	**341**	11	**383**	20	**476**	36	**499**	34	**236**	14	**1403**	88	**784**	46	**877**	43
11	**426**	22	**480**	28	**492**	18	**605**	28	**311**	13	**626**	50	**417**	27	**513**	16	**191**	9	**1581**	70	**830**	26	**1210**	27
12	**537**	23	**607**	21	**758**	45	**695**	37	**353**	11	**219**	14	**no sample***		**92**	3	**252**	16	**1663**	73	**1043**	59	**1114**	70
13	**514**	18	**536**	22	**464**	23	**808**	36			**685**	24	**532**	13	**no sample***		**251**	13	**no sample***		**1137**	175	**1455**	86
14	**605**	30	**794**	40									**242**	8	**748**	29	**334**	26	**1680**	108	**861**	44	**1278**	33
15	**528**	12											**681**	53	**no sample***		**298**	11	**no sample***		**1605**	90	**1509**	91
16													**no sample***		**293**	14	**431**	14	**1534**	87	**1452**	104	**1464**	153
17													**476**	28	**no sample***		**no sample***				**1536**	66	**906**	77
18															**203**	12	**841**	47			**1534**	90	**1626**	94
19																	**784**	38			**1143**	73	**1776**	124
20																					**1534**	87		
21																					**1403**	88		
22																					**1663**	73		
23																								
LoD	0.6		0.6		0.9		0.9		0.9		1.2		5.9		5.9		5.9		1.1		1.1		1.1	
LoQ	1.7		1.7		2.6		2.6		2.6		2.1		14.6		14.6		14.6		2.7		2.7		2.7	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 104: Phosphorous concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**110**	6														
-14					**84**	8	**97**	7	**141**	5	**76**	6												
-13			**107**	2	**185**	12	**85**	6	**112**	8	**87**	9												
-12	**146**	7	**156**	4	**100**	8	**105**	6	**111**	8	**75**	5												
-11	**107**	6	**103**	3	**114**	8	**106**	6	**119**	7	**94**	7												
-10	**90**	3	**109**	5	**142**	12	**88**	7	**138**	6	**95**	7							**102**	8				
-9	**93**	5	**113**	3	**129**	10	**89**	5	**118**	7	**99**	8							**108**	8				
-8	**124**	6	**86**	2	**132**	10	**79**	4	**111**	7	**81**	7							**104**	6				
-7	**90**	4	**134**	5	**182**	17	**96**	5	**160**	8	**90**	7							**109**	9				
-6	**99**	5	**96**	5	**no sample***		**82**	5	**137**	8	**77**	6					**103**	8	**112**	7			**110**	6
-5	**75**	7	**151**	5	**284**	20	**111**	7	**139**	9	**83**	7	**106**	9	**107**	9	**100**	8	**115**	8			**108**	7
-4	**83**	3	**115**	5	**104**	9	**88**	5	**122**	9	**74**	7	**108**	10	**106**	11	**114**	10	**105**	6	**104**	6	**110**	8
-3	**104**	6	**86**	3	**92**	7	**103**	6	**146**	6	**77**	6	**108**	10	**135**	14	**102**	9	**119**	7	**109**	6	**113**	9
-2	**84**	3	**110**	7	**142**	12	**121**	7	**146**	11	**64**	6	**109**	10	**110**	9	**106**	6	**110**	9	**107**	8	**109**	8
-1	**91**	4	**193**	10	**148**	12	**154**	7	**204**	12	**317**	29	**122**	12	**110**	9	**107**	9	**125**	7	**118**	10	**115**	7
0	**80**	5	**168**	7	**93**	6	**2057**	105	**370**	21	**4315**	249	**141**	12	**125**	9	**129**	7	**146**	9	**681**	39	**172**	11
1	**2994**	80	**1102**	33	**1972**	105	**6014**	172	**1455**	63	**7188**	302	**1791**	141	**841**	80	**893**	83	**2439**	173	**2473**	140	**1765**	85
2	**2705**	81	**5498**	116	**3332**	178	**7642**	342	**6298**	305	**7087**	315	**2600**	179	**1931**	95	**2274**	178	**3987**	173	**2854**	123	**2043**	134
3	**3448**	151	**5068**	205	**4950**	151	**10513**	273	**4982**	160	**9971**	399	**2699**	126	**978**	96	**2558**	158	**3341**	106	**3733**	129	**1806**	107
4	**4706**	69	**4972**	127	**5677**	219	**11779**	510	**11063**	431	**10728**	466	**no sample***		**2857**	206	**4094**	195	**3934**	200	**4207**	323	**2049**	52
5	**6486**	167	**7334**	178	**8569**	355	**15482**	388	**11724**	280	**11166**	409	**3847**	202	**4062**	108	**no sample***		**4500**	205	**4448**	275	**1657**	63
6	**6557**	105	**5632**	90	**9418**	549	**14589**	550	**11823**	530	**10674**	425	**no sample***		**5622**	269	**6521**	370	**4948**	162	**5275**	223	**2030**	91
7	**6882**	241	**6120**	170	**9184**	412	**14713**	415	**14045**	359	**14074**	782	**8047**	582	**7056**	459	**8281**	602	**5702**	309	**5543**	176	**1936**	80
8	**6778**	197	**7697**	257	**8993**	580	**17779**	688	**16158**	421	**10594**	795	**8959**	477	**7445**	411	**10670**	524	**6313**	269	**5482**	347	**2083**	99
9	**7093**	235	**6868**	208	**8928**	267	**20365**	300	**16210**	600	**11178**	729	**9490**	652	**8813**	720	**12430**	1068	**6813**	392	**5902**	251	**1904**	109
10	**8464**	229	**9263**	273	**11925**	366	**20891**	338	**18598**	297	**11029**	463	**10304**	478	**9689**	475	**12854**	968	**6981**	261	**5550**	108	**1993**	63
11	**8396**	146	**9757**	542	**12347**	408	**25754**	721	**19722**	597	**13433**	991	**10900**	481	**9885**	830	**13014**	751	**7694**	252	**6013**	278	**1747**	142
12	**9062**	550	**9965**	320	**13057**	424	**28630**	609	**25936**	873	**15448**	774	**no sample***		**10630**	658	**12871**	958	**7862**	114	**6349**	261	**1973**	118
13	**8802**	270	**10654**	332	**11950**	785	**30883**	1487			**20307**	450	**11659**	796	**no sample***		**14186**	654	**no sample***		**6533**	329	**828**	33
14	**10382**	191	**11827**	460									**11760**	964	**10903**	661	**14503**	711	**7509**	213	**7174**	328	**2338**	155
15	**5997**	201											**12507**	1098	**no sample***		**14434**	483	**no sample***		**7456**	337	**2666**	152
16													**no sample***		**11942**	1014	**14105**	1134	**8358**	518	**7855**	433	**4467**	156
17													**14835**	817	**no sample***		**no sample***				**8094**	533	**6094**	214
18															**13459**	744	**13661**	731			**8263**	257	**7283**	262
19																	**14548**	936			**8789**	421	**8270**	233
20																					**9059**	353	**8310**	463
21																					**9905**	540	**9170**	655
22																					**10120**	636		
23																					**10922**	653		
LoD	1.23		1.23		2.80		2.80		2.80		2.21		0.88		0.88		0.88		0.30		0.30		0.30	
LoQ	3.26		3.26		7.47		7.47		7.47		5.59		2.51		2.51		2.51		0.79		0.79		0.79	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 105: Sulfur concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in mg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**498**	24														
-14					**216**	13	**476**	28	**567**	19	**431**	24												
-13			**226**	4	**377**	25	**476**	25	**494**	30	**476**	34												
-12	**222**	5	**291**	9	**248**	15	**451**	27	**592**	32	**417**	32												
-11	**217**	7	**246**	5	**247**	12	**500**	24	**586**	31	**493**	25												
-10	**222**	5	**264**	12	**311**	19	**442**	24	**619**	20	**469**	29							**<LoD**					
-9	**223**	8	**233**	8	**268**	14	**454**	14	**549**	28	**531**	29							**<LoD**					
-8	**217**	11	**265**	6	**276**	17	**455**	18	**587**	29	**476**	31							**<LoD**					
-7	**226**	11	**246**	7	**251**	14	**519**	18	**536**	21	**525**	34							**<LoD**					
-6	**214**	9	**272**	11	**no sample***		**479**	25	**639**	29	**470**	34					**176**	9	**<LoD**				**<LoD**	
-5	**246**	21	**211**	4	**248**	12	**540**	33	**585**	26	**506**	34	**171**	12	**181**	11	**175**	7	**<LoD**				**<LoD**	
-4	**201**	8	**273**	7	**240**	13	**473**	22	**833**	49	**450**	36	**175**	17	**171**	14	**175**	10	**<LoD**		**<LoD**		**<LoD**	
-3	**213**	10	**248**	7	**263**	20	**543**	26	**696**	36	**478**	37	**176**	9	**174**	9	**174**	8	**<LoD**		**<LoD**		**<LoD**	
-2	**212**	6	**207**	10	**206**	13	**508**	20	**937**	57	**404**	30	**177**	16	**183**	10	**170**	7	**<LoD**		**<LoD**		**<LoD**	
-1	**233**	9	**271**	10	**268**	15	**604**	24	**534**	24	**597**	50	**178**	11	**176**	12	**173**	7	**<LoD**		**<LoD**		**<LoD**	
0	**208**	12	**324**	10	**254**	16	**569**	24	**631**	28	**506**	28	**180**	15	**177**	6	**170**	14	**<LoD**		**<LoD**		**<LoD**	
1	**254**	4	**275**	8	**249**	15	**631**	20	**538**	23	**535**	14	**188**	14	**184**	8	**177**	9	**<LoD**		**<LoD**		**<LoD**	
2	**251**	7	**332**	8	**247**	13	**505**	22	**569**	18	**409**	16	**186**	6	**185**	9	**175**	11	**<LoD**		**<LoD**		**<LoD**	
3	**288**	6	**336**	5	**288**	9	**488**	15	**471**	15	**462**	23	**181**	14	**177**	8	**166**	11	**<LoD**		**<LoD**		**<LoD**	
4	**262**	8	**371**	5	**262**	10	**441**	13	**487**	11	**396**	13	**no sample***		**174**	7	**153**	10	**<LoD**		**<LoD**		**<LoD**	
5	**265**	9	**348**	9	**291**	13	**463**	8	**390**	15	**343**	15	**171**	11	**163**	4	**no sample***		**<LoD**		**<LoD**		**<LoD**	
6	**253**	3	**340**	7	**271**	10	**373**	5	**336**	15	**295**	14	**no sample***		**139**	3	**129**	9	**<LoD**		**<LoD**		**<LoD**	
7	**241**	7	**326**	11	**246**	10	**355**	9	**321**	9	**328**	18	**130**	11	**125**	8	**110**	8	**<LoD**		**<LoD**		**<LoD**	
8	**247**	5	**301**	12	**225**	15	**383**	11	**320**	10	**234**	17	**111**	6	**106**	8	**82**	4	**<LoD**		**<LoD**		**<LoD**	
9	**238**	9	**280**	6	**214**	11	**369**	6	**268**	6	**222**	12	**99**	8	**84**	5	**60**	3	**<LoD**		**<LoD**		**<LoD**	
10	**255**	7	**338**	4	**248**	7	**317**	2	**266**	8	**211**	9	**89**	8	**65**	2	**47**	3	**<LoD**		**<LoD**		**<LoD**	
11	**230**	6	**306**	14	**237**	5	**295**	8	**205**	7	**218**	16	**74**	6	**54**	2	**39**	3	**<LoD**		**<LoD**		**<LoD**	
12	**238**	14	**290**	10	**233**	7	**271**	10	**193**	6	**192**	10	**no sample***		**43**	3	**25**	2	**<LoD**		**<LoD**		**<LoD**	
13	**213**	7	**256**	6	**190**	16	**258**	11			**179**	5	**48**	2	**no sample***		**13**	1	**no sample***		**<LoD**		**<LoD**	
14	**231**	7	**245**	4									**44**	3	**43**	4	**7**	0	**<LoD**		**<LoD**		**<LoD**	
15	**189**	2											**34**	1	**no sample***		**3**	0	**no sample***		**<LoD**		**<LoD**	
16													**no sample***		**30**	1	1	0	**<LoD**		**<LoD**		**<LoD**	
17													**23**	1	**no sample***		**no sample***				**<LoD**		**<LoD**	
18															**25**	1	1	0			**<LoD**		**<LoD**	
19																	2	0			**<LoD**		**<LoD**	
20																					**<LoD**		**<LoD**	
21																					**<LoD**		**<LoD**	
22																					**<LoD**			
23																					**<LoD**			
LoD	0.05		0.05		0.45		0.45		0.45		0.01		0.77		0.77		0.77		3.12		3.12		0.03	
LoQ	0.09		0.09		1.26		1.26		1.26		0.02		2.03		2.03		2.03		9.18		9.18		0.09	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 106: Manganese concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**316**	4														
-14					**21**	0	**441**	11	**386**	11	**328**	7												
-13			**26**	1	**50**	1	**442**	12	**343**	7	**342**	8												
-12	**48**	2	**41**	2	**28**	1	**424**	4	**414**	4	**297**	4												
-11	**15**	0	**23**	0	**39**	1	**486**	10	**421**	8	**361**	11												
-10	**17**	1	**23**	1	**46**	1	**448**	12	**436**	9	**321**	2							**58**	1				
-9	**13**	0	**40**	1	**31**	1	**474**	5	**405**	11	**385**	9							**60**	1				
-8	**29**	1	**14**	0	**26**	1	**479**	12	**458**	12	**331**	2							**55**	1				
-7	**19**	1	**38**	1	**125**	4	**529**	12	**436**	12	**406**	9							**52**	1				
-6	**28**	1	**18**	1	**no sample***		**503**	19	**534**	14	**356**	5					**31**	1	**53**	1			**43**	1
-5	**11**	0	**49**	1	**318**	2	**557**	12	**508**	9	**390**	10	**32**	1	**33**	0	**31**	1	**57**	1			**41**	1
-4	**14**	0	**31**	1	**126**	2	**497**	7	**555**	14	**345**	5	**32**	1	**33**	1	**35**	1	**63**	1	**50**	1	**43**	1
-3	**11**	0	**22**	1	**83**	2	**565**	15	**317**	4	**374**	8	**31**	0	**33**	0	**32**	1	**67**	1	**48**	1	**43**	1
-2	**12**	0	**51**	1	**182**	3	**544**	9	**661**	17	**343**	5	**32**	1	**33**	1	**33**	1	**67**	1	**53**	1	**42**	1
-1	**12**	0	**58**	1	**199**	3	**838**	12	**718**	8	**901**	21	**33**	0	**33**	1	**46**	1	**71**	1	**55**	1	**44**	1
0	**16**	0	**20**	0	**113**	4	**794**	10	**695**	10	**1099**	47	**32**	1	**62**	1	**418**	6	**80**	1	**154**	4	**65**	2
1	**444**	13	**217**	4	**1122**	28	**1119**	28	**613**	13	**1139**	27	**632**	7	**186**	1	**321**	3	**810**	16	**579**	13	**421**	5
2	**1334**	32	**756**	13	**3079**	113	**1167**	31	**625**	18	**824**	13	**861**	6	**491**	8	**565**	5	**739**	7	**594**	6	**400**	6
3	**1713**	57	**1161**	19	**2353**	39	**1336**	38	**589**	11	**913**	47	**917**	8	**593**	7	**573**	10	**574**	10	**640**	8	**320**	4
4	**1506**	107	**1602**	37	**2175**	29	**1093**	37	**654**	9	**554**	17	**no sample***		**896**	22	**874**	16	**581**	9	**576**	10	**314**	8
5	**1512**	29	**2807**	48	**2809**	279	**923**	39	**400**	18	**291**	7	**896**	14	**1043**	15	**no sample***		**618**	8	**534**	7	**284**	7
6	**1455**	26	**1922**	74	**2384**	33	**587**	7	**203**	7	**141**	2	**no sample***		**1244**	13	**969**	19	**640**	8	**594**	10	**311**	7
7	**1337**	30	**1857**	28	**1917**	34	**391**	14	**167**	5	**103**	2	**788**	14	**1318**	16	**887**	11	**671**	9	**609**	12	**317**	5
8	**1288**	26	**2466**	97	**1744**	59	**356**	10	**158**	3	**57**	1	**771**	12	**1195**	11	**948**	14	**674**	8	**605**	11	**335**	6
9	**1222**	41	**1489**	72	**1725**	37	**343**	4	**161**	4	**65**	1	**752**	7	**1017**	25	**887**	14	**637**	7	**587**	7	**339**	4
10	**1275**	55	**1686**	52	**2359**	109	**378**	8	**184**	5	**84**	1	**701**	10	**861**	12	**749**	15	**609**	8	**572**	8	**355**	4
11	**1153**	26	**1737**	83	**2465**	73	**520**	8	**193**	5	**97**	1	**640**	10	**728**	17	**696**	8	**580**	6	**567**	15	**306**	8
12	**1129**	10	**1797**	19	**2455**	43	**480**	12	**286**	9	**154**	4	**no sample***		**719**	13	**618**	7	**502**	5	**544**	11	**294**	6
13	**1108**	37	**1709**	45	**2084**	26	**430**	8			**257**	7	**567**	12	**no sample***		**642**	11	**no sample***		**510**	5	**236**	2
14	**1214**	25	**1667**	52									**562**	12	**740**	11	**668**	8	**515**	3	**517**	7	**345**	4
15	**1007**	33											**530**	8	**no sample***		**695**	20	**no sample***		**513**	9	**334**	4
16													**no sample***		**728**	21	**921**	18	**498**	14	**524**	8	**435**	12
17													**568**	7	**no sample***		**no sample***				**491**	9	**462**	7
18															**744**	12	**1280**	13			**466**	6	**472**	5
19																	**1203**	9			**431**	7	**489**	13
20																					**392**	3	**461**	11
21																					**370**	4	**493**	7
22																					**412**	7		
23																					**468**	8		
LoD	0.29		0.29		0.15		0.15		0.15		0.09		0.17		0.17		0.17		0.77		0.77		0.77	
LoQ	0.77		0.77		0.41		0.41		0.41		0.22		0.41		0.41		0.41		1.89		1.89		1.89	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 107: Iron concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**15**	1														
-14					**22**	0	**18**	1	**19**	0	**7**	0												
-13			**38**	1	**94**	3	**13**	1	**16**	0	**6**	0												
-12	**84**	4	**30**	1	**34**	1	**18**	1	**36**	2	**23**	0												
-11	**10**	0	**34**	1	**94**	2	**84**	3	**47**	2	**17**	1												
-10	**39**	1	**26**	1	**123**	2	**25**	1	**26**	1	**11**	0							**63**	1				
-9	**12**	0	**123**	3	**45**	1	**41**	1	**20**	1	**12**	0							**75**	2				
-8	**26**	1	**12**	0	**66**	1	**46**	1	**20**	1	**7**	0							**113**	1				
-7	**71**	2	**45**	2	**1694**	65	**19**	1	**16**	0	**40**	1							**159**	2				
-6	**109**	3	**35**	1	**no sample***		**19**	1	**19**	0	**12**	0					**13**	0	**205**	2			**43**	1
-5	**10**	0	**124**	3	**4240**	155	**23**	1	**37**	1	**12**	0	**18**	0	**29**	1	**13**	0	**170**	2			**30**	1
-4	**23**	0	**73**	1	**696**	24	**29**	1	**6**	0	**6**	0	**18**	1	**32**	0	**180**	1	**217**	3	**111**	3	**32**	0
-3	**9**	0	**37**	1	**276**	5	**25**	1	**6**	0	**12**	0	**20**	0	**40**	1	**36**	1	**311**	5	**103**	1	**41**	1
-2	**12**	0	**109**	2	**1040**	28	**125**	5	**28**	2	**25**	0	**25**	0	**62**	1	**35**	1	**275**	2	**101**	2	**45**	0
-1	**12**	1	**175**	4	**1314**	42	**2011**	45	**1687**	44	**2488**	103	**76**	1	**69**	1	**81**	2	**363**	7	**156**	2	**68**	1
0	**43**	1	**307**	6	**252**	7	**24081**	1097	**8278**	295	**18607**	798	**144**	5	**146**	4	**433**	8	**278**	6	**2300**	66	**280**	5
1	**14221**	274	**4353**	113	**22121**	419	**<LoD**		**7749**	184	**18107**	487	**5444**	177	**2887**	84	**2384**	27	**9164**	198	**9569**	477	**5446**	231
2	**8968**	98	**25347**	474	**25302**	1791	**34125**	1029	**19169**	472	**7590**	255	**7950**	288	**4927**	132	**6579**	230	**13122**	386	**9339**	140	**7137**	312
3	**10994**	403	**13235**	263	**27855**	670	**22409**	800	**5952**	247	**3042**	240	**6592**	181	**2454**	74	**5062**	352	**10183**	186	**10066**	173	**5976**	124
4	**13225**	1030	**8890**	315	**26967**	766	**12233**	216	**5854**	253	**456**	9	**no sample***		**6733**	292	**7077**	255	**10777**	255	**10984**	630	**6304**	257
5	**16115**	336	**21706**	605	**25754**	1386	**11296**	461	**3615**	272	**104**	2	**5863**	133	**7657**	178	**no sample***		**12950**	357	**11208**	36	**5569**	187
6	**14189**	221	**12470**	484	**26006**	750	**7667**	140	**531**	10	**53**	1	**no sample***		**7651**	142	**5672**	230	**13531**	471	**12775**	258	**6070**	212
7	**13121**	343	**11576**	258	**20313**	551	**2343**	81	**228**	5	**91**	3	**1610**	58	**6813**	171	**3569**	134	**15131**	402	**12938**	293	**5919**	89
8	**11215**	227	**14816**	793	**16979**	560	**1449**	56	**301**	6	**369**	7	**1443**	9	**4948**	92	**3487**	198	**15488**	414	**12711**	282	**6419**	202
9	**9961**	460	**10312**	434	**16119**	507	**1080**	19	**291**	8	**643**	14	**1477**	50	**3159**	50	**2933**	110	**14177**	652	**13015**	515	**6137**	102
10	**9236**	466	**11844**	496	**21360**	1262	**2973**	65	**342**	8	**2379**	108	**740**	9	**1977**	58	**1956**	48	**13180**	312	**13165**	278	**6535**	195
11	**7998**	312	**12075**	665	**24346**	1122	**7522**	159	**370**	9	**268**	3	**919**	14	**1560**	23	**2045**	61	**13546**	211	**12958**	438	**5571**	112
12	**7003**	182	**10858**	163	**22070**	710	**3697**	215	**1045**	22	**352**	4	**no sample***		**1562**	52	**1235**	15	**12333**	292	**12511**	447	**4970**	214
13	**6775**	300	**11060**	323	**19306**	657	**1358**	16			**1920**	50	**329**	4	**no sample***		**1372**	17	**no sample***		**12256**	298	**2287**	108
14	**7273**	100	**10562**	154									**1246**	24	**1695**	74	**955**	12	**10243**	275	**12076**	423	**6097**	218
15	**948**	30											**501**	5	**no sample***		**929**	17	**no sample***		**11159**	236	**8414**	116
16													**no sample***		**1932**	69	**2112**	57	**10155**	503	**10871**	209	**7206**	303
17													**619**	7	**no sample***		**no sample***				**8872**	206	**8246**	313
18															**2440**	144	**2786**	68			**8576**	197	**7877**	203
19																	**3862**	87			**8150**	105	**7724**	97
20																					**7248**	325	**5604**	233
21																					**6215**	307	**6261**	117
22																					**6159**	71		
23																					**7457**	176		
LoD	0.29		0.29		0.90		0.90		0.90		0.18		1.47		1.47		1.47		0.24		0.24		0.24	
LoQ	0.79		0.79		2.53		2.53		2.53		0.47		3.50		3.50		3.50		0.59		0.59		0.59	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 108: Arsenic concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**1.064**	0.079														
-14					**1.340**	0.090	**1.443**	0.112	**1.255**	0.095	**1.027**	0.092												
-13			**1.214**	0.021	**2.657**	0.195	**1.434**	0.106	**1.079**	0.061	**1.307**	0.115												
-12	**1.630**	0.104	**1.773**	0.089	**1.727**	0.095	**1.325**	0.102	**1.334**	0.107	**1.144**	0.092												
-11	**1.424**	0.097	**1.453**	0.086	**1.844**	0.071	**1.459**	0.102	**1.327**	0.100	**1.408**	0.108												
-10	**1.419**	0.030	**1.505**	0.058	**2.287**	0.175	**1.269**	0.068	**1.391**	0.078	**1.268**	0.087							**1.770**	0.145				
-9	**1.361**	0.081	**1.368**	0.051	**1.866**	0.162	**1.251**	0.120	**1.166**	0.108	**1.376**	0.136							**1.807**	0.165				
-8	**1.421**	0.107	**1.466**	0.057	**2.024**	0.085	**1.208**	0.107	**1.337**	0.101	**1.189**	0.101							**1.772**	0.131				
-7	**1.444**	0.089	**1.429**	0.077	**2.644**	0.239	**1.318**	0.122	**1.277**	0.062	**1.320**	0.100							**1.844**	0.146				
-6	**1.349**	0.070	**1.579**	0.081	**no sample***		**1.171**	0.097	**1.494**	0.079	**1.170**	0.063					**1.069**	0.092	**1.863**	0.080			**1.635**	0.104
-5	**1.430**	0.066	**1.223**	0.067	**3.959**	0.251	**1.324**	0.095	**1.441**	0.083	**1.270**	0.078	**1.127**	0.090	**1.106**	0.130	**1.052**	0.091	**1.825**	0.138			**1.553**	0.148
-4	**1.111**	0.078	**1.593**	0.073	**1.978**	0.163	**1.115**	0.082	**1.824**	0.112	**1.102**	0.055	**1.159**	0.109	**1.114**	0.117	**1.088**	0.100	**1.867**	0.119	**1.881**	0.139	**1.593**	0.081
-3	**1.229**	0.055	**1.348**	0.060	**1.915**	0.180	**1.269**	0.077	**1.718**	0.086	**1.115**	0.111	**1.151**	0.128	**1.127**	0.141	**1.088**	0.075	**2.016**	0.143	**1.776**	0.091	**1.588**	0.103
-2	**1.168**	0.051	**1.189**	0.094	**2.051**	0.128	**1.231**	0.057	**2.044**	0.112	**0.884**	0.072	**1.174**	0.125	**1.134**	0.113	**1.063**	0.042	**1.989**	0.142	**1.694**	0.155	**1.561**	0.118
-1	**1.299**	0.058	**1.666**	0.144	**2.640**	0.230	**1.583**	0.099	**1.808**	0.124	**2.049**	0.197	**1.213**	0.109	**1.117**	0.091	**1.085**	0.060	**1.972**	0.113	**1.784**	0.121	**1.574**	0.131
0	**1.130**	0.068	**2.036**	0.080	**2.180**	0.128	**3.389**	0.147	**2.233**	0.097	**1.642**	0.124	**1.195**	0.102	**1.201**	0.068	**1.413**	0.090	**1.896**	0.132	**3.054**	0.118	**1.808**	0.118
1	**20.350**	0.474	**3.680**	0.132	**20.503**	1.285	**4.170**	0.080	**1.463**	0.099	**0.938**	0.088	**3.718**	0.271	**3.540**	0.262	**2.758**	0.231	**9.707**	0.327	**7.726**	0.390	**4.688**	0.377
2	**12.956**	0.265	**21.664**	0.555	**19.856**	1.027	**2.355**	0.141	**2.600**	0.170	**0.614**	0.051	**3.316**	0.198	**2.620**	0.161	**2.842**	0.181	**7.070**	0.396	**5.502**	0.282	**3.544**	0.224
3	**13.059**	0.366	**12.133**	0.306	**18.253**	1.014	**1.341**	0.081	**1.727**	0.097	**0.781**	0.064	**1.911**	0.144	**1.797**	0.186	**1.803**	0.072	**4.431**	0.217	**4.964**	0.146	**2.824**	0.117
4	**10.546**	0.336	**8.457**	0.172	**18.740**	0.983	**0.931**	0.047	**1.315**	0.054	**0.774**	0.063	**no sample***		**1.977**	0.125	**1.256**	0.080	**4.526**	0.252	**5.007**	0.250	**2.742**	0.070
5	**9.693**	0.369	**13.805**	0.346	**11.260**	0.579	**1.377**	0.064	**1.040**	0.030	**0.879**	0.036	**1.361**	0.090	**1.472**	0.095	**no sample***		**4.677**	0.183	**4.858**	0.253	**2.320**	0.176
6	**6.457**	0.178	**4.243**	0.158	**8.652**	0.574	**1.247**	0.023	**0.913**	0.083	**0.747**	0.030	**no sample***		**1.130**	0.082	**1.070**	0.041	**4.486**	0.148	**5.572**	0.344	**2.334**	0.113
7	**5.971**	0.199	**3.726**	0.172	**5.016**	0.248	**0.900**	0.041	**1.058**	0.056	**0.966**	0.066	**0.761**	0.078	**0.986**	0.046	**0.889**	0.106	**5.231**	0.263	**4.517**	0.256	**2.439**	0.064
8	**4.179**	0.103	**11.281**	0.405	**3.388**	0.193	**1.090**	0.044	**1.120**	0.058	**0.742**	0.080	**0.707**	0.040	**0.881**	0.063	**0.917**	0.070	**4.902**	0.232	**3.578**	0.098	**2.528**	0.119
9	**2.823**	0.107	**3.800**	0.133	**4.003**	0.156	**1.293**	0.025	**1.162**	0.098	**0.836**	0.050	**0.703**	0.075	**0.778**	0.079	**0.896**	0.107	**3.780**	0.143	**3.580**	0.100	**2.150**	0.162
10	**2.959**	0.111	**2.636**	0.033	**5.383**	0.292	**1.460**	0.047	**1.340**	0.106	**1.120**	0.053	**0.750**	0.066	**0.629**	0.081	**0.865**	0.086	**2.880**	0.112	**3.256**	0.246	**1.886**	0.161
11	**2.427**	0.069	**3.365**	0.186	**5.750**	0.237	**2.132**	0.059	**1.430**	0.084	**0.784**	0.090	**0.853**	0.059	**0.682**	0.093	**0.906**	0.075	**2.567**	0.114	**2.411**	0.165	**1.956**	0.109
12	**2.427**	0.152	**2.394**	0.088	**5.158**	0.218	**1.721**	0.079	**2.126**	0.125	**0.940**	0.063	**no sample***		**0.643**	0.078	**0.863**	0.079	**2.253**	0.133	**2.010**	0.132	**2.176**	0.131
13	**2.267**	0.124	**2.634**	0.082	**4.947**	0.243	**1.739**	0.042			**1.246**	0.093	**0.837**	0.098	**no sample***		**0.902**	0.073	**no sample***		**2.001**	0.111	**2.916**	0.166
14	**2.781**	0.075	**2.311**	0.028									**0.981**	0.103	**0.748**	0.053	**0.847**	0.056	**2.102**	0.103	**1.967**	0.073	**3.224**	0.122
15	**2.865**	0.049											**0.812**	0.110	**no sample***		**0.843**	0.063	**no sample***		**1.859**	0.116	**4.997**	0.188
16													**no sample***		**0.699**	0.064	**0.880**	0.071	**1.693**	0.079	**1.811**	0.133	**2.782**	0.104
17													**0.889**	0.066	**no sample***		**no sample***				**1.678**	0.120	**2.548**	0.175
18															**1.073**	0.087	**0.760**	0.054			**1.737**	0.064	**2.235**	0.108
19																	**0.950**	0.081			**1.702**	0.066	**2.519**	0.165
20																					**1.784**	0.078	**1.594**	0.061
21																					**1.545**	0.086	**1.660**	0.131
22																					**1.651**	0.096		
23																					**1.777**	0.089		
LoD	0.047		0.047		0.085		0.085		0.085		0.058		0.057		0.057		0.057		0.089		0.089		0.089	
LoQ	0.097		0.097		0.201		0.201		0.201		0.085		0.144		0.144		0.144		0.198		0.198		0.198	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 109: Antimony concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**0.118**	0.009														
-14					**0.151**	0.014	**0.185**	0.007	**0.181**	0.006	**0.138**	0.012												
-13			0.162	0.009	**0.306**	0.010	**0.194**	0.018	**0.123**	0.010	**0.172**	0.011												
-12	0.181	0.013	0.215	0.013	**0.197**	0.017	**0.167**	0.013	**0.177**	0.013	**0.145**	0.014												
-11	0.168	0.008	0.169	0.011	**0.195**	0.013	**0.200**	0.005	**0.200**	0.014	**0.193**	0.010												
-10	0.181	0.015	0.187	0.011	**0.279**	0.020	**0.182**	0.039	**0.186**	0.018	**0.152**	0.013							0.156	0.012				
-9	0.179	0.010	0.158	0.013	**0.238**	0.019	**0.163**	0.010	**0.167**	0.016	**0.182**	0.018							0.148	0.017				
-8	0.173	0.014	0.187	0.044	**0.220**	0.015	**0.163**	0.014	**0.178**	0.012	**0.157**	0.012							0.164	0.018				
-7	0.182	0.015	0.163	0.004	**0.249**	0.020	**0.187**	0.017	**0.170**	0.013	**0.181**	0.015							0.140	0.018				
-6	0.161	0.006	0.189	0.014	**no sample***		**0.170**	0.013	**0.210**	0.008	**0.151**	0.014					0.088	<LoD	0.168	0.019			0.124	0.016
-5	0.194	0.023	0.137	0.006	**0.278**	0.024	**0.178**	0.014	**0.186**	0.013	**0.175**	0.011	0.098	0.022	0.083	0.015	0.088	<LoD	0.142	0.012			0.128	0.019
-4	0.145	0.015	0.178	0.020	**0.227**	0.013	**0.177**	0.007	**0.235**	0.018	**0.145**	0.010	0.088	0.022	0.088	<LoD	0.088	<LoD	0.162	0.021	0.136	0.022	0.141	0.024
-3	0.170	0.022	0.166	0.019	**0.224**	0.022	**0.186**	0.016	**0.171**	0.011	**0.147**	0.012	0.113	0.024	0.088	<LoD	0.088	<LoD	0.158	0.018	0.163	0.031	0.139	0.016
-2	0.153	0.017	0.139	0.008	**0.188**	0.019	**0.157**	0.015	**0.267**	0.019	**0.123**	0.007	0.093	0.035	0.088	<LoD	0.088	<LoD	0.181	0.018	0.176	0.022	0.132	0.020
-1	0.171	0.011	0.187	0.013	**0.270**	0.004	**0.157**	0.011	**0.163**	0.008	**0.147**	0.010	0.093	0.026	0.081	0.025	0.088	<LoD	0.161	0.016	0.145	0.017	0.147	0.017
0	0.148	0.005	0.218	0.009	**0.223**	0.012	**0.112**	0.007	**0.134**	0.012	**0.085**	0.008	0.098	0.030	0.079	0.014	0.088	0.020	0.198	0.013	0.159	0.025	0.141	0.017
1	0.204	0.018	0.209	0.010	**0.255**	0.017	**0.097**	0.009	**0.110**	0.011	**0.093**	0.008	0.088	<LoD	0.085	0.025	0.088	<LoD	0.141	<LoD	0.141	<LoD	0.141	<LoD
2	0.117	0.008	0.234	0.012	**0.161**	0.014	**0.074**	0.008	**0.120**	0.009	**0.066**	0.005	0.088	<LoD	0.088	<LoD	0.088	<LoD	0.141	<LoD	0.141	<LoD	0.141	<LoD
3	0.134	0.012	0.105	0.022	**0.170**	0.013	**0.097**	0.008	**0.080**	0.007	**0.081**	0.004	0.088	<LoD	0.088	<LoD	0.088	<LoD	0.141	<LoD	0.141	<LoD	0.141	<LoD
4	0.116	0.009	0.145	<LoD	**0.147**	0.014	**0.053**	0.005	**0.102**	0.009	**0.071**	0.005	0.000		0.088	<LoD	0.088	<LoD	0.141	<LoD	0.141	<LoD	0.141	<LoD
5	0.145	<LoD	0.173	0.006	**0.168**	0.008	**0.081**	0.009	**0.095**	0.014	**0.073**	0.004	0.088	<LoD	0.088	<LoD	0.000		0.141	<LoD	0.141	<LoD	0.141	<LoD
6	0.145	<LoD	0.145	<LoD	**0.202**	0.020	**0.063**	0.008	**0.073**	0.006	**0.058**	0.005	0.000		0.088	<LoD	0.088	<LoD	0.141	<LoD	0.141	<LoD	0.141	<LoD
7	0.145	<LoD	0.103	0.011	**0.162**	0.015	**0.069**	0.004	**0.091**	0.009	**0.081**	0.006	0.088	<LoD	0.088	<LoD	0.088	<LoD	0.141	<LoD	0.141	<LoD	0.141	<LoD
8	0.145	<LoD	0.123	0.014	**0.157**	0.010	**0.092**	0.012	**0.113**	0.007	**0.064**	0.005	0.088	<LoD	0.088	<LoD	0.088	<LoD	0.137	0.009	0.141	<LoD	0.141	<LoD
9	0.145	<LoD	0.145	<LoD	**0.184**	0.007	**0.107**	0.007	**0.094**	0.001	**0.071**	0.008	0.088	<LoD	0.088	<LoD	0.088	<LoD	0.145	0.026	0.141	<LoD	0.141	<LoD
10	0.145	<LoD	0.120	0.018	**0.225**	0.017	**0.093**	0.005	**0.136**	0.004	**0.070**	0.005	0.088	<LoD	0.088	<LoD	0.088	<LoD	0.172	0.029	0.141	<LoD	0.141	<LoD
11	0.145	<LoD	0.130	0.022	**0.250**	0.024	**0.106**	0.007	**0.133**	0.013	**0.069**	0.012	0.088	<LoD	0.088	<LoD	0.088	<LoD	0.157	0.008	0.141	<LoD	0.141	<LoD
12	0.145	<LoD	0.113	0.010	**0.214**	0.011	**0.113**	0.006	**0.168**	0.011	**0.068**	0.007	0.000		0.088	<LoD	0.088	<LoD	0.179	0.021	0.141	<LoD	0.141	<LoD
13	0.145	<LoD	0.145	<LoD	**0.162**	0.016	**0.133**	0.009			**0.097**	0.005	0.082	0.024	0.000		0.088	<LoD	**no sample***		0.141	<LoD	0.141	<LoD
14	0.145	<LoD	0.145	<LoD									0.084	0.011	0.088	<LoD	0.088	<LoD	0.237	0.026	0.136	0.020	0.141	<LoD
15	**0.773**	0.032											0.094	0.017	0.000		0.088	<LoD	**no sample***		0.141	<LoD	0.141	<LoD
16													0.000		0.088	<LoD	0.088	<LoD	0.227	0.010	0.128	0.014	0.141	<LoD
17													0.106	0.027	0.000		0.000				0.141	<LoD	0.141	<LoD
18															0.088	<LoD	0.088	<LoD			0.141	<LoD	0.131	0.028
19																	0.088	<LoD			0.141	<LoD	0.148	0.016
20																					0.128	0.006	0.146	0.005
21																					0.141	<LoD	0.149	0.016
22																					0.141	<LoD		
23																					0.135	0.015		
LoD	0.103		0.103		0.013		0.013		0.013		0.011		0.078		0.078		0.078		0.120		0.120		0.120	
LoQ	0.290		0.290		0.033		0.033		0.033		0.024		0.176		0.176		0.176		0.282		0.282		0.282	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 110: Cadmium concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**0.057**	0.007														
-14					**0.044**	0.004	**0.077**	0.004	**0.076**	0.011	**0.053**	0.004												
-13			**0.047**	0.005	**0.105**	0.009	**0.069**	0.005	**0.066**	0.003	**0.063**	0.003												
-12	**0.076**	0.008	**0.070**	0.008	**0.065**	0.007	**0.064**	0.006	**0.074**	0.009	**0.054**	0.004												
-11	**0.039**	0.003	**0.050**	0.007	**0.077**	0.006	**0.066**	0.005	**0.073**	0.012	**0.054**	0.003												
-10	**0.052**	0.006	**0.054**	0.003	**0.102**	0.007	**0.060**	0.002	**0.070**	0.007	**0.056**	0.004							**0.052**	0.005				
-9	**0.043**	0.006	**0.066**	0.007	**0.078**	0.006	**0.058**	0.003	**0.060**	0.005	**0.071**	0.005							**0.050**	0.002				
-8	**0.057**	0.005	**0.047**	0.010	**0.080**	0.004	**0.051**	0.005	**0.069**	0.008	**0.053**	0.004							**0.056**	0.007				
-7	**0.080**	0.004	**0.060**	0.004	**0.330**	0.020	**0.056**	0.004	**0.061**	0.009	**0.060**	0.004							**0.050**	0.005				
-6	**0.073**	0.004	**0.054**	0.005	**no sample***		**0.052**	0.004	**0.071**	0.006	**0.051**	0.003					**0.023**	0.004	**0.065**	0.007			**0.055**	0.009
-5	**0.056**	0.004	**0.066**	0.003	**0.777**	0.055	**0.061**	0.003	**0.072**	0.008	**0.050**	0.004	**0.027**	0.007	**0.024**	0.003	**0.023**	0.002	**0.047**	0.007			**0.054**	0.006
-4	**0.044**	0.004	**0.059**	0.008	**0.132**	0.010	**0.053**	0.005	**0.074**	0.013	**0.045**	0.004	**0.029**	0.003	**0.026**	0.002	**0.033**	0.003	**0.047**	0.005	**0.059**	0.007	**0.050**	0.005
-3	**0.045**	0.004	**0.049**	0.003	**0.094**	0.008	**0.057**	0.007	**0.091**	0.015	**0.043**	0.004	**0.025**	0.003	**0.025**	0.002	**0.025**	0.006	**0.049**	0.005	**0.061**	0.004	**0.053**	0.005
-2	**0.042**	0.004	**0.068**	0.010	**0.184**	0.018	**0.084**	0.010	**0.098**	0.014	**0.034**	0.004	**0.022**	0.003	**0.025**	0.004	**0.022**	0.003	**0.046**	0.005	**0.058**	0.006	**0.051**	0.004
-1	**0.042**	0.004	**0.089**	0.004	**0.167**	0.014	**0.042**	0.009	**0.168**	0.014	**0.030**	0.003	**0.025**	0.004	**0.021**	0.005	**0.021**	0.002	**0.050**	0.010	**0.054**	0.007	**0.048**	0.004
0	**0.061**	0.004	**0.062**	0.004	**0.120**	0.012	**0.008**	0.001	**0.019**	0.007	**0.006**	0.002	**0.033**	0.006	**0.025**	0.004	**0.016**	0.003	**0.146**	0.013	**0.045**	0.009	**0.073**	0.007
1	**0.169**	0.013	**0.073**	0.007	**0.117**	0.008	0.003	<LoD	**0.021**	0.005	0.003	0.001	**0.009**	0.002	**0.041**	0.005	**0.085**	0.011	**0.010**	0.002	**0.033**	0.004	**0.009**	0.003
2	0.006	<LoD	**0.058**	0.007	0.004	0.004	**0.018**	0.003	**0.008**	0.006	**0.008**	0.001	0.004	<LoD	**0.018**	0.004	0.004	<LoD	**0.007**	0.002	**0.015**	0.003	**0.007**	0.003
3	0.006	<LoD	0.006	<LoD	0.003	0.004	0.005	0.001	0.003	0.005	0.003	<LoD	0.003	0.002	**0.017**	0.005	**0.012**	0.002	**0.010**	0.001	**0.008**	0.002	**0.009**	0.002
4	0.006	<LoD	0.006	<LoD	0.003	0.003	0.003	<LoD	0.003	<LoD	0.003	<LoD	**no sample***		0.006	0.001	**0.033**	0.005	**0.009**	0.002	**0.009**	0.003	**0.010**	0.003
5	0.006	<LoD	0.009	0.004	**0.017**	0.001	0.003	<LoD	**0.007**	0.005	0.003	<LoD	0.008	0.003	0.004	0.002	**no sample***		**0.007**	0.002	**0.009**	0.002	**0.012**	0.002
6	0.006	<LoD	0.006	<LoD	**0.169**	0.009	0.003	<LoD	0.003	<LoD	0.003	0.003	**no sample***		0.006	0.002	**0.051**	0.008	**0.014**	0.002	**0.019**	0.001	**0.012**	0.003
7	0.006	<LoD	0.009	0.003	**0.051**	0.006	0.003	<LoD	0.003	<LoD	0.003	<LoD	**0.016**	0.003	0.006	0.002	**0.018**	0.004	**0.012**	0.003	**0.019**	0.002	**0.016**	0.001
8	0.006	<LoD	0.006	<LoD	**0.231**	0.007	0.003	<LoD	**0.028**	0.006	**0.060**	0.001	**0.011**	0.003	**0.021**	0.005	**0.017**	0.002	**0.034**	0.004	**0.015**	0.003	**0.011**	0.003
9	0.006	<LoD	0.008	0.003	**0.536**	0.009	0.003	<LoD	0.003	<LoD	**0.180**	0.015	**0.009**	0.001	**0.020**	0.004	**0.016**	0.002	**0.095**	0.007	**0.013**	0.003	**0.010**	0.002
10	0.009	0.002	**0.017**	0.004	**0.522**	0.027	0.003	<LoD	0.003	<LoD	**0.381**	0.022	**0.022**	0.002	**0.009**	0.003	**0.013**	0.003	**0.062**	0.002	**0.019**	0.003	**0.025**	0.002
11	**0.021**	0.001	**0.015**	0.004	**0.467**	0.014	0.003	<LoD	0.003	<LoD	**0.034**	0.004	**0.062**	0.006	0.007	0.003	**0.010**	0.003	**0.020**	0.002	**0.014**	0.003	**0.010**	0.003
12	**0.038**	0.006	**0.017**	0.004	**0.098**	0.009	**0.013**	0.004	**0.021**	0.008	**0.043**	0.005	**no sample***		0.008	0.002	**0.016**	0.005	**0.019**	0.002	**0.023**	0.006	**0.015**	0.004
13	**0.063**	0.004	**0.015**	0.006	**0.037**	0.004	**0.090**	0.007			**0.049**	0.004	**0.019**	0.002	**no sample***		**0.012**	0.004	**no sample***		**0.034**	0.003	**0.008**	0.003
14	**0.047**	0.004	**0.023**	0.003									**0.151**	0.024	**0.013**	0.004	**0.010**	0.002	**0.030**	0.004	**0.021**	0.003	**0.017**	0.002
15	0.007	0.002											**0.020**	0.005	**no sample***		**0.009**	0.003	**no sample***		**0.020**	0.005	**0.067**	0.006
16													**no sample***		**0.047**	0.002	**0.013**	0.002	**0.054**	0.007	**0.026**	0.002	**0.022**	0.004
17													**0.019**	0.004	**no sample***		**no sample***				**0.026**	0.005	**0.031**	0.004
18															**0.393**	0.031	**0.012**	0.003			**0.026**	0.001	**0.283**	0.018
19																	**0.058**	0.006			**0.027**	0.002	**0.612**	0.028
20																					**0.026**	0.005	**0.194**	0.012
21																					**0.037**	0.004	**0.263**	0.018
22																					**0.039**	0.006		
23																					**0.047**	0.002		
LoD	0.005		0.005		0.003		0.003		0.003		0.003		0.003		0.003		0.003		0.001		0.001		0.001	
LoQ	0.012		0.012		0.007		0.007		0.007		0.006		0.008		0.008		0.008		0.002		0.002		0.002	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 111: Chromium concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**0.183**	0.006														
-14					0.099	0.006	**0.623**	0.044	**0.174**	0.017	**0.186**	0.009												
-13			**0.210**	0.022	**0.417**	0.034	**0.250**	0.023	0.129	0.012	0.100	0.019												
-12	**0.300**	0.025	**0.169**	0.015	**0.285**	0.031	**0.289**	0.018	**0.192**	0.016	0.095	0.022												
-11	**0.140**	0.013	**0.309**	0.025	**0.225**	0.024	**0.357**	0.028	**1.066**	0.035	0.096	0.006												
-10	**0.188**	0.014	**0.231**	0.028	**0.335**	0.014	**0.381**	0.017	**0.220**	0.019	0.089	0.021							0.493	0.054				
-9	**0.118**	0.004	**0.300**	0.030	**0.279**	0.027	**0.393**	0.032	**0.158**	0.010	0.113	0.011							**0.683**	0.045				
-8	**0.206**	0.017	**0.142**	0.019	**1.319**	0.118	**0.306**	0.025	**0.291**	0.026	0.090	0.022							**0.652**	0.057				
-7	**0.169**	0.015	**0.438**	0.025	**1.258**	0.108	**0.268**	0.027	**0.192**	0.017	0.089	0.015							**0.732**	0.038				
-6	**0.260**	0.023	**0.189**	0.006	**no sample***		**0.424**	0.030	**0.220**	0.021	0.100	0.014					0.488	<LoD	**0.861**	0.057			0.507	0.024
-5	**0.145**	0.007	**0.183**	0.025	**2.890**	0.184	**0.412**	0.030	**0.397**	0.035	0.094	0.013	0.506	0.022	0.488	<LoD	0.488	<LoD	**0.631**	0.075			0.387	0.028
-4	**0.100**	0.010	**0.169**	0.012	**1.017**	0.045	**0.319**	0.032	**0.238**	0.034	0.078	0.013	0.570	0.066	0.531	0.050	0.665	0.080	0.388	0.053	0.474	0.035	0.426	0.042
-3	**0.143**	0.010	**0.213**	0.012	**0.861**	0.066	**0.268**	0.015	0.118	0.040	0.073	0.020	0.557	0.043	0.488	<LoD	0.488	<LoD	**0.575**	0.061	**0.805**	0.048	0.354	0.052
-2	**0.109**	0.008	**0.285**	0.029	**1.012**	0.097	**0.247**	0.007	0.083	0.026	0.085	0.015	0.555	0.072	0.527	0.061	0.488	<LoD	**0.565**	0.048	**0.618**	0.025	0.423	0.035
-1	**0.117**	0.011	**0.283**	0.019	**1.332**	0.097	**0.561**	0.052	**0.891**	0.083	0.087	0.018	0.760	0.098	0.455	0.041	0.488	<LoD	0.482	0.067	**0.599**	0.063	**0.576**	0.028
0	**0.106**	0.008	**0.178**	0.010	**0.243**	0.023	**0.482**	0.033	**0.156**	0.013	**0.805**	0.044	0.454	0.034	0.488	<LoD	0.488	<LoD	0.385	0.042	0.439	0.051	0.505	0.080
1	**0.458**	0.042	**0.120**	0.006	**0.188**	0.011	**1.004**	0.061	**0.664**	0.064	**1.454**	0.107	0.488	<LoD	0.488	<LoD	0.488	<LoD	**0.607**	0.021	**0.529**	0.043	**1.103**	0.062
2	**0.206**	0.013	**0.332**	0.032	**0.358**	0.027	**1.131**	0.035	**1.204**	0.072	**1.493**	0.095	0.521	0.049	0.460	0.046	0.763	0.083	**0.712**	0.067	**1.746**	0.136	**0.747**	0.047
3	**0.344**	0.025	**0.376**	0.022	**0.483**	0.026	**2.981**	0.113	**1.257**	0.092	**2.163**	0.162	0.968	0.111	0.488	<LoD	0.651	0.032	**0.647**	0.049	**0.986**	0.042	0.456	0.046
4	**0.329**	0.014	**0.342**	0.025	**0.518**	0.031	**2.392**	0.091	**2.852**	0.113	**2.792**	0.093	**no sample***		0.575	0.056	**1.092**	0.071	**0.670**	0.028	**0.655**	0.040	**0.651**	0.119
5	**0.449**	0.037	**0.598**	0.056	**0.985**	0.058	**1.993**	0.114	**3.024**	0.070	**2.146**	0.168	0.859	0.090	0.773	0.057	**no sample***		**0.818**	0.047	**0.597**	0.019	0.501	0.035
6	**0.549**	0.031	**0.734**	0.028	**1.945**	0.096	**2.389**	0.045	**2.916**	0.177	**1.951**	0.111	**no sample***		**1.279**	0.135	**1.524**	0.078	**0.968**	0.045	**0.765**	0.012	**0.679**	0.089
7	**0.585**	0.050	**0.889**	0.086	**1.341**	0.093	**3.094**	0.113	**3.723**	0.213	**2.775**	0.139	**42.933**	3.653	**1.286**	0.096	**1.550**	0.207	**2.987**	0.228	**0.817**	0.024	**0.554**	0.084
8	**0.571**	0.024	**0.635**	0.040	**2.126**	0.140	**7.117**	0.225	**4.062**	0.242	**2.163**	0.157	**1.449**	0.138	**1.646**	0.105	**1.963**	0.126	**1.202**	0.079	**0.851**	0.091	**0.703**	0.053
9	**0.617**	0.025	**0.784**	0.050	**2.509**	0.097	**4.401**	0.194	**3.898**	0.189	**2.348**	0.184	**1.776**	0.196	**1.639**	0.144	**2.139**	0.208	**1.251**	0.046	**0.860**	0.062	**0.623**	0.076
10	**0.716**	0.054	**1.246**	0.049	**3.075**	0.079	**3.688**	0.092	**4.642**	0.367	**3.673**	0.305	**1.823**	0.137	**2.154**	0.214	**2.167**	0.196	**1.353**	0.089	**1.018**	0.059	**0.825**	0.077
11	**0.817**	0.057	**1.099**	0.109	**2.730**	0.146	**3.436**	0.051	**4.260**	0.242	**2.601**	0.216	**2.337**	0.160	**2.009**	0.298	**3.139**	0.243	**1.624**	0.125	**1.175**	0.108	**0.610**	0.062
12	**1.021**	0.066	**1.232**	0.089	**5.363**	0.071	**5.038**	0.117	**4.564**	0.125	**2.624**	0.188	**no sample***		**2.100**	0.249	**2.100**	0.233	**1.588**	0.065	**1.256**	0.139	**2.025**	0.159
13	**1.022**	0.052	**1.189**	0.117	**1.458**	0.102	**9.329**	0.179			**3.636**	0.234	**2.354**	0.305	**no sample***		**2.183**	0.182	**no sample***		**1.314**	0.064	0.343	0.030
14	**1.100**	0.033	**1.404**	0.094									**2.732**	0.292	**1.971**	0.209	**2.262**	0.209	**2.226**	0.164	**1.490**	0.163	**0.844**	0.099
15	**0.599**	0.025											**2.528**	0.324	**no sample***		**2.104**	0.195	**no sample***		**1.576**	0.193	**0.909**	0.106
16													**no sample***		**2.016**	0.223	**2.045**	0.199	**2.793**	0.154	**1.671**	0.065	**1.595**	0.085
17													**2.472**	0.185	**no sample***		**no sample***				**1.848**	0.129	**1.490**	0.132
18															**3.220**	0.308	**2.075**	0.138			**1.838**	0.112	**2.745**	0.222
19																	**2.395**	0.201			**2.044**	0.086	**3.517**	0.216
20																					**2.130**	0.142	**2.968**	0.130
21																					**2.304**	0.178	**3.296**	0.260
22																					**222.502**	11.136		
23																					**2.919**	0.196		
LoD	0.025		0.025		0.049		0.049		0.049		0.047		0.449		0.449		0.449		0.232		0.232		0.232	
LoQ	0.060		0.060		0.132		0.132		0.132		0.117		0.977		0.977		0.977		0.514		0.514		0.514	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 112: Cobalt concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**0.792**	0.030														
-14					**0.159**	0.006	**0.912**	0.077	**0.941**	0.059	**0.659**	0.053												
-13			**0.216**	0.007	**0.332**	0.018	**0.929**	0.059	**0.824**	0.064	**0.742**	0.049												
-12	**0.230**	0.017	**0.291**	0.019	**0.186**	0.012	**0.902**	0.044	**1.004**	0.064	**0.604**	0.030												
-11	**0.148**	0.010	**0.204**	0.015	**0.244**	0.021	**0.986**	0.072	**1.096**	0.055	**0.708**	0.064												
-10	**0.161**	0.009	**0.229**	0.022	**0.334**	0.029	**0.909**	0.021	**1.133**	0.020	**0.649**	0.048							**0.196**	0.030				
-9	**0.146**	0.011	**0.266**	0.017	**0.233**	0.021	**0.945**	0.054	**1.017**	0.086	**0.735**	0.067							**0.196**	0.028				
-8	**0.173**	0.011	**0.218**	0.020	**0.274**	0.025	**0.929**	0.080	**1.140**	0.057	**0.648**	0.058							**0.180**	0.028				
-7	**0.174**	0.014	**0.257**	0.008	**0.819**	0.054	**1.064**	0.051	**1.074**	0.058	**0.755**	0.034							**0.185**	0.029				
-6	**0.196**	0.018	**0.234**	0.020	**no sample***		**0.975**	0.041	**1.250**	0.045	**0.679**	0.043					**0.172**	0.019	**0.201**	0.021			**0.165**	0.020
-5	**0.155**	0.015	**0.270**	0.018	**1.683**	0.090	**1.110**	0.060	**1.238**	0.077	**0.714**	0.061	**0.147**	0.011	**0.154**	0.016	**0.160**	0.026	**0.172**	0.029			**0.175**	0.030
-4	**0.132**	0.009	**0.260**	0.024	**0.500**	0.024	**0.993**	0.108	**1.472**	0.083	**0.649**	0.062	**0.171**	0.026	**0.139**	0.016	**0.292**	0.053	**0.187**	0.026	**0.351**	0.025	**0.187**	0.040
-3	**0.139**	0.008	**0.226**	0.022	**0.308**	0.008	**1.144**	0.043	**0.836**	0.020	**0.675**	0.017	**0.161**	0.015	**0.163**	0.026	**0.184**	0.014	**0.197**	0.032	**0.248**	0.029	**0.174**	0.020
-2	**0.134**	0.010	**0.249**	0.022	**0.550**	0.054	**1.109**	0.060	**1.572**	0.024	**0.597**	0.007	**0.149**	0.018	**0.163**	0.015	**0.144**	0.018	**0.193**	0.014	**0.176**	0.020	**0.172**	0.032
-1	**0.157**	0.014	**0.356**	0.013	**0.572**	0.050	**2.430**	0.084	**2.113**	0.135	**1.574**	0.106	**0.159**	0.028	**0.170**	0.028	**0.291**	0.043	**0.195**	0.031	**0.202**	0.011	**0.161**	0.019
0	**0.138**	0.014	**0.277**	0.012	**0.304**	0.024	**2.260**	0.075	**2.043**	0.132	**1.886**	0.099	**0.163**	0.009	**0.194**	0.012	**0.656**	0.059	**0.223**	0.012	**0.246**	0.018	**0.205**	0.014
1	**0.510**	0.018	**0.323**	0.025	**0.679**	0.038	**2.024**	0.166	**1.168**	0.052	**1.116**	0.082	**0.535**	0.043	**0.420**	0.052	**0.616**	0.055	**0.332**	0.029	**0.244**	0.022	**0.166**	0.016
2	**0.400**	0.024	**0.588**	0.022	**0.616**	0.036	**1.091**	0.057	**0.826**	0.051	**0.639**	0.056	**0.221**	0.023	**0.301**	0.016	**0.308**	0.055	**0.140**	0.018	**0.122**	0.012	**0.091**	0.018
3	**0.475**	0.029	**0.264**	0.029	**0.428**	0.039	**0.730**	0.023	**0.761**	0.047	**0.817**	0.064	**0.209**	0.038	**0.313**	0.038	**0.285**	0.032	**0.127**	0.020	**0.154**	0.016	**0.084**	0.008
4	**0.275**	0.023	**0.243**	0.017	**0.407**	0.022	**0.641**	0.033	**1.103**	0.065	**0.835**	0.080	**no sample***		**0.262**	0.022	**0.282**	0.020	**0.141**	0.017	**0.127**	0.017	**0.074**	0.016
5	**0.258**	0.020	**0.513**	0.042	**0.478**	0.024	**0.870**	0.044	**1.174**	0.067	**0.773**	0.058	**0.175**	0.031	**0.289**	0.025	**no sample***		**0.154**	0.034	**0.134**	0.005	**0.065**	0.013
6	**0.247**	0.019	**0.244**	0.020	**0.729**	0.057	**0.831**	0.048	**1.101**	0.068	**0.724**	0.060	**no sample***		**0.331**	0.040	**0.474**	0.047	**0.164**	0.023	**0.169**	0.016	**0.076**	0.006
7	**0.248**	0.024	**0.294**	0.021	**0.500**	0.035	**0.875**	0.043	**1.317**	0.091	**0.905**	0.047	**0.655**	0.053	**0.407**	0.045	**0.418**	0.037	**0.208**	0.031	**0.191**	0.022	**0.076**	0.007
8	**0.235**	0.021	**0.820**	0.058	**0.795**	0.036	**1.102**	0.055	**1.477**	0.114	**0.726**	0.040	**0.393**	0.038	**0.490**	0.058	**0.595**	0.045	**0.289**	0.018	**0.194**	0.012	**0.072**	0.015
9	**0.222**	0.013	**0.374**	0.009	**1.136**	0.047	**1.216**	0.071	**1.407**	0.055	**0.863**	0.079	**0.486**	0.070	**0.588**	0.042	**0.706**	0.100	**0.339**	0.032	**0.196**	0.009	**0.079**	0.018
10	**0.274**	0.011	**0.485**	0.034	**1.290**	0.072	**1.248**	0.040	**1.488**	0.072	**1.301**	0.107	**0.596**	0.087	**0.620**	0.051	**0.756**	0.046	**0.300**	0.019	**0.209**	0.021	**0.086**	0.011
11	**0.296**	0.026	**0.553**	0.041	**1.412**	0.089	**1.574**	0.073	**1.406**	0.076	**0.855**	0.081	**0.769**	0.073	**0.699**	0.073	**0.764**	0.070	**0.302**	0.028	**0.225**	0.018	**0.081**	0.018
12	**0.393**	0.033	**0.576**	0.041	**0.909**	0.042	**1.718**	0.093	**1.603**	0.073	**0.889**	0.027	**no sample***		**0.740**	0.091	**0.907**	0.068	**0.262**	0.014	**0.236**	0.020	**0.111**	0.006
13	**0.411**	0.015	**0.601**	0.019	**0.718**	0.054	**2.130**	0.091			**1.067**	0.059	**0.661**	0.092	**no sample***		**0.932**	0.067	**no sample***		**0.284**	0.021	**0.121**	0.024
14	**0.452**	0.025	**0.693**	0.046									**1.130**	0.055	**0.782**	0.107	**0.961**	0.070	**0.354**	0.015	**0.289**	0.027	**0.131**	0.021
15	**0.426**	0.014											**0.884**	0.119	**no sample***		**1.030**	0.109	**no sample***		**0.341**	0.035	**0.184**	0.023
16													**no sample***		**0.844**	0.075	**1.043**	0.102	**0.436**	0.030	**0.350**	0.033	**0.202**	0.016
17													**1.062**	0.070	**no sample***		**no sample***				**0.369**	0.040	**0.245**	0.023
18															**1.338**	0.091	**1.157**	0.102			**0.387**	0.039	**0.650**	0.075
19																	**1.412**	0.167			**0.443**	0.036	**1.293**	0.089
20																					**0.482**	0.053	**0.791**	0.022
21																					**0.508**	0.025	**1.009**	0.082
22																					**2.901**	0.116		
23																					**0.630**	0.072		
LoD	0.005		0.005		0.010		0.010		0.010		0.004		0.009		0.009		0.009		0.005		0.005		0.005	
LoQ	0.011		0.011		0.028		0.028		0.028		0.011		0.025		0.025		0.025		0.014		0.014		0.014	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 113: Copper concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**2.203**	0.116														
-14					**2.704**	0.064	**2.021**	0.083	**2.465**	0.075	**1.288**	0.011												
-13			**1.927**	0.087	**4.279**	0.252	**1.959**	0.063	**2.190**	0.107	**2.426**	0.191												
-12	**2.156**	0.084	**2.612**	0.087	**2.906**	0.047	**1.831**	0.069	**2.671**	0.020	**2.173**	0.105												
-11	**1.849**	0.101	**2.066**	0.025	**3.685**	0.113	**2.104**	0.019	**2.749**	0.059	**2.177**	0.113												
-10	**2.074**	0.099	**2.261**	0.091	**3.962**	0.279	**1.858**	0.014	**2.754**	0.095	**2.088**	0.033							**1.040**	0.066				
-9	**2.280**	0.111	**2.622**	0.084	**3.457**	0.310	**2.185**	0.100	**2.668**	0.117	**2.322**	0.071							**1.127**	0.024				
-8	**2.592**	0.074	**2.594**	0.076	**3.596**	0.142	**2.116**	0.073	**2.801**	0.079	**2.059**	0.026							**1.056**	0.023				
-7	**2.550**	0.045	**2.204**	0.045	**9.163**	0.437	**2.271**	0.118	**2.840**	0.118	**2.711**	0.147							**0.984**	0.036				
-6	**2.458**	0.064	**2.397**	0.109	**no sample***		**2.684**	0.190	**3.476**	0.200	**2.167**	0.084					**0.838**	0.029	**1.144**	0.028			**1.015**	0.051
-5	**2.411**	0.077	**2.175**	0.074	17.847	0.630	**2.994**	0.193	**3.359**	0.063	**2.366**	0.068	**0.851**	0.024	**0.868**	0.015	0.825	0.058	**0.921**	0.027			**0.981**	0.042
-4	**2.171**	0.084	**3.280**	0.047	**6.107**	0.249	**2.365**	0.059	**3.489**	0.103	**2.144**	0.055	**0.892**	0.037	0.811	0.019	**1.554**	0.034	**0.973**	0.048	**0.921**	0.042	**0.984**	0.036
-3	**2.143**	0.089	**1.878**	0.061	**3.842**	0.104	**2.502**	0.063	**4.164**	0.070	**2.346**	0.065	0.829	0.032	0.819	0.055	0.808	0.027	**1.172**	0.078	**0.873**	0.010	**0.993**	0.065
-2	**1.997**	0.017	**2.270**	0.048	**4.672**	0.071	**2.771**	0.138	**4.322**	0.157	**2.032**	0.086	0.831	0.031	**0.834**	0.037	**1.014**	0.042	**1.089**	0.033	**1.036**	0.047	**0.914**	0.057
-1	**2.154**	0.027	**2.939**	0.060	**5.298**	0.135	**2.374**	0.051	**4.164**	0.120	**2.316**	0.091	**0.869**	0.041	0.808	0.038	**1.757**	0.071	**0.811**	0.028	**0.955**	0.046	**1.387**	0.043
0	**2.116**	0.077	**2.721**	0.045	**2.963**	0.218	**2.055**	0.058	**2.756**	0.069	**1.427**	0.096	0.793	0.014	0.706	0.055	**5.463**	0.096	**1.055**	0.038	**0.688**	0.031	**0.913**	0.028
1	**2.778**	0.080	**1.750**	0.042	**2.721**	0.164	**2.285**	0.081	**2.989**	0.125	**1.671**	0.122	**1.354**	0.039	0.722	0.020	**2.281**	0.147	**0.049**	0.013	**0.628**	0.052	**0.203**	0.058
2	**0.800**	0.028	**2.119**	0.085	**0.872**	0.041	**2.958**	0.128	**3.193**	0.163	**2.365**	0.138	0.416	<LoD	0.349	0.023	0.416	<LoD	0.026	0.033	**0.126**	0.024	**0.215**	0.029
3	**0.655**	0.038	**0.259**	0.022	**0.663**	0.063	**3.269**	0.164	**3.517**	0.182	**2.894**	0.279	0.416	<LoD	0.416	<LoD	0.416	<LoD	**0.059**	0.023	**0.087**	0.020	**0.108**	0.028
4	**0.440**	0.031	**0.265**	0.022	0.333	0.036	**1.574**	0.117	**2.677**	0.119	**3.038**	0.114	**no sample***		0.416	<LoD	0.511	0.038	0.019	<LoD	0.017	0.030	**0.094**	0.008
5	**0.386**	0.015	**0.563**	0.054	0.289	0.089	**1.448**	0.051	**6.406**	0.525	**3.261**	0.085	0.499	0.032	0.416	<LoD	**no sample***		0.019	<LoD	**0.072**	0.012	0.020	0.016
6	**0.296**	0.021	0.066	<LoD	**2.159**	0.028	**1.331**	0.127	**2.989**	0.106	**2.952**	0.101	**no sample***		0.416	<LoD	**0.862**	0.051	**0.094**	0.022	**0.110**	0.018	**0.626**	0.026
7	**0.280**	0.023	**0.236**	0.021	**0.457**	0.024	**1.417**	0.147	**2.305**	0.044	**3.837**	0.064	0.416	<LoD	0.416	<LoD	0.356	0.056	**0.064**	0.023	**0.130**	0.039	**0.149**	0.033
8	**0.382**	0.026	**0.172**	0.047	**2.348**	0.156	**1.442**	0.084	**2.325**	0.117	**3.736**	0.105	0.416	<LoD	0.416	<LoD	0.401	0.031	**0.385**	0.029	**0.069**	0.026	**0.116**	0.019
9	**0.294**	0.033	0.066	<LoD	**4.541**	0.134	**1.587**	0.108	**1.887**	0.162	**4.173**	0.121	0.416	<LoD	0.416	<LoD	0.416	<LoD	**1.440**	0.029	0.019	<LoD	**0.384**	0.042
10	**0.212**	0.018	0.066	<LoD	**5.910**	0.321	**1.125**	0.084	**1.986**	0.111	**7.639**	0.199	0.463	0.041	0.416	<LoD	0.416	<LoD	**0.424**	0.021	**0.069**	0.021	**0.281**	0.027
11	**0.675**	0.042	**0.193**	0.021	**4.033**	0.201	**1.223**	0.108	**1.591**	0.104	**3.511**	0.145	0.416	<LoD	0.416	<LoD	0.416	<LoD	**0.142**	0.014	**0.069**	0.036	**0.058**	0.031
12	**0.556**	0.016	0.066	<LoD	**0.787**	0.029	**1.478**	0.048	**2.176**	0.127	**3.315**	0.138	**no sample***		0.542	0.048	0.416	<LoD	**0.077**	0.023	**0.258**	0.025	**0.254**	0.024
13	**0.768**	0.048	0.066	<LoD	0.209	0.033	**2.265**	0.038			**3.872**	0.147	0.616	0.048	**no sample***		0.416	<LoD	**no sample***		**0.351**	0.026	**0.381**	0.029
14	**0.577**	0.047	**0.182**	0.046									0.416	<LoD	0.416	<LoD	0.416	<LoD	**0.373**	0.035	**0.041**	0.022	**0.151**	0.024
15	**3.045**	0.162											0.530	0.062	**no sample***		0.416	<LoD	**no sample***		**0.042**	0.024	**0.768**	0.037
16													**no sample***		0.062		0.416	<LoD	**0.805**	0.057	0.020	0.019	**0.141**	0.045
17													0.416	<LoD	**no sample***		**no sample***				0.019	<LoD	**0.208**	0.026
18															**3.993**	0.087	0.480	0.021			0.033	0.012	**2.817**	0.108
19																	**0.948**	0.027			**0.151**	0.031	0.019	<LoD
20																					0.019	<LoD	**1.826**	0.063
21																					0.035	0.017	**3.081**	0.103
22																					0.019	<LoD		
23																					**0.197**	0.019		
LoD	0.059		0.059		0.159		0.159		0.159		0.141		0.319		0.319		0.319		0.016		0.016		0.016	
LoQ	0.133		0.133		0.379		0.379		0.379		0.410		0.833		0.833		0.833		0.038		0.038		0.038	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 114: Lead concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**0.037**	0.001														
-14					**0.456**	0.010	**0.178**	0.010	**0.093**	0.003	**0.062**	0.005												
-13			**1.014**	0.027	**1.840**	0.072	**0.047**	0.003	**0.104**	0.007	**0.068**	0.005												
-12	**2.124**	0.070	**0.881**	0.032	**0.785**	0.043	**0.138**	0.009	**0.085**	0.007	**0.070**	0.003												
-11	**0.168**	0.007	**0.835**	0.021	**1.727**	0.051	**0.061**	0.005	**0.131**	0.009	**0.067**	0.002												
-10	**0.950**	0.024	**0.763**	0.010	**2.207**	0.057	**0.172**	0.012	**0.080**	0.003	**0.080**	0.005							**0.218**	0.005				
-9	**0.384**	0.009	**1.779**	0.036	**0.857**	0.025	**0.059**	0.005	**0.119**	0.009	**0.052**	0.003							**0.205**	0.005				
-8	**0.839**	0.008	**0.354**	0.010	**1.044**	0.046	**0.280**	0.018	**0.063**	0.004	**0.065**	0.005							**0.288**	0.007				
-7	**1.683**	0.051	**1.377**	0.042	**21.983**	0.507	**0.181**	0.015	**0.205**	0.012	**0.067**	0.002							**0.412**	0.013				
-6	**2.737**	0.031	**1.369**	0.029	**no sample***		**0.202**	0.015	**0.149**	0.015	**0.062**	0.004					0.048	0.004	**0.743**	0.025			**0.266**	0.009
-5	**0.474**	0.011	**3.913**	0.110	**31.076**	0.239	**0.143**	0.009	**0.445**	0.033	**0.053**	0.004	**0.158**	0.005	**0.159**	0.008	0.039	0.005	**0.303**	0.012			**0.183**	0.009
-4	**0.683**	0.009	**2.132**	0.057	**10.348**	0.176	**0.107**	0.008	**0.034**	0.003	**0.058**	0.004	**0.147**	0.002	**0.169**	0.001	**2.238**	0.032	**0.210**	0.013	**0.334**	0.008	**0.207**	0.009
-3	**0.356**	0.018	**1.106**	0.042	**2.222**	0.045	**0.167**	0.011	**0.179**	0.023	**0.070**	0.003	**0.174**	0.017	**0.179**	0.009	**0.174**	0.009	**0.240**	0.008	**0.727**	0.016	**0.266**	0.016
-2	**0.412**	0.011	**3.233**	0.076	**15.326**	0.232	**1.868**	0.051	**0.207**	0.021	**0.073**	0.002	**0.169**	0.013	**0.269**	0.008	**0.161**	0.007	**0.352**	0.002	**0.586**	0.013	**0.294**	0.012
-1	**0.385**	0.021	**4.416**	0.055	**13.003**	0.205	**0.031**	0.003	**10.088**	1.866	**0.129**	0.008	**0.368**	0.019	**0.359**	0.005	**0.207**	0.009	**0.215**	0.012	**0.829**	0.013	**0.383**	0.010
0	**0.901**	0.013	**0.718**	0.035	**0.961**	0.026	**0.298**	0.013	**0.479**	0.011	**0.042**	0.002	**0.379**	0.014	**0.425**	0.018	**0.394**	0.020	**0.382**	0.009	**0.461**	0.012	**0.673**	0.008
1	**1.955**	0.049	**0.674**	0.022	**0.276**	0.011	**0.177**	0.009	**1.597**	0.026	**0.068**	0.005	**0.140**	0.005	**0.582**	0.012	**0.210**	0.012	**0.211**	0.009	**0.688**	0.015	**0.182**	0.007
2	**0.855**	0.009	**0.629**	0.018	**0.394**	0.014	**2.118**	0.085	**0.808**	0.021	**0.397**	0.009	**0.141**	0.004	**0.575**	0.020	**0.196**	0.012	**0.100**	0.008	**0.329**	0.010	**0.104**	0.005
3	**0.648**	0.029	**0.664**	0.013	**0.563**	0.022	**0.114**	0.007	**0.326**	0.009	**0.039**	0.004	**0.244**	0.007	**0.483**	0.012	**0.656**	0.015	**0.193**	0.004	**0.068**	0.002	**0.067**	0.007
4	**0.198**	0.010	**0.448**	0.015	**0.232**	0.014	**0.077**	0.003	**0.375**	0.018	**0.054**	0.002	**no sample***		**0.211**	0.005	**1.649**	0.023	**0.101**	0.005	**0.094**	0.007	**0.047**	0.006
5	**0.364**	0.014	**0.491**	0.014	**0.980**	0.048	**0.163**	0.014	**0.770**	0.027	**0.056**	0.001	**0.112**	0.004	**0.174**	0.004	**no sample***		**0.106**	0.004	**0.119**	0.010	**0.040**	0.006
6	**0.271**	0.009	**0.316**	0.011	**12.078**	0.235	**0.213**	0.011	**0.035**	0.004	**0.134**	0.004	**no sample***		**0.346**	0.015	**2.569**	0.044	**0.208**	0.008	**0.414**	0.009	**0.190**	0.003
7	**0.511**	0.008	**0.488**	0.009	**2.614**	0.077	**0.145**	0.013	**0.194**	0.009	**0.045**	0.002	**0.313**	0.008	**0.125**	0.008	**0.583**	0.017	**0.135**	0.008	**0.526**	0.017	**0.389**	0.006
8	**0.323**	0.009	**1.926**	0.065	**15.314**	0.293	**0.327**	0.016	**2.579**	0.053	**3.881**	0.047	**0.236**	0.010	**0.924**	0.015	**0.854**	0.029	**0.942**	0.014	**0.241**	0.006	**0.094**	0.006
9	**0.267**	0.020	**0.418**	0.017	**32.635**	0.939	**0.144**	0.007	**0.220**	0.012	**8.482**	1.365	**0.188**	0.009	**0.514**	0.008	**0.371**	0.013	**1.923**	0.028	**0.092**	0.004	**0.049**	0.005
10	**0.378**	0.016	**0.412**	0.024	**28.400**	1.386	**0.118**	0.007	**0.097**	0.011	**26.710**	0.419	**1.204**	0.027	**0.126**	0.006	**0.292**	0.008	**1.067**	0.019	**0.296**	0.005	**0.350**	0.017
11	**1.730**	0.033	**0.894**	0.031	**25.805**	0.564	**0.709**	0.021	**0.231**	0.006	**1.911**	0.025	**no sample***	no samp	**0.134**	0.008	0.047	0.005	**0.384**	0.006	**0.097**	0.004	**0.057**	0.004
12	**3.521**	0.056	**0.409**	0.013	**4.636**	0.123	**0.644**	0.018	**0.962**	0.023	**2.041**	0.020	**no sample***		**0.647**	0.028	**0.324**	0.018	**0.123**	0.005	**0.235**	0.008	**0.354**	0.010
13	**2.765**	0.064	**0.420**	0.008	**2.471**	0.120	**10.782**	1.677			**3.038**	0.069	**0.687**	0.017	**no sample***		**0.128**	0.008	**no sample***		**0.494**	0.014	**0.061**	0.002
14	**4.209**	0.127	**1.764**	0.038									**no sample***	no samp	**0.334**	0.008	0.047	0.005	**0.696**	0.028	**0.233**	0.012	**0.270**	0.013
15	**0.372**	0.017											**0.907**	0.017	**no sample***		0.047	0.002	**no sample***		**0.183**	0.008	**2.066**	0.040
16													**no sample***		**1.913**	0.052	**0.169**	0.010	**1.782**	0.033	**0.151**	0.007	**0.265**	0.011
17													**0.607**	0.023	**no sample***		**no sample***				**0.398**	0.014	**0.695**	0.017
18															**14.267**	0.186	**0.080**	0.008			**0.219**	0.005	**8.599**	0.240
19																	**2.965**	0.039			**0.187**	0.005	0.005	<LoD
20																					**0.111**	0.005	**6.413**	0.145
21																					**0.128**	0.006	**9.687**	0.165
22																					**0.141**	0.009		
23																					**0.485**	0.009		
LoD	0.013		0.013		0.009		0.009		0.009		0.006		0.024		0.024		0.024		0.004		0.004		0.004	
LoQ	0.038		0.038		0.023		0.023		0.023		0.017		0.052		0.052		0.052		0.009		0.009		0.009	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 115: Molybdenum concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**4.9**	0.2														
-14					**3.3**	0.2	**6.6**	0.4	**5.8**	0.3	**4.7**	0.3												
-13			**4.8**	0.2	**6.5**	0.3	**6.6**	0.3	**5.0**	0.3	**5.8**	0.4												
-12	**4.3**	0.2	**6.5**	0.2	**4.1**	0.3	**6.3**	0.3	**6.2**	0.3	**5.0**	0.4												
-11	**4.4**	0.2	**5.3**	0.1	**4.2**	0.3	**6.8**	0.3	**6.2**	0.3	**6.2**	0.5												
-10	**4.5**	0.1	**6.0**	0.3	**5.5**	0.3	**5.9**	0.3	**6.6**	0.2	**5.5**	0.4							**4.2**	0.4				
-9	**4.7**	0.3	**5.0**	0.3	**4.6**	0.3	**5.9**	0.3	**5.7**	0.4	**6.3**	0.5							**4.3**	0.3				
-8	**4.7**	0.2	**5.7**	0.2	**4.7**	0.4	**5.8**	0.5	**6.3**	0.3	**5.2**	0.4							**4.2**	0.2				
-7	**4.7**	0.2	**5.3**	0.4	**4.2**	0.3	**6.3**	0.4	**5.6**	0.3	**6.1**	0.4							**4.2**	0.2				
-6	**4.3**	0.1	**5.9**	0.3	**no sample***		**5.8**	0.3	**6.9**	0.3	**5.2**	0.4					**3.7**	0.1	**4.1**	0.2			**4.1**	0.3
-5	**5.5**	0.5	**4.3**	0.2	**4.0**	0.2	**6.3**	0.4	**6.5**	0.2	**5.6**	0.4	**3.6**	0.3	**3.7**	0.4	**3.6**	0.3	**4.1**	0.3			**4.0**	0.3
-4	**4.0**	0.2	**5.9**	0.3	**4.0**	0.3	**5.5**	0.4	**8.5**	0.2	**5.0**	0.4	**3.8**	0.3	**3.7**	0.3	**3.8**	0.4	**4.1**	0.3	**4.2**	0.3	**4.1**	0.2
-3	**4.6**	0.2	**5.1**	0.2	**4.4**	0.4	**6.1**	0.3	**6.9**	0.1	**5.3**	0.3	**3.6**	0.2	**3.7**	0.4	**3.7**	0.3	**4.1**	0.3	**4.1**	0.2	**4.0**	0.3
-2	**4.5**	0.2	**4.1**	0.3	**3.3**	0.3	**5.5**	0.2	**9.2**	0.6	**4.3**	0.3	**3.6**	0.3	**3.7**	0.3	**3.7**	0.4	**4.1**	0.3	**3.9**	0.3	**4.0**	0.2
-1	**5.1**	0.4	**5.8**	0.1	**4.8**	0.3	**6.5**	0.3	**5.6**	0.3	**6.6**	0.6	**3.6**	0.3	**3.7**	0.4	**3.8**	0.4	**3.9**	0.2	**3.9**	0.2	**3.8**	0.2
0	**4.4**	0.2	**7.0**	0.2	**4.8**	0.3	**4.1**	0.1	**5.6**	0.3	**2.2**	0.1	**3.6**	0.3	**3.7**	0.2	**5.1**	0.4	**3.9**	0.3	**4.0**	0.2	**3.9**	0.3
1	**5.9**	0.2	**5.9**	0.2	**5.2**	0.3	**2.2**	0.1	**3.4**	0.2	**0.8**	0.1	**3.9**	0.3	**3.9**	0.2	**4.6**	0.4	**3.9**	0.1	**3.9**	0.2	**3.6**	0.2
2	**6.1**	0.2	**7.5**	0.3	**5.5**	0.3	**0.9**	0.1	**3.2**	0.2	**0.4**	0.0	**3.6**	0.3	**3.3**	0.2	**3.8**	0.4	**3.3**	0.2	**3.6**	0.2	**3.5**	0.3
3	**7.1**	0.2	**7.3**	0.4	**4.9**	0.3	**0.6**	0.0	**2.1**	0.1	**0.7**	0.1	**3.1**	0.2	**3.3**	0.2	**3.5**	0.2	**3.1**	0.2	**3.4**	0.1	**3.6**	0.2
4	**5.5**	0.2	**7.4**	0.2	**3.7**	0.2	**0.4**	0.0	**0.9**	0.0	**0.5**	0.0	**no sample***		**2.6**	0.3	**1.6**	0.1	**3.0**	0.2	**3.3**	0.2	**3.4**	0.2
5	**4.5**	0.2	**6.4**	0.2	**2.4**	0.1	**0.5**	0.0	**0.6**	0.0	**0.7**	0.1	**1.7**	0.1	**1.9**	0.2	**no sample***		**2.9**	0.1	**3.0**	0.2	**3.5**	0.3
6	**3.1**	0.1	**4.1**	0.1	**1.6**	0.1	**0.4**	0.0	**0.6**	0.0	**0.4**	0.0	**no sample***		**1.2**	0.1	**0.9**	0.0	**2.5**	0.1	**2.7**	0.2	**3.4**	0.2
7	**2.4**	0.1	**2.8**	0.1	**1.0**	0.0	**0.4**	0.0	**0.5**	0.0	**0.4**	0.0	**0.9**	0.1	**0.7**	0.1	**0.5**	0.0	**2.2**	0.2	**2.3**	0.1	**3.3**	0.2
8	**2.0**	0.1	**2.6**	0.1	**0.5**	0.0	**0.5**	0.0	**0.5**	0.0	**0.3**	0.0	0.1	0.0	**0.5**	0.0	**0.2**	0.0	**1.8**	0.1	**2.0**	0.1	**3.3**	0.2
9	**1.6**	0.1	**1.5**	0.1	**0.6**	0.0	**0.6**	0.0	**0.5**	0.0	**0.3**	0.0	0.1	0.0	**0.3**	0.0	0.1	0.0	**1.5**	0.1	**1.6**	0.0	**3.2**	0.2
10	**1.3**	0.1	**1.2**	0.1	**0.7**	0.1	**0.5**	0.0	**0.6**	0.0	**0.4**	0.0	0.1	0.0	0.2	0.0	0.1	0.0	**1.1**	0.1	**1.3**	0.1	**3.1**	0.2
11	**0.9**	0.0	**0.9**	0.1	**0.8**	0.0	**0.4**	0.0	**0.6**	0.0	**0.3**	0.0	0.1	0.0	0.2	0.0	0.2	0.0	**0.9**	0.1	**1.0**	0.0	**3.2**	0.2
12	**0.9**	0.0	**0.7**	0.0	**0.8**	0.0	**0.4**	0.0	**0.7**	0.0	**0.3**	0.0	**no sample***		0.1	0.0	0.2	0.0	**0.8**	0.0	**0.7**	0.0	**3.1**	0.1
13	**0.7**	0.0	**0.5**	0.0	**0.6**	0.0	**0.3**	0.0			**0.2**	0.0	0.1	0.0	**no sample***		0.1	0.0	**no sample***		**0.6**	0.0	**3.7**	0.2
14	**0.9**	0.0	**0.6**	0.0									0.1	0.0	**0.2**	0.0	0.1	0.0	**0.5**	0.0	**0.5**	0.0	**2.8**	0.1
15	**0.9**	0.0											0.1	0.0	**no sample***		0.1	0.0	**no sample***		**0.4**	0.0	**3.3**	0.1
16													**no sample***		0.1	0.0	0.1	0.0	**0.3**	0.0	**0.3**	0.0	**1.9**	0.1
17													0.2	0.0	**no sample***		**no sample***				**0.3**	0.0	**1.6**	0.1
18															0.2	0.0	0.1	0.0			**0.3**	0.0	**1.0**	0.1
19																	0.2	0.0			**0.2**	0.0	**0.5**	0.0
20																					**0.2**	0.0	**0.3**	0.0
21																					**0.2**	0.0	**0.2**	0.0
22																					**2.1**	0.1		
23																					**0.3**	0.0		
LoD	0.04		0.04		0.09		0.09		0.09		0.06		0.07		0.07		0.07		0.01		0.01		0.01	
LoQ	0.12		0.12		0.26		0.26		0.26		0.16		0.20		0.20		0.20		0.03		0.03		0.03	
* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.																								

Table A3. 116: Nickel concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**0.5**	0.0														
-14					**0.5**	0.1	**1.0**	0.1	**0.7**	0.1	1.0	<LoD												
-13			**16.5**	0.6	**1.2**	0.1	**1.0**	0.1	**0.6**	0.1	1.0	<LoD												
-12	0.7	0.0	**18.8**	1.6	**0.6**	0.0	**0.8**	0.1	**0.9**	0.0	1.0	<LoD												
-11	0.8	<LoD	**15.2**	0.9	**1.0**	0.1	**1.0**	0.1	**1.3**	0.1	1.0	<LoD												
-10	1.0	0.3	**20.6**	1.6	**3.3**	0.1	**0.8**	0.1	**0.8**	0.1	1.0	<LoD							**0.6**	0.1				
-9	0.7	0.2	**14.7**	0.9	**3.5**	0.1	**0.9**	0.1	**0.7**	0.1	1.0	<LoD							**1.7**	0.1				
-8	0.8	<LoD	**15.6**	1.1	**5.0**	0.1	**0.7**	0.1	**0.9**	0.1	1.0	<LoD							**0.6**	0.1				
-7	0.8	<LoD	**17.2**	1.1	**4.2**	0.3	**0.8**	0.1	**0.6**	0.1	0.9	0.1							**0.6**	0.1				
-6	0.8	<LoD	**14.0**	0.5	**no sample***		**1.0**	0.1	**1.0**	0.1	1.0	<LoD					**0.4**	0.1	**0.6**	0.1			**0.6**	0.0
-5	1.1	0.1	**12.4**	1.1	**2.7**	0.1	**0.9**	0.1	**0.8**	0.1	1.1	0.2	**0.5**	0.1	**0.4**	0.1	**0.4**	0.1	**0.6**	0.0			**0.5**	0.1
-4	1.3	0.1	**13.9**	0.6	**1.0**	0.1	**0.7**	0.0	**0.8**	0.1	1.0	0.1	**0.5**	0.1	**0.4**	0.0	**0.7**	0.1	**0.5**	0.1	**7.4**	0.2	**0.7**	0.1
-3	**2.1**	0.1	**12.9**	0.6	**0.8**	0.1	**1.0**	0.1	**0.8**	0.1	1.6	0.1	**0.5**	0.1	**1.9**	0.1	**0.4**	0.1	**0.6**	0.1	**2.5**	0.1	**0.6**	0.1
-2	**2.9**	0.2	**12.6**	0.7	**1.0**	0.0	**0.8**	0.1	**1.1**	0.1	1.3	0.1	**0.5**	0.0	**0.5**	0.1	**0.5**	0.0	**0.5**	0.1	**0.6**	0.1	**0.7**	0.1
-1	**3.5**	0.1	**15.1**	1.0	**3.3**	0.2	**1.1**	0.1	**1.2**	0.1	1.7	0.1	**0.6**	0.1	**0.5**	0.1	**6.2**	0.4	**0.5**	0.1	**0.5**	0.1	**0.7**	0.1
0	**4.1**	0.1	**12.9**	0.8	**3.5**	0.2	**0.9**	0.1	**1.2**	0.1	1.1	0.1	**0.5**	0.1	**0.5**	0.0	**11.8**	0.3	**0.6**	0.1	**0.5**	0.1	**0.6**	0.1
1	**5.2**	0.1	**10.9**	0.4	**2.6**	0.1	**1.1**	0.0	**0.8**	0.1	1.2	0.1	**0.5**	0.1	**0.5**	0.1	**14.1**	0.7	**0.6**	0.0	**0.5**	0.0	**0.6**	0.1
2	**5.3**	0.2	**9.7**	0.1	**1.0**	0.1	**1.1**	0.0	**0.8**	0.1	1.5	0.8	**0.3**	0.1	**0.6**	0.1	**0.5**	0.1	0.4	0.1	**0.5**	0.0	0.3	0.1
3	**5.2**	0.2	**8.1**	0.9	**0.9**	0.1	**0.8**	0.1	**0.5**	0.0	1.0	<LoD	**0.4**	0.0	**0.4**	0.1	**0.4**	0.1	0.3	0.0	**0.7**	0.0	0.3	0.0
4	**5.3**	0.4	**6.3**	0.6	**0.7**	0.1	**0.6**	0.0	**1.6**	0.0	**2.5**	0.2	**no sample***		**0.4**	0.1	**0.5**	0.1	0.3	0.0	0.2	0.0	0.3	0.1
5	**5.0**	0.2	**5.5**	0.5	**0.6**	0.0	**0.5**	0.0	**0.7**	0.0	1.0	0.1	**0.4**	0.1	**0.4**	0.0	**no sample***		0.4	0.1	0.3	0.0	0.2	0.0
6	**5.1**	0.2	**5.9**	0.3	**1.1**	0.1	**0.4**	0.0	**0.5**	0.0	1.2	0.1	**no sample***		**0.5**	0.1	**0.7**	0.1	0.3	0.1	0.3	0.0	0.2	0.0
7	**4.7**	0.2	**5.9**	0.5	**0.6**	0.1	**0.3**	0.0	**0.5**	0.1	1.8	0.1	**19.3**	4.4	**0.4**	0.0	**1.0**	0.1	**0.4**	0.0	0.3	0.0	0.3	0.1
8	**4.9**	0.3	**4.3**	0.4	**0.7**	0.1	**1.4**	0.1	**0.6**	0.1	**3.1**	0.3	**0.3**	0.1	**0.6**	0.1	**0.8**	0.0	0.4	0.1	0.3	0.0	0.3	0.0
9	**5.3**	0.3	**2.5**	0.1	**1.2**	0.1	**0.6**	0.1	**0.7**	0.1	**4.0**	0.1	**0.4**	0.0	**0.4**	0.1	**0.7**	0.0	0.4	0.1	0.2	0.0	0.3	0.0
10	**7.7**	0.6	**3.3**	0.4	**1.8**	0.1	**0.3**	0.0	**0.6**	0.1	**7.4**	0.6	**0.5**	0.0	**0.4**	0.1	**0.6**	0.1	0.4	0.0	0.2	0.0	0.3	0.0
11	**6.7**	0.3	**1.8**	0.1	**1.2**	0.1	**0.6**	0.0	**0.6**	0.1	**6.0**	0.2	**0.9**	0.1	**0.5**	0.1	**1.6**	0.1	0.4	0.1	0.2	0.0	0.2	0.0
12	**7.0**	0.5	1.5	0.1	**1.7**	0.2	**0.8**	0.1	**1.0**	0.1	**7.2**	0.3	**no sample***		**0.4**	0.0	**0.8**	0.1	0.2	0.0	0.3	0.0	0.3	0.0
13	**6.8**	0.4	1.4	0.1	**0.4**	0.0	**2.0**	0.2			**7.3**	0.1	**0.6**	0.0	**no sample***		**0.6**	0.0	**no sample***		0.3	0.0	0.3	0.0
14	**7.2**	0.3	1.3	0.1									**1.4**	0.1	**0.5**	0.1	**0.6**	0.0	0.3	0.0	0.2	0.0	0.2	0.0
15	**8.3**	0.7											**0.6**	0.1	**no sample***		**0.5**	0.1	**no sample***		0.2	0.0	0.4	0.0
16													**no sample***		**1.4**	0.1	**0.6**	0.1	**0.5**	0.0	0.3	0.0	0.4	0.1
17													**0.5**	0.1	**no sample***		**no sample***				0.3	0.0	0.3	0.1
18															**1.3**	0.1	**0.5**	0.0			0.2	0.1	**0.8**	0.1
19																	**1.9**	0.1			0.3	0.0	**2.0**	0.1
20																					0.3	0.0	**1.0**	0.1
21																					0.4	0.1	**1.3**	0.0
22																					0.2	<LoD		
23																					0.4	0.0		
LoD	0.65		0.65		0.06		0.06		0.06		0.80		0.08		0.08		0.08		0.16		0.16		0.16	
LoQ	1.57		1.57		0.16		0.16		0.16		2.03		0.19		0.19		0.19		0.42		0.42		0.42	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 117: Selenium concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									0.455	<LoD														
-14					0.455	<LoD	0.349	0.098	0.416	0.179	**0.220**	0.063												
-13			0.155	0.054	0.357	0.107	0.455	<LoD	0.384	0.110	**0.355**	0.033												
-12	0.198	0.073	0.252	0.059	0.455	<LoD	0.455	<LoD	0.420	0.057	**0.301**	0.036												
-11	0.208	0.018	0.250	0.089	0.455	<LoD	0.411	0.087	0.483	0.091	**0.463**	0.089												
-10	0.196	0.056	0.287	0.051	0.455	<LoD	0.378	0.045	0.501	0.148	**0.341**	0.080							0.364	0.073				
-9	0.205	0.072	0.285	0.043	0.455	<LoD	0.381	0.122	0.413	0.096	**0.380**	0.037							0.348	0.107				
-8	0.188	0.079	0.276	0.114	0.455	<LoD	0.414	0.127	0.634	0.084	**0.371**	0.032							0.450	0.135				
-7	0.171	0.043	0.230	0.065	0.455	<LoD	0.418	0.038	0.434	0.076	**0.377**	0.022							0.379	0.096				
-6	0.206	<LoD	0.245	0.104	**no sample***		0.455	<LoD	0.493	0.155	**0.380**	0.034					0.571	<LoD	0.402	0.178			0.368	0.165
-5	0.210	0.095	0.179	0.056	0.455	<LoD	0.393	0.130	0.446	0.124	**0.323**	0.026	0.571	<LoD	0.571	<LoD	0.571	<LoD	0.451	0.120			0.386	0.140
-4	0.206	<LoD	0.290	0.077	0.455	<LoD	0.375	0.090	0.641	0.094	**0.367**	0.020	0.571	<LoD	0.571	<LoD	0.571	<LoD	0.370	0.100	0.358	<LoD	0.392	0.064
-3	0.192	0.098	0.279	0.055	0.455	<LoD	0.443	0.162	0.558	0.084	**0.358**	0.040	0.571	<LoD	0.571	<LoD	0.571	<LoD	0.358	<LoD	0.387	0.138	0.413	0.068
-2	0.206	<LoD	0.245	0.063	0.455	<LoD	0.408	0.127	0.796	0.111	**0.433**	0.001	0.571	<LoD	0.571	<LoD	0.571	<LoD	0.424	0.141	0.398	0.017	0.434	0.103
-1	0.206	<LoD	0.253	0.032	0.350	0.049	0.430	0.083	0.421	0.088	**0.353**	0.034	0.571	<LoD	0.571	<LoD	0.571	<LoD	0.425	0.175	0.356	0.074	0.358	<LoD
0	0.218	0.043	0.305	0.059	0.455	<LoD	0.455	<LoD	0.515	0.171	**0.361**	0.027	0.571	<LoD	0.571	<LoD	0.571	<LoD	0.497	0.046	0.358	<LoD	0.348	0.099
1	0.239	0.083	0.248	0.096	0.455	<LoD	0.455	<LoD	0.617	0.142	**0.478**	0.030	0.571	<LoD	0.571	<LoD	0.571	<LoD	0.590	0.104	0.343	0.120	0.407	0.053
2	0.198	0.081	0.322	0.116	0.361	0.046	0.369	0.078	0.476	0.192	**0.432**	0.021	0.571	<LoD	0.571	<LoD	0.571	<LoD	0.507	0.116	0.361	0.067	0.343	0.101
3	0.241	0.058	0.378	0.002	0.387	0.057	0.540	0.126	0.563	0.056	**0.530**	0.032	0.571	<LoD	0.571	<LoD	0.571	<LoD	0.536	0.085	0.334	0.100	0.341	0.156
4	0.268	0.063	0.372	0.035	0.397	0.112	0.498	0.163	0.780	0.201	**0.653**	0.045	**no sample***		0.571	<LoD	0.571	<LoD	0.451	0.111	0.414	0.086	0.419	0.188
5	0.219	0.059	**0.428**	0.116	0.427	0.045	0.577	0.083	0.803	0.172	**0.626**	0.013	0.571	<LoD	0.571	<LoD	**no sample***		0.520	0.059	0.373	0.164	0.346	0.135
6	0.217	0.062	**0.463**	0.073	0.508	0.110	0.555	0.074	0.877	0.228	**1.025**	0.077	**no sample***		0.571	<LoD	0.571	<LoD	0.473	0.128	0.375	0.093	0.358	<LoD
7	0.224	0.058	0.390	0.060	0.586	0.086	0.484	0.064	**1.338**	0.155	**1.423**	0.068	0.571	<LoD	0.571	<LoD	0.571	<LoD	0.454	0.111	0.362	0.048	0.373	0.102
8	0.240	0.081	**0.425**	0.107	0.445	0.073	0.660	0.126	**2.085**	0.327	**0.950**	0.109	0.559	0.150	0.529	0.085	0.571	<LoD	0.644	0.188	0.456	0.134	0.387	0.140
9	0.302	0.048	0.359	0.079	0.474	0.066	0.778	0.209	**1.925**	0.255	**1.083**	0.072	0.558	0.176	0.571	<LoD	0.571	<LoD	0.662	0.148	0.459	0.094	0.454	0.079
10	0.269	0.057	**0.541**	0.098	0.629	0.069	0.713	0.060	**2.003**	0.114	**0.770**	0.074	0.571	<LoD	0.576	0.087	0.571	<LoD	0.666	0.068	0.386	0.168	0.384	0.095
11	0.299	0.038	**0.529**	0.106	0.624	0.108	0.648	0.063	**1.303**	0.226	**1.301**	0.068	0.690	0.124	0.751	0.217	0.571	<LoD	0.624	0.109	0.546	0.135	0.395	0.164
12	0.334	0.077	**0.592**	0.112	0.696	0.079	0.790	0.078	**0.993**	0.139	**0.764**	0.070	**no sample***		0.639	0.150	0.587	0.140	0.543	0.097	0.442	0.109	0.454	0.096
13	0.353	0.103	**0.602**	0.111	0.560	0.154	**1.842**	0.149			**0.834**	0.077	0.854	0.167	**no sample***		0.691	0.044	**no sample***		0.450	0.190	0.394	0.053
14	0.402	0.067	**0.673**	0.179									0.957	0.258	0.613	0.185	0.571	<LoD	0.452	0.076	0.559	0.053	0.500	0.027
15	0.261	0.075											1.100	0.174	**no sample***		0.596	0.080	**no sample***		0.525	0.270	0.411	0.041
16													**no sample***		0.571	<LoD	0.641	0.131	0.518	0.188	0.494	0.080	0.502	0.122
17													**1.184**	0.185	**no sample***		**no sample***				0.583	0.101	0.589	0.110
18															0.571	<LoD	0.617	0.274			0.571	0.188	0.612	0.155
19																	0.640	0.217			0.567	0.082	0.526	0.143
20																					0.702	0.128	0.693	0.069
21																					0.635	0.141	0.710	0.068
22																					0.654	0.125		
23																					0.717	0.070		
LoD	0.152		0.152		0.345		0.345		0.345		0.083		0.529		0.529		0.529		0.330		0.330		0.330	
LoQ	0.411		0.411		0.910		0.910		0.910		0.193		1.141		1.141		1.141		0.717		0.717		0.717	
* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.																								

Table A3. 118: Silver concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									0.008	<LoD														
-14					0.008	<LoD	0.008	<LoD	0.008	<LoD	0.005	0.001												
-13			0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.005	0.001												
-12	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	<LoD												
-11	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	<LoD												
-10	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	0.001							0.026	<LoD				
-9	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.013	0.003	0.008	<LoD	0.004	<LoD							0.026	<LoD				
-8	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	0.001							0.026	<LoD				
-7	0.024	<LoD	0.024	<LoD	**0.033**	0.006	0.008	<LoD	0.008	<LoD	0.004	0.001							0.026	<LoD				
-6	0.024	<LoD	0.024	<LoD	**no sample***		0.008	<LoD	0.008	<LoD	0.004	<LoD					0.079	<LoD	0.026	<LoD			0.026	<LoD
-5	0.024	<LoD	0.024	<LoD	**0.134**	0.007	0.008	<LoD	0.008	<LoD	0.004	0.001	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD			**0.396**	0.027
-4	0.024	<LoD	0.024	<LoD	0.009	0.004	0.008	<LoD	0.008	<LoD	0.004	<LoD	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	**0.163**	0.006
-3	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.006	0.001	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
-2	0.024	<LoD	0.024	<LoD	**0.020**	0.006	0.008	<LoD	0.008	<LoD	0.004	<LoD	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
-1	0.024	<LoD	0.024	<LoD	0.012	0.005	0.008	<LoD	0.007	0.003	0.004	<LoD	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
0	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	<LoD	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
1	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	<LoD	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
2	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	<LoD	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
3	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	<LoD	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
4	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	<LoD	**no sample***		0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
5	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	<LoD	0.079	<LoD	0.079	<LoD	**no sample***		0.026	<LoD	0.026	<LoD	0.026	<LoD
6	0.024	<LoD	0.024	<LoD	0.014	0.004	0.008	<LoD	0.008	<LoD	0.004	<LoD	**no sample***		0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
7	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	<LoD	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
8	0.024	<LoD	0.024	<LoD	**0.017**	0.002	0.008	<LoD	0.008	<LoD	0.009	0.003	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
9	0.024	<LoD	0.024	<LoD	**0.042**	0.002	0.008	<LoD	0.008	<LoD	0.008	0.000	0.079	<LoD	0.079	<LoD	**0.217**	0.009	0.026	<LoD	0.026	<LoD	0.026	<LoD
10	0.024	<LoD	0.024	<LoD	**0.050**	0.002	0.008	<LoD	0.008	<LoD	**0.019**	0.004	0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
11	0.024	<LoD	0.024	<LoD	**0.039**	0.003	0.008	<LoD	0.008	<LoD	0.005	0.002	0.079	<LoD	0.079	<LoD	**0.273**	0.015	0.026	<LoD	0.026	<LoD	0.026	<LoD
12	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD	0.008	<LoD	0.004	0.001	**no sample***		0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
13	0.024	<LoD	0.024	<LoD	0.008	<LoD	0.008	<LoD			**0.009**	0.002	0.079	<LoD	**no sample***		0.079	<LoD	**no sample***		0.026	<LoD	0.026	<LoD
14	0.024	<LoD	0.024	<LoD									0.079	<LoD	0.079	<LoD	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
15	0.024	<LoD											0.079	<LoD	**no sample***		0.079	<LoD	**no sample***		0.026	<LoD	0.026	<LoD
16													**no sample***		0.075	0.005	0.079	<LoD	0.026	<LoD	0.026	<LoD	0.026	<LoD
17													0.079	<LoD	**no sample***		**no sample***				0.026	<LoD	0.026	<LoD
18															0.107	0.011	0.079	<LoD			0.026	<LoD	0.026	<LoD
19																	0.079	<LoD			0.026	<LoD	**0.054**	0.009
20																					0.026	<LoD	0.026	<LoD
21																					0.026	<LoD	0.031	0.006
22																					0.026	<LoD		
23																					0.026	<LoD		
LoD	0.018		0.018		0.006		0.006		0.006		0.003		0.067		0.067		0.067		0.028		0.028		0.028	
LoQ	0.049		0.049		0.015		0.015		0.015		0.009		0.158		0.158		0.158		0.052		0.052		0.052	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 119: Tin concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									0.178	<LoD														
-14					0.178	<LoD	0.178	<LoD	0.185	0.068	0.193	<LoD												
-13			0.136	<LoD	0.178	<LoD	0.178	<LoD	0.178	<LoD	0.193	<LoD												
-12	0.136	<LoD	0.136	<LoD	0.178	<LoD	0.178	<LoD	0.178	<LoD	0.193	<LoD												
-11	0.136	<LoD	0.116	0.039	0.178	<LoD	0.178	<LoD	0.178	<LoD	0.193	<LoD												
-10	0.136	<LoD	0.136	<LoD	0.178	<LoD	0.178	<LoD	0.178	<LoD	0.193	<LoD							0.046	<LoD				
-9	0.136	<LoD	0.147	0.067	0.178	<LoD	0.178	<LoD	0.178	<LoD	0.193	<LoD							0.046	<LoD				
-8	0.136	<LoD	0.136	<LoD	0.178	<LoD	0.178	<LoD	0.178	<LoD	0.193	<LoD							0.046	<LoD				
-7	0.136	<LoD	0.098	0.038	**0.613**	0.064	0.178	<LoD	0.178	<LoD	0.193	<LoD							0.046	<LoD				
-6	0.136	<LoD	0.136	<LoD	**no sample***		0.178	<LoD	0.178	<LoD	0.193	<LoD					0.105	<LoD	0.065	0.034			0.046	<LoD
-5	0.136	<LoD	0.136	<LoD	**1.468**	0.084	0.178	<LoD	0.178	<LoD	0.193	<LoD	0.105	<LoD	0.105	<LoD	0.105	<LoD	0.046	<LoD			0.046	<LoD
-4	0.136	<LoD	0.101	0.037	0.346	0.079	0.178	<LoD	0.178	<LoD	0.193	<LoD	0.105	<LoD	0.105	<LoD	0.136	0.039	0.046	<LoD	0.046	<LoD	0.046	<LoD
-3	0.136	<LoD	0.119	0.032	0.189	0.054	0.178	<LoD	0.178	<LoD	0.193	<LoD	0.105	<LoD	0.105	<LoD	0.105	<LoD	0.046	<LoD	0.046	<LoD	0.046	<LoD
-2	0.136	<LoD	0.136	<LoD	**0.389**	0.057	0.178	<LoD	0.178	<LoD	0.193	<LoD	0.105	<LoD	0.105	<LoD	0.105	<LoD	0.046	<LoD	0.046	<LoD	0.046	<LoD
-1	0.136	<LoD	0.105	0.071	**0.483**	0.051	0.178	<LoD	**0.401**	0.039	0.193	<LoD	0.105	<LoD	0.105	<LoD	0.105	<LoD	0.046	<LoD	0.046	<LoD	0.046	<LoD
0	0.136	<LoD	0.136	<LoD	0.178	<LoD	0.178	<LoD	0.178	<LoD	0.193	<LoD	0.105	<LoD	0.105	<LoD	0.105	<LoD	0.046	<LoD	0.046	<LoD	0.046	<LoD
1	0.136	<LoD	0.136	<LoD	0.178	<LoD	0.178	<LoD	0.145	0.069	0.193	<LoD	0.105	<LoD	0.105	<LoD	0.105	<LoD	0.042	0.028	**0.113**	0.016	0.046	0.032
2	0.136	<LoD	0.145	0.043	0.164	0.084	0.178	<LoD	0.136	0.109	0.193	<LoD	0.105	<LoD	0.105	<LoD	0.105	<LoD	**0.104**	0.040	**0.168**	0.066	0.063	0.038
3	0.160	0.046	0.211	0.051	0.190	0.061	0.146	0.059	0.178	<LoD	0.193	<LoD	0.105	<LoD	0.105	<LoD	0.105	<LoD	**0.094**	0.040	0.088	0.036	0.067	0.051
4	0.147	0.014	0.182	0.072	0.263	0.070	0.178	<LoD	0.275	0.094	0.193	<LoD	**no sample***		0.105	<LoD	0.156	0.031	**0.122**	0.040	**0.129**	0.057	0.082	0.041
5	0.253	0.034	**0.458**	0.043	**0.457**	0.039	0.178	<LoD	0.178	0.082	0.193	<LoD	0.109	0.043	0.095	0.022	**no sample***		**0.129**	0.031	0.089	0.024	0.077	0.047
6	**0.274**	0.013	**0.572**	0.012	**1.034**	0.119	0.178	<LoD	0.178	<LoD	0.193	<LoD	**no sample***		0.115	0.038	**0.225**	0.044	**0.219**	0.057	**0.213**	0.015	0.081	0.071
7	**0.340**	0.018	**0.538**	0.053	**0.845**	0.163	0.172	0.075	0.178	<LoD	0.193	<LoD	0.196	0.102	0.150	0.035	0.169	0.050	**0.251**	0.035	**0.173**	0.034	0.083	0.019
8	**0.294**	0.020	**0.285**	0.024	**1.172**	0.116	0.172	0.104	0.178	<LoD	0.193	<LoD	0.161	0.028	0.188	0.048	**0.271**	0.074	**0.271**	0.093	**0.241**	0.089	**0.131**	0.040
9	**0.362**	0.017	**0.478**	0.045	**1.629**	0.078	0.178	<LoD	0.178	<LoD	0.193	<LoD	0.206	0.062	**0.218**	0.071	**0.253**	0.080	**0.403**	0.040	**0.213**	0.026	0.091	0.042
10	**0.469**	0.050	**0.782**	0.074	**1.948**	0.136	0.146	0.033	0.187	0.135	**0.390**	0.064	0.193	0.059	0.172	0.069	**0.277**	0.054	**0.333**	0.056	**0.258**	0.072	**0.106**	0.015
11	**0.538**	0.063	**0.805**	0.033	**1.694**	0.112	0.150	0.112	0.252	0.054	0.193	<LoD	**0.258**	0.045	0.203	0.066	**0.234**	0.059	**0.396**	0.057	**0.296**	0.084	**0.097**	0.051
12	**0.626**	0.080	**0.848**	0.075	**0.970**	0.050	0.345	0.039	**0.563**	0.108	0.193	<LoD	**no sample***		**0.233**	0.105	**0.243**	0.034	**0.388**	0.026	**0.334**	0.078	**0.107**	0.051
13	**0.782**	0.128	**0.790**	0.189	**0.604**	0.051	**0.486**	0.059			0.272	0.049	**0.228**	0.063	**no sample***		**0.289**	0.069	**no sample***		**0.356**	0.055	0.041	0.035
14	**0.724**	0.102	**0.907**	0.099									**0.327**	0.096	**0.241**	0.078	**0.221**	0.078	**0.448**	0.145	**0.369**	0.038	**0.189**	0.055
15	**0.308**	0.078											**0.264**	0.062	**no sample***		**0.282**	0.083	**no sample***		**0.312**	0.081	**0.195**	0.059
16													**no sample***		**0.330**	0.063	**0.268**	0.079	**0.657**	0.148	**0.498**	0.065	**0.342**	0.079
17													**0.283**	0.021	**no sample***		**no sample***				**0.427**	0.091	**0.347**	0.059
18															**0.600**	0.097	**0.331**	0.076			**0.491**	0.044	**0.823**	0.156
19																	**0.324**	0.055			**0.471**	0.100	**1.086**	0.175
20																					**0.476**	0.111	**0.847**	0.139
21																					**0.609**	0.075	**0.975**	0.108
22																					**0.814**	0.039		
23																					**0.882**	0.126		
LoD	0.096		0.096		0.136		0.136		0.136		0.146		0.085		0.085		0.085		0.036		0.036		0.036	
LoQ	0.273		0.273		0.356		0.356		0.356		0.385		0.210		0.210		0.210		0.092		0.092		0.092	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 120: Titanium concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									0.098	<LoD														
-14					0.137	0.019	0.089	0.016	0.091	0.011	0.177	<LoD												
-13			**0.895**	0.043	**0.581**	0.032	**0.259**	0.028	0.077	0.025	0.177	<LoD												
-12	**1.325**	0.076	**0.894**	0.031	0.193	0.032	0.098	<LoD	0.098	<LoD	0.177	<LoD												
-11	**0.410**	0.039	**0.779**	0.056	**0.643**	0.044	0.098	<LoD	0.098	<LoD	0.177	<LoD												
-10	**0.891**	0.057	**0.861**	0.046	**0.862**	0.050	**0.307**	0.043	0.098	<LoD	0.129	0.020							0.172	<LoD				
-9	**0.615**	0.019	**2.054**	0.088	**0.297**	0.030	0.081	0.011	0.107	0.026	0.142	0.036							0.172	<LoD				
-8	**0.850**	0.052	**0.736**	0.051	**0.773**	0.054	**1.254**	0.058	0.077	0.024	0.177	<LoD							0.172	<LoD				
-7	**1.328**	0.076	**1.015**	0.070	**10.547**	0.576	0.098	<LoD	0.133	0.025	0.177	<LoD							0.172	<LoD				
-6	**1.476**	0.088	**1.085**	0.067	**no sample***		0.113	0.032	0.195	0.039	0.177	<LoD					0.077	<LoD	**0.548**	0.083			0.172	<LoD
-5	**0.831**	0.071	**1.194**	0.093	**30.484**	1.921	0.098	<LoD	**0.571**	0.098	0.177	<LoD	0.150	0.013	0.144	0.056	0.077	<LoD	0.172	<LoD			0.172	<LoD
-4	**0.795**	0.049	**1.050**	0.093	**4.735**	0.292	0.097	0.024	**0.431**	0.026	0.177	<LoD	**0.190**	0.043	0.111	0.031	**2.384**	0.221	0.172	<LoD	0.172	<LoD	0.172	<LoD
-3	**0.695**	0.069	**0.924**	0.048	**1.703**	0.131	0.096	0.021	0.188	0.014	0.177	<LoD	**0.221**	0.024	0.095	0.032	**0.235**	0.035	0.172	<LoD	0.172	<LoD	0.172	<LoD
-2	**0.583**	0.010	**1.638**	0.141	**5.720**	0.436	**1.471**	0.104	**0.271**	0.025	0.142	0.020	0.114	0.025	**0.244**	0.057	**0.518**	0.061	0.172	0.046	0.172	<LoD	0.172	<LoD
-1	**0.616**	0.057	**1.448**	0.060	**6.279**	0.357	**0.272**	0.023	**8.024**	0.462	0.276	0.041	**0.262**	0.035	**0.313**	0.065	0.075	0.020	0.172	<LoD	0.172	<LoD	0.172	<LoD
0	**0.973**	0.070	**0.958**	0.064	0.158	0.024	**1.723**	0.074	**1.391**	0.117	**2.340**	0.131	0.117	0.060	**0.168**	0.031	**0.311**	0.052	**0.428**	0.100	0.172	<LoD	0.172	<LoD
1	**1.417**	0.020	**1.324**	0.071	0.146	0.022	**1.269**	0.056	**2.893**	0.195	**4.827**	0.310	**0.221**	0.055	**0.343**	0.017	**0.169**	0.040	0.172	<LoD	**0.774**	0.067	0.172	<LoD
2	**1.218**	0.089	**1.432**	0.045	**0.487**	0.046	**3.358**	0.183	**3.947**	0.284	**5.927**	0.325	**0.591**	0.057	**1.106**	0.094	**0.506**	0.063	**0.377**	0.055	**0.609**	0.202	0.200	0.037
3	**1.542**	0.071	**1.877**	0.048	**0.625**	0.033	**4.583**	0.170	**3.479**	0.225	**7.964**	0.436	**1.144**	0.079	**1.559**	0.153	**2.034**	0.151	**0.643**	0.079	0.306	0.058	0.172	<LoD
4	**1.252**	0.058	**1.333**	0.056	**0.776**	0.045	**3.940**	0.134	**8.089**	0.387	**9.140**	0.445	**no sample***		**1.032**	0.137	**5.541**	0.323	**0.485**	0.053	**0.563**	0.059	0.178	0.041
5	**1.539**	0.043	**2.588**	0.060	**1.882**	0.129	**4.807**	0.136	**8.911**	0.274	**8.632**	0.563	**2.119**	0.201	**1.347**	0.188	**no sample***		**0.839**	0.382	**0.496**	0.054	0.191	0.060
6	**1.674**	0.067	**2.611**	0.119	**9.114**	0.337	**6.148**	0.251	**9.577**	0.573	**7.708**	0.474	**no sample***		**2.341**	0.200	**8.061**	0.499	**0.995**	0.089	**1.050**	0.094	**0.543**	0.091
7	**2.286**	0.113	**2.723**	0.118	**3.779**	0.124	**8.878**	0.349	**11.758**	0.570	**9.637**	0.439	**4.471**	0.365	**3.023**	0.253	**4.851**	0.386	**1.086**	0.105	**1.422**	0.109	**0.734**	0.089
8	**2.089**	0.056	**2.037**	0.044	**9.351**	0.484	**10.678**	0.228	**14.558**	0.734	**12.506**	1.010	**4.297**	0.364	**4.576**	0.326	**6.500**	0.418	**2.980**	0.118	**1.109**	0.047	0.332	0.042
9	**2.357**	0.088	**2.589**	0.117	**17.190**	0.830	**12.365**	0.249	**13.139**	0.568	**17.315**	1.011	**4.618**	0.403	**4.433**	0.376	**6.484**	0.542	**3.762**	0.183	**1.134**	0.086	**0.346**	0.052
10	**2.712**	0.150	**4.302**	0.146	**17.645**	0.491	**8.950**	0.154	**14.169**	0.635	**41.385**	4.475	**7.446**	0.865	**4.257**	0.224	**7.041**	0.622	**3.167**	0.111	**1.677**	0.149	**0.919**	0.139
11	**3.367**	0.098	**3.974**	0.210	**15.256**	0.566	**7.479**	0.347	**14.442**	0.603	**13.011**	1.013	**16.101**	7.078	**4.763**	0.675	**6.392**	0.356	**2.359**	0.188	**1.635**	0.200	**0.597**	0.103
12	**4.224**	0.180	**4.354**	0.134	**6.305**	0.165	**10.788**	0.428	**13.910**	0.550	**11.964**	0.620	**no sample***		**4.869**	0.437	**7.473**	0.595	**1.921**	0.071	**1.995**	0.086	**0.778**	0.079
13	**4.999**	0.285	**3.563**	0.104	**3.789**	0.316	**24.599**	1.103			**17.773**	0.682	**7.697**	0.667	**no sample***		**7.282**	0.624	**no sample***		**2.461**	0.117	0.172	<LoD
14	**4.734**	0.120	**3.912**	0.322									**24.729**	2.147	**5.589**	0.553	**6.781**	0.416	**3.563**	0.335	**2.301**	0.153	**0.837**	0.045
15	**1.143**	0.059											**8.814**	1.202	**no sample***		**7.112**	0.721	**no sample***		**2.702**	0.244	**3.206**	0.310
16													**no sample***		**7.289**	0.547	**7.007**	0.665	**4.923**	0.308	**2.671**	0.104	**2.021**	0.244
17													**7.837**	0.212	**no sample***		**no sample***				**3.241**	0.248	**2.624**	0.265
18															**22.937**	2.013	**6.917**	0.443			**3.219**	0.370	**14.003**	1.275
19																	**10.788**	0.894			**3.387**	0.084	**29.032**	1.491
20																					**3.680**	0.149	**11.629**	0.518
21																					**4.359**	0.312	**15.061**	1.168
22																					**5.210**	0.293		
23																					**5.974**	0.213		
LoD	0.151		0.151		0.076		0.076		0.076		0.123		0.075		0.075		0.075		0.153		0.153		0.153	
LoQ	0.408		0.408		0.197		0.197		0.197		0.355		0.153		0.153		0.153		0.345		0.345		0.345	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 121: Vanadium concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**0.463**	0.023														
-14					**0.693**	0.066	**0.597**	0.048	**0.582**	0.020	**0.477**	0.029												
-13			**0.610**	0.017	**1.587**	0.106	**0.609**	0.043	**0.490**	0.026	**0.643**	0.032												
-12	**0.769**	0.033	**0.869**	0.024	**0.937**	0.088	**0.562**	0.046	**0.613**	0.034	**0.499**	0.043												
-11	**0.648**	0.025	**0.716**	0.024	**1.034**	0.094	**0.608**	0.035	**0.607**	0.044	**0.640**	0.053												
-10	**0.675**	0.014	**0.761**	0.025	**1.366**	0.097	**0.519**	0.029	**0.641**	0.021	**0.554**	0.045							**0.601**	0.036				
-9	**0.651**	0.033	**0.754**	0.034	**1.065**	0.098	**0.515**	0.027	**0.558**	0.041	**0.693**	0.044							**0.634**	0.053				
-8	**0.656**	0.037	**0.722**	0.022	**1.105**	0.092	**0.552**	0.044	**0.613**	0.030	**0.542**	0.039							**0.614**	0.043				
-7	**0.707**	0.037	**0.716**	0.028	**2.424**	0.196	**0.612**	0.042	**0.547**	0.032	**0.575**	0.048							**0.607**	0.050				
-6	**0.705**	0.042	**0.781**	0.040	**no sample***		**0.528**	0.031	**0.693**	0.045	**0.482**	0.046					**0.662**	0.067	**0.641**	0.041			**0.610**	0.038
-5	**0.711**	0.068	**0.670**	0.022	**4.697**	0.309	**0.567**	0.034	**0.685**	0.029	**0.527**	0.047	**0.685**	0.058	**0.700**	0.071	**0.674**	0.054	**0.631**	0.051			**0.604**	0.056
-4	**0.521**	0.036	**0.847**	0.035	**1.579**	0.137	**0.475**	0.033	**0.734**	0.050	**0.448**	0.042	**0.704**	0.058	**0.710**	0.067	**0.832**	0.086	**0.602**	0.041	**0.618**	0.037	**0.614**	0.039
-3	**0.587**	0.039	**0.709**	0.030	**1.295**	0.119	**0.559**	0.038	**0.936**	0.031	**0.480**	0.047	**0.708**	0.061	**0.703**	0.084	**0.694**	0.056	**0.587**	0.044	**0.667**	0.050	**0.631**	0.056
-2	**0.550**	0.019	**0.628**	0.047	**1.758**	0.125	**0.633**	0.031	**0.892**	0.074	**0.383**	0.038	**0.693**	0.058	**0.736**	0.069	**0.712**	0.050	**0.627**	0.062	**0.679**	0.059	**0.640**	0.048
-1	**0.639**	0.022	**0.948**	0.040	**2.245**	0.188	**0.468**	0.030	**1.230**	0.081	**0.482**	0.026	**0.718**	0.082	**0.752**	0.070	**0.717**	0.072	**0.604**	0.041	**0.704**	0.056	**0.669**	0.051
0	**0.563**	0.038	**1.004**	0.044	**1.189**	0.072	**1.099**	0.061	**0.678**	0.046	**2.161**	0.133	**0.722**	0.069	**0.784**	0.049	**0.806**	0.055	**0.694**	0.045	**0.708**	0.039	**0.755**	0.061
1	**3.380**	0.094	**1.235**	0.050	**3.315**	0.245	**2.196**	0.054	**1.640**	0.073	**4.031**	0.213	**0.691**	0.062	**1.219**	0.124	**0.964**	0.083	**0.524**	0.028	**0.856**	0.045	**0.537**	0.027
2	**0.542**	0.025	**2.972**	0.085	**1.666**	0.103	**2.975**	0.158	**3.539**	0.157	**4.104**	0.199	**0.814**	0.064	**0.724**	0.052	**0.673**	0.063	**1.142**	0.083	**0.856**	0.046	**0.696**	0.041
3	**0.851**	0.016	**1.244**	0.035	**2.330**	0.138	**4.737**	0.142	**3.253**	0.115	**5.810**	0.343	**1.235**	0.103	**0.501**	0.053	**0.954**	0.074	**1.033**	0.045	**0.947**	0.029	**0.603**	0.055
4	**0.986**	0.022	**1.276**	0.037	**2.876**	0.163	**4.801**	0.104	**7.570**	0.161	**6.480**	0.298	**no sample***		**0.823**	0.068	**1.935**	0.105	**1.062**	0.078	**1.448**	0.100	**0.629**	0.017
5	**1.490**	0.052	**3.337**	0.102	**5.096**	0.270	**5.995**	0.153	**7.858**	0.144	**6.837**	0.412	**1.760**	0.136	**1.302**	0.078	**no sample***		**1.486**	0.097	**1.340**	0.092	**0.557**	0.020
6	**1.737**	0.042	**2.173**	0.046	**7.002**	0.422	**6.526**	0.208	**7.291**	0.260	**5.311**	0.336	**no sample***		**1.804**	0.154	**2.809**	0.139	**1.658**	0.094	**1.609**	0.089	**0.584**	0.038
7	**1.819**	0.066	**2.514**	0.065	**6.495**	0.305	**7.804**	0.326	**8.568**	0.332	**7.008**	0.368	**2.954**	0.235	**2.144**	0.111	**2.897**	0.226	**1.984**	0.122	**1.737**	0.103	**0.597**	0.038
8	**1.732**	0.044	**1.978**	0.081	**6.445**	0.401	**9.741**	0.207	**9.752**	0.387	**5.485**	0.474	**2.840**	0.256	**2.306**	0.150	**3.667**	0.226	**2.475**	0.132	**1.743**	0.144	**0.614**	0.042
9	**1.660**	0.060	**2.249**	0.075	**7.524**	0.241	**10.744**	0.355	**10.284**	0.412	**6.516**	0.540	**2.749**	0.206	**2.621**	0.214	**3.963**	0.310	**2.532**	0.112	**1.841**	0.124	**0.625**	0.043
10	**2.156**	0.089	**3.387**	0.067	**9.931**	0.441	**8.431**	0.078	**11.440**	0.584	**9.406**	0.626	**3.280**	0.259	**2.814**	0.246	**4.064**	0.308	**2.430**	0.155	**1.932**	0.132	**0.685**	0.024
11	**2.184**	0.081	**3.347**	0.160	**8.942**	0.386	**7.459**	0.191	**12.574**	0.523	**6.708**	0.582	**3.757**	0.213	**2.996**	0.278	**4.077**	0.306	**2.522**	0.123	**1.982**	0.136	**0.623**	0.039
12	**2.432**	0.155	**3.508**	0.098	**7.370**	0.211	**9.487**	0.178	**13.235**	0.395	**7.702**	0.489	**no sample***		**3.116**	0.289	**3.766**	0.307	**1.903**	0.049	**1.959**	0.097	**0.667**	0.039
13	**2.457**	0.078	**3.073**	0.094	**5.403**	0.237	**15.178**	0.430			**10.646**	0.476	**3.499**	0.351	**no sample***		**3.941**	0.201	**no sample***		**1.970**	0.098	**0.384**	0.021
14	**2.846**	0.101	**3.401**	0.103									**4.648**	0.438	**3.194**	0.252	**3.761**	0.309	**2.531**	0.091	**2.010**	0.116	**0.904**	0.063
15	**1.745**	0.028											**3.671**	0.350	**no sample***		**3.828**	0.204	**no sample***		**2.181**	0.127	**0.841**	0.053
16													**no sample***		**3.144**	0.257	**3.704**	0.292	**2.670**	0.141	**2.289**	0.145	**1.449**	0.052
17													**3.846**	0.254	**no sample***		**no sample***				**2.308**	0.165	**1.637**	0.039
18															**3.901**	0.262	**3.377**	0.240			**2.303**	0.061	**2.647**	0.094
19																	**3.909**	0.225			**2.508**	0.087	**4.188**	0.155
20																					**2.672**	0.125	**3.271**	0.211
21																					**2.868**	0.093	**3.827**	0.294
22																					**4.078**	0.260		
23																					**3.463**	0.260		
LoD	0.012		0.012		0.124		0.124		0.124		0.044		0.143		0.143		0.143		0.067		0.067		0.067	
LoQ	0.023		0.023		0.363		0.363		0.363		0.092		0.365		0.365		0.365		0.125		0.125		0.125	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 122: Zink concentrations across the SWI in dialyses-based *in-situ* pore water samples and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L. Statistically identified outliers (Grubbs test) marked in grey.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4					
Depth	Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3		Peeper 1		Peeper 2		Peeper 3	
cm	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
-15									**7.7**	0.3														
-14					**10.1**	0.3	**15.4**	0.4	**10.2**	0.5	**8.2**	0.3												
-13			**9.2**	0.6	**16.9**	1.0	**10.5**	0.5	**8.4**	0.5	**8.7**	0.1												
-12	**16.4**	0.9	**15.2**	0.8	**11.3**	0.7	**13.2**	0.2	**9.9**	0.6	**8.5**	0.1												
-11	**7.6**	0.2	**8.5**	0.6	**16.4**	0.5	**15.1**	0.6	**9.7**	0.5	**8.4**	0.2												
-10	**7.2**	0.4	**7.5**	0.3	**15.8**	0.6	**11.2**	0.5	**9.8**	0.7	**8.8**	0.3							**13.4**	0.2				
-9	**6.1**	0.4	**9.9**	0.4	**13.3**	0.6	**10.9**	0.3	**9.1**	0.2	**10.0**	0.3							**15.0**	0.6				
-8	**12.8**	0.3	**7.0**	0.6	**12.2**	0.4	**9.7**	0.4	**10.0**	0.8	**8.1**	0.3							**14.1**	0.7				
-7	**9.5**	0.3	**13.2**	0.5	**43.9**	1.6	**14.8**	0.5	**10.7**	0.3	**9.6**	0.3							**12.1**	0.4				
-6	**9.9**	0.4	**7.5**	0.5	**no sample***		**10.7**	0.4	**10.9**	0.5	**9.5**	0.2					**6.4**	0.2	**14.8**	0.4			**12.5**	0.3
-5	**8.1**	0.2	**25.3**	0.5	**98.5**	2.4	**13.1**	0.3	**10.7**	0.6	**8.4**	0.3	**6.8**	0.4	**5.8**	0.2	**5.7**	0.3	**11.7**	0.2			**13.6**	0.1
-4	**6.4**	0.3	**17.1**	0.6	**24.3**	0.9	**10.0**	0.5	**1.6**	0.1	**7.8**	0.3	**7.0**	0.6	**6.7**	0.5	**11.6**	1.0	**11.8**	0.4	**12.5**	0.4	**13.4**	0.3
-3	**5.4**	0.4	**10.5**	0.2	**15.0**	0.5	**11.6**	0.4	**0.9**	0.1	**8.7**	0.5	**8.2**	0.4	**8.4**	0.4	**5.9**	0.4	**12.7**	0.4	**12.2**	0.1	**13.0**	0.4
-2	**5.6**	0.2	**19.7**	0.2	**33.0**	0.7	**16.1**	0.8	**1.6**	0.2	**7.1**	0.2	**7.2**	0.5	**6.1**	0.2	**6.5**	0.3	**13.0**	0.4	**15.0**	0.4	**12.9**	0.3
-1	**5.6**	0.3	**20.4**	0.6	**29.1**	0.8	**13.3**	0.3	**30.7**	1.1	**6.9**	0.3	**7.6**	0.3	**6.0**	0.5	**5.7**	0.3	**12.0**	0.3	**12.9**	0.3	**12.3**	0.5
0	**8.2**	0.3	**8.6**	0.2	**13.8**	0.7	**9.3**	0.3	**15.5**	0.7	**2.8**	0.1	**10.2**	0.7	**6.5**	0.4	**6.9**	0.4	**26.5**	0.9	**12.9**	0.3	**18.8**	0.5
1	**53.8**	2.0	**12.2**	0.6	**45.8**	0.7	**5.5**	0.2	**5.3**	0.3	**4.2**	0.1	**8.3**	0.6	**14.6**	1.0	**21.5**	1.5	**5.5**	0.2	**13.2**	0.2	**4.8**	0.3
2	**5.6**	0.3	**31.7**	0.7	**5.0**	0.2	**7.2**	0.7	**10.7**	0.5	**2.5**	0.2	**3.1**	0.5	**4.4**	0.4	**2.5**	0.2	**1.1**	0.1	**4.3**	0.1	**2.2**	0.2
3	**3.9**	0.2	**2.6**	0.2	**5.7**	0.4	**2.0**	0.1	**4.4**	0.3	**1.7**	0.2	**2.2**	0.2	**10.0**	0.3	**4.6**	0.4	**3.1**	0.1	**2.5**	0.2	**3.5**	0.3
4	**2.0**	0.2	**1.5**	0.1	**5.0**	0.2	**3.3**	0.2	**1.5**	0.1	**3.9**	0.3	**no sample***		**1.9**	0.3	**5.7**	0.4	**2.5**	0.2	**1.0**	0.1	**2.6**	0.2
5	**2.0**	0.1	**12.4**	0.4	**3.9**	0.2	**3.2**	0.2	**2.4**	0.2	**1.7**	0.1	**7.2**	0.6	**1.1**	0.1	**no sample***		**1.8**	0.1	**1.8**	0.1	**1.5**	0.1
6	**1.2**	0.1	**0.8**	0.1	**22.7**	0.9	**1.1**	0.1	**0.9**	0.1	**2.1**	0.2	**no sample***		**2.7**	0.1	**10.1**	0.4	**3.0**	0.2	**2.3**	0.2	**3.6**	0.3
7	**2.5**	0.2	**1.8**	0.1	**6.9**	0.1	**1.8**	0.2	**2.1**	0.2	**2.4**	0.2	**1.8**	0.2	**1.7**	0.2	**4.4**	0.3	**2.6**	0.2	**1.8**	0.2	**10.4**	0.6
8	**1.8**	0.2	**18.3**	1.0	**25.8**	2.0	**7.8**	0.5	**10.6**	0.7	**13.2**	0.6	**2.1**	0.3	**3.5**	0.5	**3.9**	0.2	**5.6**	0.3	**1.5**	0.2	**4.9**	0.4
9	**1.0**	0.1	**2.8**	0.2	**54.2**	1.8	**1.5**	0.1	**1.0**	0.1	**28.3**	0.5	**2.9**	0.3	**2.2**	0.1	**3.6**	0.2	**13.7**	0.6	**1.4**	0.3	**2.9**	0.2
10	**1.3**	0.0	**0.7**	0.0	**51.8**	2.3	**2.8**	0.2	**0.8**	0.1	**75.7**	1.1	**5.3**	0.5	**1.9**	0.1	**2.0**	0.1	**6.1**	0.2	**2.3**	0.2	**7.5**	0.7
11	**3.4**	0.2	**1.6**	0.1	**49.8**	3.4	**3.9**	0.2	**1.2**	0.1	**7.6**	0.4	**13.3**	0.4	**3.8**	0.4	**4.0**	0.3	**2.9**	0.2	**2.1**	0.2	**3.5**	0.3
12	**5.5**	0.1	**0.6**	0.1	**10.7**	0.4	**5.9**	0.4	**3.1**	0.2	**8.0**	0.2	**no sample***		**7.3**	0.1	**2.1**	0.2	**2.0**	0.1	**4.1**	0.3	**3.1**	0.1
13	**7.0**	0.6	**1.7**	0.1	**5.1**	0.3	**16.5**	0.6			**10.3**	0.3	**20.0**	0.3	**no sample***		**1.7**	0.1	**no sample***		**4.6**	0.2	**3.8**	0.4
14	**7.6**	0.3	**7.6**	0.4									**27.5**	0.9	**6.9**	0.4	**2.0**	0.2	**5.5**	0.3	**2.5**	0.2	**2.9**	0.2
15	**2.8**	0.2											**5.4**	0.3	**no sample***		**1.3**	0.2	**no sample***		**0.8**	0.1	**9.4**	0.2
16													**no sample***		**19.7**	0.7	**1.5**	0.1	**9.1**	0.4	**1.1**	0.1	**3.2**	0.1
17													**5.1**	0.4	**no sample***		**no sample***				**7.5**	0.2	**5.5**	0.1
18															**56.9**	3.0	**4.4**	0.2			**1.2**	0.1	**29.9**	0.4
19																	**8.4**	0.7			**1.7**	0.1	**68.7**	2.0
20																					**1.0**	0.1	**20.8**	0.8
21																					**1.4**	0.1	**32.3**	0.6
22																					**0.9**	0.2		
23																					**3.2**	0.4		
LoD	0.12		0.12		0.12		0.12		0.12		0.03		0.13		0.13		0.13		0.10		0.10		0.10	
LoQ	0.32		0.32		0.31		0.31		0.31		0.08		0.31		0.31		0.31		0.26		0.26		0.26	

* individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.

Table A3. 123: Phosphate concentrations across the SWI in dialyses-based *in-situ* pore water samples. All values in mg/L.

Depth	Sampling Site 1			Sampling Site 2			Sampling Site 3			Sampling Site 4		
(cm)	Peeper 1	Peeper 2	Peeper 3	Peeper 1	Peeper 2	Peeper 3	Peeper 1	Peeper 2	Peeper 3	Peeper 1	Peeper 2	Peeper 3
-15					5.40							
-14			0.69	0.35	5.05	0.04						
-13		0.59	0.74	0.40	5.15	0.46						
-12	0.62	0.69	0.89	0.30	5.05	0.56						
-11	0.52	0.84	0.44	0.20	5.15	0.04						
-10	0.97	0.49	0.44	0.60	4.90	0.56				0.70		
-9	1.12	0.59	0.79	0.40	5.35	0.36				0.65		
-8	0.72	0.69	0.69	0.20	0.00	0.26				0.60		
-7	0.97	0.54	0.06	0.24	0.40	0.61				0.60		
-6		0.16	missing*	0.54	0.20	0.45			0.70	0.80		0.55
-5	0.94	0.01	0.41	0.24	0.10	0.30	0.85	0.80	0.70	0.55		0.60
-4	0.59	0.06	0.16	0.04	0.35	0.80	0.70	0.95	0.60	0.65	0.60	0.80
-3	0.74	0.14	0.21	0.14	0.60	0.30	0.70	0.90	0.80	0.60	0.55	0.60
-2	2.01	0.14	0.26	1.44	0.40	0.25	0.80	0.85	0.70	0.60	0.45	0.70
-1	0.39	0.01	0.06	0.01	0.20	0.70	0.75	0.95	0.70	0.95	0.45	0.85
0	0.39	0.01	0.16	0.06	0.35	1.20	0.85	1.00	0.50	0.35	0.55	0.75
1	0.09	0.26	0.31	0.01	0.55	3.45	0.75	1.20	0.05	0.50	0.50	0.85
2	0.21	0.11	0.56	0.36	0.45	7.75	0.95	1.95	0.45	1.20	0.55	1.00
3	0.66	0.56	0.86	4.02	4.00	13.65	2.55	2.30	0.35	0.55	0.50	0.65
4	0.26	0.91	2.21	10.62	3.05	17.20	missing*	3.35	0.55	5.75	0.45	1.00
5	1.36	0.91	4.51	14.47	12.35	17.65	2.40	7.90	missing*	12.40	0.55	0.45
6	2.91	1.71	4.31	22.32	3.36	18.45	missing*	3.80	0.50	16.35	0.10	4.20
7	4.96	1.86	9.66	24.42	9.86	16.55	1.60	4.95	0.40	6.10	0.10	7.90
8	2.86	1.21	2.46	22.32	11.21	20.70	4.40	7.65	0.55	12.15	1.35	7.60
9	7.31	3.71	7.01	1.37	19.71	20.00	2.75	6.35	0.60	17.05	4.00	5.55
10	8.66	4.51	6.31	30.32	11.06	18.60	6.25	4.10	4.15	19.70	7.40	7.95
11	4.86	3.21	5.21	24.97	13.36	28.30	5.30	4.85	13.05	missing*	8.00	7.60
12	2.66	6.46	3.71	24.22	7.26	26.35	missing*	4.95	11.70	22.50	7.15	14.90
13	4.66	9.91	4.81	34.92		38.10	5.55	missing*	12.50	missing*	22.85	13.65
14	11.91	0.09					7.75	7.45	9.60	15.70	18.10	26.00
15	5.61						5.90	missing*	13.30		22.80	19.45
16							missing*	15.00	12.05		16.80	15.00
17							3.80	missing*	14.15		18.10	11.30
18								13.95	missing*		17.45	7.15
19									18.00		18.10	18.10
20									16.90		8.95	15.30
21											27.95	
22											36.75	
23												
*** individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.**												
**** individual samples are missing due to handling error**												

Table A3. 124: Sulfate concentrations across the SWI in dialyses-based *in-situ* pore water samples. All values in mg/L.

Depth	Sampling Site 1			Sampling Site 2			Sampling Site 3			Sampling Site 4		
(cm)	Peeper 1	Peeper 2	Peeper 3	Peeper 1	Peeper 2	Peeper 3	Peeper 1	Peeper 2	Peeper 3	Peeper 1	Peeper 2	Peeper 3
-15					888							
-14			260	476	404	1055						
-13		281	478	293	480	1051						
-12	275	251	602	1054	314	1052						
-11	268	241	298	1035	296	1052						
-10	95	245	538	972	1343	1044				735		
-9	334	239	666	1011	463	1053				451		
-8	204	284	701	863	744	1048				570		
-7	371	733	566	821	657	1056				673		
-6	306	297	missing*	1086	617	1009			666	537		810
-5	567	558	701	810	434	969	373	912	556	661		746
-4	465	244	746	1010	435	1043	744	914	350	708	416	614
-3	320	275	692	1800	1022	1041	284	915	703	568	416	720
-2	442	321	666	1080	405	1034	556	543	518	577	324	696
-1	510	468	550	1006	475	1030	312	686	621	666	493	799
0	253	321	317	683	317	1013	584	486	436	541	599	484
1	295	362	706	308	269	955	512	600	566	510	535	1013
2	361	377	423	731	149	839	484	449	700	772	528	667
3	653	288	495	897	736	819	479	780	764	545	405	801
4	393	338	734	754	255	750	missing*	673	534	569	524	560
5	477	320	531	725	527	686	378	731	missing*	249	182	702
6	586	561	436	737	227	622	missing*	809	405	160	442	664
7	759	432	688	681	393	566	314	648	477	562	447	711
8	467	254	231	645	347	545	615	629	268	211	703	752
9	713	595	476	148	435	504	868	551	200	448	607	635
10	649	589	452	563	241	483	350	344	121	264	305	436
11	439	453	366	427	244	463	359	208	132	244	300	538
12	199	516	201	359	148	439	134	387	134	300	236	454
13	345	508	310	375		414	223	missing*	111	missing*	279	648
14	544	125					missing*	201	missing*	159	285	636
15	449						177	missing*	45	missing*	230	530
16							missing*	129	29	40	349	362
17							69	missing*			138	398
18								51			174	320
19											86	170
20											44	94
21											16	32
22												
23												
*** individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.**												
**** individual samples are missing due to handling error**												

Table A3. 125: Ammonium concentrations across the SWI in dialyses-based *in-situ* pore water samples. All values in mg/L.

Depth	Sampling Site 1			Sampling Site 2			Sampling Site 3			Sampling Site 4		
(cm)	Peeper 1	Peeper 2	Peeper 3	Peeper 1	Peeper 2	Peeper 3	Peeper 1	Peeper 2	Peeper 3	Peeper 1	Peeper 2	Peeper 3
-15					0.64							
-14			0.74	1.20	0.84	-0.59						
-13		0.33	1.64	0.62	0.57	-0.56						
-12	0.86	0.97	1.53	-0.05	1.08	-0.59						
-11	0.85	0.08	1.77	-0.12	1.13	-0.59						
-10	0.85	0.97	0.88	-0.04	0.35	-0.55				1.48		
-9	1.30	0.57	1.03	-0.17	0.15	-0.55				1.82		
-8	0.34	0.72	0.83	-0.17	1.45	-0.57				2.50		
-7	0.74	0.32	0.89	0.26	0.36	-0.48				1.06		
-6	0.54	0.78	missing*	0.32	0.11	-0.55			1.62	1.90		2.18
-5	1.03	0.96	0.74	0.85	0.15	-0.45	1.96	1.97	0.60	2.30		1.29
-4	0.55	0.57	0.92	0.42	-0.02	-0.44	4.25	2.10	0.86	1.38	2.52	1.10
-3	0.30	0.46	0.87	0.93	0.55	-0.46	3.06	2.25	1.19	2.12	1.95	1.38
-2	0.34	0.71	1.19	0.02	0.58	-0.41	2.59	2.15	0.57	1.25	1.46	1.19
-1	0.17	0.91	1.66	0.38	1.00	-0.13	3.93	3.38	0.96	0.56	3.02	1.34
0	0.74	0.60	0.15	0.89	0.81	1.46	3.07	1.18	0.92	1.76	2.31	0.89
1	0.77	0.65	0.89	2.52	1.21	2.90	2.85	3.20	1.15	2.90	2.68	2.17
2	1.19	0.86	2.66	3.93	1.76	4.37	2.13	1.41	1.94	4.05	2.48	2.28
3	1.00	1.58	2.90	5.50	2.21	5.70	2.97	2.62	1.65	3.23	3.71	2.52
4	1.40	1.50	3.41	6.46	2.35	7.21	missing*		2.04	4.18	3.94	2.58
5	1.94	1.27	4.55	7.95	2.85	8.82	2.13	2.87	missing*	4.57	4.75	2.91
6	2.40	1.77	5.24	8.83	2.84	10.38	missing*	4.22	1.33	4.57	4.56	2.46
7	2.54	2.02	5.57	10.34	3.52	11.49	3.48	5.59	5.50	6.08	4.83	3.12
8	3.03	2.48	6.91	11.97	3.58	12.63	2.98	7.15	8.50	5.18	5.58	3.33
9	3.19	2.60	6.44	13.78	4.46	13.65	4.79	8.85	10.48	6.43	5.01	4.24
10	3.88	3.31	7.07	15.54	3.63	13.53	4.08	10.80	12.94	6.60	6.37	3.99
11	3.94	3.56	7.10	17.78	5.17	15.69	9.41	10.92	13.72	7.26	5.55	3.12
12	4.82	4.65	8.50	17.29	6.90	16.67	missing*	13.42	14.52	7.58	6.31	2.50
13	3.99	6.52	10.76	19.21		18.35	12.23	missing*	15.16	6.63	7.20	2.26
14	5.53	6.98					11.83	16.57	16.13	missing*	7.05	4.27
15	7.26						13.13	missing*	17.13	18.65	7.57	5.11
16							4.89	24.47	17.91	missing*	8.64	7.97
17							16.06	missing*	missing*	25.28	10.79	10.15
18							16.29	19.91	20.12		10.50	12.32
19							21.35				11.64	15.18
20							14.91				11.66	17.36
21							missing*				12.93	20.82
22							20.56				11.88	
23							15.56				13.84	
*** individual samples are missing due to damage to the membrane during deployment or recovery of the peeper.**												
**** individual samples are missing due to handling error**												

A4 Measured concentrations in mesocosm samples

Table A3. 126: Carbon concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**119**	4	24	1	**42**	2	**143**	7	**30**	2	**16**	1	**25**	1	**21**	1	**57**	2	**59**	2	**<LoD**	
2	**143**	3	36	2	**41**	3	**230**	13	**23**	2	**17**	2	**23**	1	**20**	1	**102**	2	**39**	1	**41**	2
3	**42**	2	15	1	**16**	1	**48**	3	**26**	2	**18**	1	**54**	2	**38**	1	**114**	6	**31**	1	**56**	2
4	**38**	1	14	1	**12**	1	**38**	2	**27**	2	**12**	1	**60**	1	**20**	1	**36**	1	**15**	1	22	2
5	**32**	1	14	1	**14**	1	**42**	2	**28**	3	**13**	1	**78**	2	**21**	1	**130**	3	**13**	1	30	1
6	**35**	2	15	1	**13**	1	**39**	1	**29**	2	**14**	1	**47**	1	**20**	1	**84**	4	**15**	1	37	3
7	**32**	2	16	2	**15**	1	**37**	1	**24**	2	**15**	1	**<LoD**		**20**	1	**60**	2	**20**	1	24	1
8	**17**	1	17	1	**11**	1	**24**	2	**23**	1	**15**	1	**<LoD**		**50**	2	**31**	1	**27**	2	20	2
LoD	4		15		1		4		8		2		1		7		5		5		15	
LoQ	11		40		3		11		18		5		3		13		9		9		40	

Table A3. 127: Phosphorous concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**895**	46	**96**	4	**1011**	49	**590**	18	**62**	4	**361**	22	**7250**	293	**11**	0	**150**	8	**17**	1	**179**	4
2	**918**	38	**98**	4	**1120**	77	**503**	26	**52**	4	**333**	34	**98**	8	**8**	0	**152**	7	**20**	2	**200**	11
3	**181**	14	**14**	1	**124**	11	**295**	20	**17**	1	**131**	3	**107**	8	**9**	0	**29**	2	**64**	2	**48**	2
4	**179**	10	**13**	2	**139**	12	**280**	17	**15**	1	**91**	10	**99**	5	**7**	0	**46**	3	**43**	3	**50**	5
5	**122**	11	**10**	1	**206**	18	**242**	10	**15**	1	**73**	8	**<LoD**		**9**	0	**8**	0	**32**	3	**13**	1
6	**121**	8	**10**	1	**236**	19	**273**	12	**14**	1	**84**	9	**<LoD**		**7**	0	**8**	1	**33**	3	**8**	0
7	**217**	14	**8**	1	**224**	17	**241**	16	**11**	1	**98**	3	**<LoD**		**7**	0	**9**	1	**20**	2	**8**	1
8	**204**	9	**12**	1	**226**	16	**310**	12	**9**	1	**85**	4	**120**	5	**7**	0	**6**	1	**19**	2	**9**	1
LoD	1		1		1		1		0		9		1		2		1		1		1	
LoQ	3		4		1		3		0		24		1		6		1		1		4	

Table A3. 128: Sulfur concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**209**	7	**310**	8	**629**	20	**218**	10	**256**	12	**302**	10	**517**	15	**644**	13	**509**	31	**334**	23	**120**	5
2	**218**	7	**336**	15	**646**	41	**247**	11	**250**	12	**291**	23	**561**	18	**682**	14	**481**	22	**348**	15	**115**	5
3	**510**	16	**687**	31	**666**	30	**614**	53	**532**	20	**576**	18	**843**	26	**1225**	27	**590**	35	**570**	24	**186**	13
4	**535**	48	**640**	19	**645**	28	**619**	32	**546**	32	**488**	19	**852**	56	**883**	29	**528**	26	**372**	23	**200**	16
5	**537**	21	**693**	37	**666**	22	**607**	23	**1293**	90	**525**	40	**1053**	26	**1158**	81	**680**	21	**379**	28	**280**	23
6	**557**	30	**762**	29	**672**	23	**617**	35	**1135**	51	**550**	40	**695**	28	**1047**	33	**588**	29	**415**	25	**317**	24
7	**586**	14	**799**	48	**744**	17	**643**	45	**1136**	57	**737**	24	**<LoD**		**1212**	47	**699**	36	**474**	29	**356**	27
8	**575**	20	**823**	38	**751**	25	**650**	62	**928**	27	**705**	15	**940**	44	**1094**	47	**606**	29	**451**	33	**389**	42
LoD	1		1		0		1		3		2		0		9		2		2		1	
LoQ	2		4		1		2		9		5		1		24		6		6		4	

Table A3. 129: Manganese concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**1175**	24	**2478**	28	**6165**	275	**116**	4	**120**	2	**198**	10	**2621**	134	**3131**	121	**2304**	46	**1161**	48	**148**	2
2	**1320**	46	**2677**	54	**6810**	191	**123**	6	**117**	2	**163**	5	**2669**	82	**3289**	158	**2126**	41	**743**	6	**150**	1
3	**2839**	90	**4426**	110	**3943**	81	**671**	40	**736**	8	**622**	3	**203**	4	**236**	3	**2522**	199	**578**	31	**574**	14
4	**2803**	150	**4097**	88	**3700**	84	**697**	36	**686**	9	**526**	5	**92**	2	**86**	2	**2537**	32	**461**	16	**696**	26
5	**3176**	203	**4214**	116	**3400**	153	**637**	32	**206**	81	**692**	28	**<LoD**		**23**	1	**866**	25	**501**	18	**862**	27
6	**3103**	138	**4570**	115	**3383**	67	**565**	16	**1497**	23	**692**	36	**<LoD**		**20**	0	**667**	29	**524**	19	**491**	18
7	**3721**	315	**4161**	213	**3672**	163	**38**	1	**59**	2	**308**	7	**<LoD**		**16**	1	**132**	5	**632**	27	**384**	4
8	**3697**	101	**3454**	135	**3528**	118	14	1	**33**	1	**296**	10	**<LoD**		14	1	**65**	3	**583**	10	**415**	29
LoD	8		6		1		8		1		10		1		6		17		17		6	
LoQ	22		16		3		22		3		28		3		15		48		48		16	

Table A3. 130: Iron concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**1661**	33	**3791**	191	**2729**	86	**507**	13	**337**	4	**346**	5	**49733**	890	**281**	6	**12454**	1338	**41**	0	**901**	18
2	**2024**	49	**4758**	206	**8204**	195	**619**	9	**272**	4	**399**	5	**1076**	21	**39**	1	**14388**	591	**20**	0	**818**	20
3	**67**	3	**142**	2	**131**	2	**7**	0	**5375**	127	**131**	2	**21**	0	**7**	0	**13974**	266	**73**	3	**3582**	679
4	**57**	1	**91**	1	**89**	1	**6**	0	**4762**	150	**77**	1	**13**	0	4	0	**13412**	292	**59**	1	**4820**	753
5	**38**	1	**43**	2	**30**	0	**3**	0	**36**	11	**25**	0	**<LoD**		**5**	0	**33**	7	**45**	1	**155**	10
6	**37**	1	**36**	4	**30**	0	**3**	0	**102**	3	**9**	0	**<LoD**		4	0	**9**	0	**44**	1	**4**	0
7	**19**	1	**8**	0	**14**	0	**2**	0	**<LoD**		**5**	0	**<LoD**		**6**	1	**6**	0	**12**	1	**5**	1
8	**14**	1	**7**	0	**14**	0	**2**	0	**<LoD**		**4**	0	**13**	1	4	0	**8**	0	**11**	0	**5**	0
LoD	0		2		0		0		5		1		0		2		1		1		2	
LoQ	1		4		1		1		13		2		1		4		3		3		4	

Table A3. 131: Arsenic concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**14.754**	0.509	**11.082**	0.641	**16.386**	0.419	**2.917**	0.146	**3.911**	0.118	**1.509**	0.079	**34.488**	0.872	**1.340**	0.032	**11.828**	0.477	**1.638**	0.140	**26.296**	1.897
2	**17.436**	0.435	**13.468**	0.644	**21.730**	1.270	**2.969**	0.144	**3.689**	0.243	**1.652**	0.125	**1.286**	0.048	**1.676**	0.062	**13.339**	0.606	**5.186**	0.298	**27.262**	1.677
3	**1.866**	0.066	**0.980**	0.044	**2.734**	0.119	**0.448**	0.021	**1.798**	0.104	**0.517**	0.019	**1.561**	0.077	**1.702**	0.043	**10.182**	0.567	**4.182**	0.164	**6.598**	0.095
4	**1.675**	0.045	**1.003**	0.050	**2.875**	0.151	**0.436**	0.025	**1.812**	0.090	**0.477**	0.043	**1.576**	0.084	**1.270**	0.033	**10.187**	0.439	**2.688**	0.187	**9.674**	1.066
5	**1.215**	0.059	**1.088**	0.057	**2.422**	0.091	**0.434**	0.037	**1.724**	0.098	**0.406**	0.031	**<LoD**		**1.582**	0.057	**1.040**	0.043	**2.195**	0.195	**0.979**	0.087
6	**1.205**	0.072	**1.098**	0.084	**2.581**	0.128	**0.495**	0.041	**1.414**	0.073	**0.426**	0.038	**1.449**	0.048	**1.371**	0.096	**0.944**	0.052	**2.380**	0.199	**0.983**	0.089
7	**1.205**	0.061	**1.362**	0.079	**2.571**	0.113	**0.501**	0.044	**0.790**	0.057	**0.516**	0.046	**1.875**	0.052	**1.421**	0.087	**0.935**	0.068	**2.413**	0.175	**1.163**	0.082
8	**1.296**	0.034	**1.493**	0.078	**2.617**	0.143	**0.473**	0.043	**0.746**	0.031	**0.494**	0.030	**2.277**	0.087	**1.307**	0.041	**0.712**	0.053	**2.240**	0.209	**1.127**	0.081
LoD	0.069		0.097		0.031		0.069		0.026		0.032		0.031		0.031		0.053		0.053		0.097	
LoQ	0.189		0.232		0.068		0.189		0.071		0.085		0.068		0.087		0.145		0.145		0.232	

Table A3. 132: Antimony concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**<LoD**		**0.328**	0.038	**0.592**	0.045	1.603	0.133	**1.672**	0.098	**2.559**	0.196	**1.547**	0.024	**1.179**	0.032	**0.397**	0.029	**2.384**	0.239	**0.081**	0.009
2	**<LoD**		**0.294**	0.022	**0.480**	0.052	1.418	0.083	**1.503**	0.105	**2.380**	0.222	**1.112**	0.054	**1.303**	0.057	**0.351**	0.023	**0.405**	0.056	**0.059**	0.005
3	**<LoD**		**0.802**	0.058	**0.367**	0.031	**<LoD**		**0.492**	0.040	**0.593**	0.030	**6.039**	0.260	**6.434**	0.081	**0.281**	0.028	**0.739**	0.048	**0.267**	0.032
4	**<LoD**		**0.808**	0.049	**0.377**	0.028	**<LoD**		**0.484**	0.056	**0.427**	0.036	**5.840**	0.230	**4.485**	0.138	**0.256**	0.025	**0.484**	0.059	**0.215**	0.016
5	3.203	0.159	**1.962**	0.079	**1.537**	0.098	1.857	0.119	**0.934**	0.073	**1.108**	0.107	**7.425**	0.290	**5.377**	0.183	**4.949**	0.303	**2.343**	0.215	**0.869**	0.068
6	**3.891**	0.111	**4.644**	0.325	**1.865**	0.136	2.084	0.051	**0.959**	0.082	**1.360**	0.121	**4.951**	0.186	**4.703**	0.165	**4.396**	0.317	**3.007**	0.270	**4.583**	0.283
7	**8.046**	0.372	**7.060**	0.436	**6.047**	0.308	2.641	0.097	**3.646**	0.225	**7.362**	0.195	**<LoD**		**4.139**	0.112	**3.941**	0.329	**6.638**	0.495	**4.900**	0.389
8	**8.375**	0.237	**6.938**	0.398	**6.165**	0.430	2.604	0.185	**3.358**	0.113	**7.616**	0.252	**<LoD**		**3.659**	0.077	**3.188**	0.288	**6.283**	0.597	**5.237**	0.335
LoD	1.397		0.012		0.036		1.397		0.022		0.035		0.036		0.014		0.025		0.025		0.012	
LoQ	3.475		0.033		0.099		3.475		0.056		0.092		0.099		0.046		0.068		0.068		0.033	

Table A3. 133: Cadmium concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**0.016**	0.008	**0.014**	0.002	0.006	0.002	**<LoD**		**0.032**	0.003	0.011	0.002	**0.585**	0.013	**0.012**	0.001	0.006	0.003	**0.030**	0.005	0.009	0.003
2	0.012	0.002	**0.014**	0.002	**<LoD**		**<LoD**		0.004	0.001	**<LoD**		**0.075**	0.007	**0.017**	0.001	0.004	0.001	**0.008**	0.001	0.005	0.001
3	**<LoD**		**0.009**	0.002	**0.011**	0.003	**<LoD**		**0.011**	0.001	**<LoD**		**1.234**	0.054	**0.207**	0.014	0.004	0.001	0.006	0.001	**0.012**	0.001
4	0.009	0.004	**0.011**	0.002	**<LoD**		**<LoD**		0.005	0.002	0.012	0.003	**1.506**	0.075	**0.101**	0.004	0.004	0.002	0.003	0.001	0.007	0.005
5	**<LoD**		**0.016**	0.002	**0.016**	0.002	**<LoD**		**0.048**	0.005	0.010	0.005	**3.668**	0.107	**4.066**	0.205	**1.035**	0.053	0.006	0.001	**0.014**	0.003
6	0.011	0.002	**0.040**	0.002	**0.011**	0.001	**<LoD**		**0.026**	0.002	0.016	0.003	**2.250**	0.078	**4.084**	0.148	**1.190**	0.085	0.007	0.002	**1.848**	0.094
7	**0.156**	0.021	**0.899**	0.045	**0.171**	0.006	0.008	0.005	**0.716**	0.053	**0.302**	0.010	**2.398**	0.058	**7.947**	0.184	**7.363**	0.564	**1.039**	0.058	**3.356**	0.206
8	**0.186**	0.017	**0.829**	0.035	**0.190**	0.010	0.009	0.005	**1.138**	0.037	**0.392**	0.024	**3.126**	0.162	**7.748**	0.292	**7.483**	0.522	**0.940**	0.076	**3.972**	0.193
LoD	0.006		0.004		0.006		0.006		0.002		0.006		0.006		0.003		0.003		0.003		0.004	
LoQ	0.014		0.009		0.010		0.014		0.005		0.018		0.010		0.008		0.008		0.008		0.009	

Table A3. 134: Chromium concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**0.237**	0.045	0.106	0.013	**0.127**	0.017	**0.292**	0.042	**0.333**	0.031	0.367	0.053	**0.791**	0.033	**<LoD**		**0.299**	0.016	0.273	0.056	**0.293**	0.049
2	**0.225**	0.042	0.127	0.025	**0.110**	0.017	**0.259**	0.043	**0.278**	0.024	**<LoD**		**0.036**	0.007	**<LoD**		**<LoD**		0.225	0.049	0.174	0.016
3	0.050	0.074	0.073	0.031	**0.046**	0.004	0.091	0.042	0.086	0.011	**<LoD**		**0.544**	0.050	**<LoD**		**<LoD**		0.161	0.022	0.190	0.014
4	0.071	0.045	0.070	0.014	**0.044**	0.008	**<LoD**		0.095	0.034	**<LoD**		**0.085**	0.012	**<LoD**		**<LoD**		**<LoD**		0.121	0.053
5	0.063	0.039	0.060	0.013	**0.075**	0.012	0.103	0.038	**0.235**	0.051	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**	
6	0.063	0.072	0.041	0.018	**0.045**	0.010	0.056	0.056	0.116	0.018	0.258	0.054	**0.321**	0.030	**<LoD**		**<LoD**		**<LoD**		0.085	0.024
7	**0.163**	0.030	0.020	0.024	**0.063**	0.014	0.093	0.059	**0.165**	0.030	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		0.136	0.022
8	0.052	0.069	0.048	0.008	**0.052**	0.010	**0.113**	0.037	0.061	0.023	**<LoD**		**0.411**	0.031	**<LoD**		**<LoD**		**<LoD**		**<LoD**	
LoD	0.043		0.085		0.013		0.043		0.052		0.241		0.013		0.282		0.062		0.119		0.085	
LoQ	0.109		0.191		0.028		0.109		0.125		0.756		0.028		0.801		0.139		0.290		0.191	

Table A3. 135: Cobalt concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	0.097	0.022	**0.179**	0.018	**14.794**	0.606	0.105	0.014	**0.159**	0.022	**0.493**	0.038	**1.168**	0.030	**0.707**	0.041	**0.184**	0.021	**0.960**	0.090	**0.129**	0.013
2	0.080	0.016	**0.150**	0.012	**13.886**	0.941	0.116	0.015	**0.084**	0.012	**0.312**	0.011	**0.547**	0.034	**1.289**	0.099	**0.118**	0.021	**0.467**	0.033	**0.110**	0.014
3	**0.337**	0.037	**0.371**	0.032	**1.659**	0.085	**0.733**	0.067	**0.521**	0.031	**0.495**	0.015	**4.217**	0.139	**7.349**	0.216	**0.278**	0.024	**0.346**	0.037	**0.177**	0.015
4	**0.346**	0.027	**0.331**	0.011	**1.360**	0.064	**0.759**	0.055	**0.480**	0.034	**0.501**	0.031	**2.968**	0.155	**3.017**	0.102	**0.251**	0.019	**0.215**	0.016	**0.154**	0.020
5	**0.886**	0.060	**1.145**	0.086	**1.491**	0.065	**2.637**	0.135	**5.060**	0.359	**0.869**	0.084	**2.902**	0.024	**1.487**	0.136	**16.203**	0.842	**0.316**	0.029	**0.386**	0.044
6	**1.127**	0.100	**3.019**	0.155	**1.618**	0.101	**2.797**	0.124	**5.327**	0.376	**0.987**	0.118	**1.286**	0.028	**1.258**	0.103	**13.117**	1.064	**0.369**	0.023	**5.883**	0.134
7	**6.899**	0.436	**11.090**	0.911	**5.198**	0.301	**2.059**	0.074	**2.934**	0.125	**15.987**	0.544	**<LoD**		**0.977**	0.038	**2.954**	0.079	**4.235**	0.350	**6.273**	0.478
8	**7.524**	0.175	**10.742**	0.433	**4.941**	0.239	**0.911**	0.055	**1.740**	0.094	**16.156**	0.677	**<LoD**		**0.836**	0.038	**1.581**	0.117	**4.120**	0.371	**6.459**	0.414
LoD	0.052		0.038		0.004		0.052		0.009		0.035		0.004		0.095		0.026		0.026		0.038	
LoQ	0.146		0.109		0.011		0.146		0.025		0.095		0.011		0.239		0.068		0.068		0.109	

Table A3. 136: Copper concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**<LoD**		0.16	0.01	0.82	0.02	**<LoD**		1.66	0.07	**<LoD**		**3.98**	0.06	0.61	0.05	**<LoD**		1.28	0.08	**<LoD**	
2	**<LoD**		0.11	0.02	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**2.02**	0.06	0.54	0.07	**<LoD**		**<LoD**		**<LoD**	
3	**<LoD**		0.76	0.04	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**3.33**	0.11	**2.93**	0.22	**<LoD**		**<LoD**		**<LoD**	
4	**5.40**	0.27	1.05	0.07	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**3.04**	0.09	**1.85**	0.07	**<LoD**		**<LoD**		**<LoD**	
5	**<LoD**		0.53	0.06	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**4.93**	0.11	**4.16**	0.12	1.96	0.04	**<LoD**		**<LoD**	
6	**<LoD**		1.41	0.09	0.51	0.10	**<LoD**		**<LoD**		**<LoD**		**3.47**	0.10	**3.94**	0.18	2.08	0.08	**<LoD**		**<LoD**	
7	1.28	0.10	3.23	0.18	**2.19**	0.05	**<LoD**		2.03	0.08	**<LoD**		**4.62**	0.18	**5.92**	0.57	**3.88**	0.14	**3.36**	0.19	2.92	0.21
8	1.60	0.06	3.10	0.19	**2.22**	0.04	**<LoD**		2.22	0.09	**<LoD**		**4.60**	0.15	**5.73**	0.19	**6.85**	0.34	**3.13**	0.11	3.31	0.10
LoD	0.81		2.00		0.50		0.81		0.95		1.12		0.50		0.50		1.26		1.26		2.00	
LoQ	1.98		5.02		1.33		1.98		2.31		3.09		1.33		0.78		3.08		3.08		5.02	

Table A3. 137: Lead concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**0.096**	0.008	**0.070**	0.006	**0.353**	0.010	**0.049**	0.005	**0.494**	0.008	0.028	0.017	**10.924**	0.053	**0.186**	0.010	**0.042**	0.006	**0.187**	0.008	**0.127**	0.008
2	**0.097**	0.006	**0.154**	0.006	**0.102**	0.005	**<LoD**		**0.021**	0.004	0.012	0.001	**0.055**	0.006	**0.119**	0.008	**0.037**	0.006	**0.165**	0.008	0.044	0.004
3	**0.115**	0.008	0.039	0.004	0.020	0.002	0.017	0.007	**<LoD**		0.016	0.002	**0.059**	0.003	**0.139**	0.009	0.029	0.003	**0.125**	0.006	**0.094**	0.002
4	**0.307**	0.023	**0.262**	0.007	0.019	0.002	**<LoD**		**<LoD**		0.010	0.001	0.026	0.003	**0.064**	0.007	0.018	0.004	**0.187**	0.006	**0.063**	0.004
5	**0.047**	0.008	**0.135**	0.006	0.033	0.001	**<LoD**		**<LoD**		0.023	0.004	**<LoD**		**0.125**	0.007	**0.045**	0.004	**0.235**	0.016	**0.108**	0.002
6	**0.043**	0.009	**0.158**	0.012	**0.051**	0.001	0.016	0.008	0.010	0.003	**0.050**	0.004	**<LoD**		**0.095**	0.009	**0.037**	0.005	**0.240**	0.012	0.022	0.005
7	**0.043**	0.006	**0.095**	0.020	0.018	0.002	**<LoD**		0.014	0.002	0.028	0.005	**<LoD**		**0.168**	0.015	0.034	0.004	**0.090**	0.003	0.023	0.004
8	**0.100**	0.007	**0.070**	0.003	0.020	0.001	**0.053**	0.007	0.010	0.002	0.013	0.001	**<LoD**		**0.137**	0.005	**0.071**	0.003	**0.080**	0.003	**0.069**	0.015
LoD	0.010		0.016		0.016		0.010		0.009		0.009		0.016		0.009		0.014		0.014		0.016	
LoQ	0.025		0.046		0.046		0.025		0.019		0.032		0.046		0.030		0.036		0.036		0.046	

Table A3. 138: Molybdenum concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**18.346**	0.928	**24.140**	1.051	**22.006**	0.681	**42.759**	2.755	**64.771**	4.159	**79.120**	4.619	**27.585**	0.769	**56.813**	1.768	**47.600**	2.434	**16.891**	1.369	**4.573**	0.245
2	**18.377**	0.531	**24.891**	0.981	**22.357**	1.510	**47.087**	2.007	**64.129**	4.199	**70.326**	4.936	**32.669**	0.789	**54.984**	2.287	**43.393**	1.919	**21.364**	1.481	**4.941**	0.153
3	**24.328**	1.017	**24.204**	0.721	**28.229**	1.193	**13.909**	0.807	**51.375**	2.737	**64.188**	1.498	**92.450**	3.134	**77.776**	0.750	**46.746**	2.937	**39.234**	1.142	**10.500**	0.317
4	**25.471**	0.672	**22.099**	1.162	**29.337**	1.366	**15.362**	0.686	**45.123**	3.015	**49.685**	3.551	**93.196**	5.282	**57.099**	2.636	**43.301**	2.323	**24.978**	1.454	**10.495**	1.097
5	**25.791**	1.154	**24.732**	1.412	**39.304**	1.205	**17.760**	0.680	**15.016**	0.968	**46.121**	3.270	**123.265**	2.711	**73.381**	4.056	**35.804**	1.761	**26.177**	2.343	**8.887**	0.615
6	**26.072**	0.937	**26.510**	1.056	**39.154**	1.913	**18.927**	0.689	**13.866**	0.977	**48.529**	4.227	**80.465**	2.685	**63.950**	2.692	**31.115**	1.742	**28.375**	2.138	**9.936**	0.831
7	**29.210**	1.031	**36.130**	1.977	**47.507**	2.055	**18.634**	0.242	**33.478**	1.794	**44.402**	1.524	**100.226**	2.274	**72.461**	2.127	**37.885**	2.767	**32.470**	2.058	**10.793**	0.811
8	**28.759**	0.808	**32.150**	0.777	**47.699**	1.879	**22.324**	1.419	**34.428**	1.255	**44.400**	1.914	**119.503**	6.884	**64.564**	2.253	**32.805**	2.547	**30.558**	2.396	**14.968**	1.852
LoD	0.075		0.041		0.039		0.075		0.180		0.226		0.039		0.234		0.258		0.258		0.041	
LoQ	0.206		0.100		0.099		0.206		0.513		0.631		0.099		0.665		0.730		0.730		0.100	

Table A3. 139: Nickel concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**0.87**	0.05	1.17	0.08	**6.51**	0.33	**2.48**	0.08	**5.72**	0.23	2.17	0.06	**9.62**	0.42	**2.26**	0.20	**3.58**	0.17	**3.54**	0.27	1.01	0.09
2	**0.51**	0.04	1.84	0.22	**8.42**	0.16	**1.58**	0.12	1.39	0.05	1.61	0.07	**3.60**	0.16	**2.55**	0.20	**3.15**	0.11	1.27	0.08	**<LoD**	
3	**0.73**	0.08	1.29	0.04	**2.06**	0.05	**2.23**	0.17	**3.43**	0.14	2.04	0.05	**16.92**	0.44	**7.97**	1.97	**4.72**	0.37	1.34	0.15	1.32	0.14
4	**0.72**	0.03	1.22	0.09	**1.95**	0.05	**2.17**	0.06	**3.15**	0.04	1.59	0.07	**15.05**	0.49	**4.96**	0.21	**4.81**	0.23	1.17	0.11	1.06	0.08
5	**0.96**	0.05	1.60	0.09	**2.35**	0.08	**2.46**	0.09	1.47	0.57	1.60	0.10	**19.98**	0.84	**17.06**	0.36	**19.09**	0.66	1.27	0.06	**<LoD**	
6	**0.95**	0.09	**6.12**	0.17	**2.17**	0.12	**2.18**	0.07	**7.56**	0.42	1.69	0.04	**13.30**	0.49	**20.46**	1.84	**19.73**	0.97	1.39	0.09	**4.26**	0.17
7	**2.90**	0.17	**4.84**	0.23	**2.96**	0.15	**3.16**	0.18	**13.32**	0.42	**11.02**	0.28	**18.15**	1.00	**28.43**	4.00	**61.32**	2.28	**5.08**	0.74	**6.66**	0.48
8	**5.89**	0.19	**4.29**	0.39	**2.77**	0.15	**3.08**	0.21	**11.73**	0.32	**14.64**	0.44	**18.91**	1.05	**26.10**	0.90	**58.87**	2.02	**3.39**	0.20	**9.50**	0.62
LoD	0.07		0.92		0.20		0.07		0.70		1.29		0.20		0.06		0.72		0.72		0.92	
LoQ	0.16		2.46		0.56		0.16		1.80		3.72		0.56		0.12		2.04		2.04		2.46	

Table A3. 140: Selenium concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	0.748	0.381	0.477	0.041	0.680	0.100	**<LoD**		**0.671**	0.094	**<LoD**		0.884	0.042	**<LoD**		0.979	0.116	**<LoD**		**<LoD**	
2	0.807	0.263	0.474	0.037	0.493	0.052	**<LoD**		**0.709**	0.117	**<LoD**		**<LoD**		**<LoD**		0.872	0.110	**<LoD**		**<LoD**	
3	**<LoD**		0.479	0.054	0.453	0.095	0.982	0.399	**0.757**	0.087	1.696	0.070	**1.421**	0.151	0.262	0.028	0.938	0.181	0.973	0.176	**<LoD**	
4	**<LoD**		0.561	0.077	**<LoD**		1.008	0.169	**0.780**	0.100	**<LoD**		**1.356**	0.084	0.189	0.017	1.047	0.041	**<LoD**		**<LoD**	
5	**<LoD**		0.588	0.103	**<LoD**		**<LoD**		**0.733**	0.131	**<LoD**		**1.892**	0.081	0.250	0.015	1.575	0.140	**<LoD**		**<LoD**	
6	0.890	0.169	0.681	0.100	0.488	0.059	0.916	0.361	**0.848**	0.107	**<LoD**		**<LoD**		0.217	0.025	1.383	0.133	**<LoD**		**<LoD**	
7	0.882	0.272	0.765	0.095	0.731	0.045	0.758	0.572	**0.861**	0.131	1.154	0.094	**1.510**	0.099	0.208	0.014	1.640	0.106	1.059	0.156	**<LoD**	
8	**<LoD**		0.840	0.079	0.806	0.114	1.125	0.158	**0.810**	0.093	1.171	0.166	**1.695**	0.104	0.211	0.016	1.506	0.116	0.986	0.153	**<LoD**	
LoD	0.676		0.945		0.414		0.676		0.396		0.978		0.414		0.147		0.843		0.843		0.945	
LoQ	1.628		2.171		0.893		1.628		0.670		2.303		0.893		0.341		1.862		1.862		2.171	

Table A3. 141: Silver concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**<LoD**		0.014	0.002	**0.006**	0.001	**<LoD**		**0.029**	0.004	**1.359**	0.062	**0.100**	0.003	**0.868**	0.028	0.002	0.001	**0.008**	0.007	**<LoD**	
2	**<LoD**		0.010	0.002	0.004	0.001	**<LoD**		**<LoD**		**1.379**	0.103	**0.008**	0.002	**<LoD**		**<LoD**		0.001	0.001	**<LoD**	
3	**<LoD**		**0.043**	0.004	0.003	0.001	**<LoD**		**<LoD**		**1.594**	0.025	0.002	0.001	**0.241**	0.009	**0.006**	0.001	**<LoD**		**<LoD**	
4	0.011	0.004	**0.040**	0.003	**0.005**	0.001	**<LoD**		**<LoD**		**1.123**	0.082	0.002	0.001	**<LoD**		0.002	0.001	**<LoD**		**<LoD**	
5	**<LoD**		0.008	0.001	**0.010**	0.002	**<LoD**		0.005	0.003	**0.826**	0.047	**<LoD**		0.035	0.001	**0.016**	0.002	**<LoD**		**<LoD**	
6	**<LoD**		0.013	0.002	**0.006**	0.001	**<LoD**		**<LoD**		**1.003**	0.084	**<LoD**		**0.050**	0.004	**0.017**	0.002	**<LoD**		**0.016**	0.002
7	**<LoD**		0.011	0.001	**0.020**	0.002	**<LoD**		**0.011**	0.002	**0.056**	0.002	**<LoD**		**2.088**	0.079	**0.015**	0.002	**0.007**	0.000	**<LoD**	
8	**<LoD**		0.005	0.001	**0.011**	0.001	**<LoD**		0.004	0.001	**0.066**	0.003	0.002	0.001	**<LoD**		**0.017**	0.003	0.001	0.000	**<LoD**	
LoD	0.011		0.005		0.003		0.011		0.004		0.009		0.003		0.012		0.001		0.001		0.005	
LoQ	0.015		0.015		0.005		0.015		0.009		0.023		0.005		0.037		0.003		0.003		0.015	

Table A3. 142: Tin concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	0.318	0.063	0.114	0.015	**<LoD**		**<LoD**		0.050	0.012	**<LoD**		**<LoD**		0.047	0.046	**0.101**	0.036	0.044	0.018	0.130	0.038
2	0.441	0.109	**0.163**	0.057	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		0.047	0.029	0.043	0.035	0.139	0.036
3	**<LoD**		0.073	0.014	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		0.053	0.019	**<LoD**		**0.095**	0.034	**0.279**	0.093
4	**<LoD**		**0.146**	0.048	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		0.057	0.016	0.068	0.031	0.129	0.078
5	**<LoD**		0.054	0.029	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		0.079	0.029	0.045	0.021	0.033	0.030	**<LoD**	
6	**<LoD**		0.101	0.038	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		0.059	0.029	**0.161**	0.082
7	**<LoD**		0.093	0.030	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		0.069	0.049	0.069	0.031	**0.160**	0.038	**0.161**	0.093
8	**<LoD**		0.056	0.039	**<LoD**		**<LoD**		**<LoD**		**<LoD**		**<LoD**		0.067	0.039	0.076	0.053	0.056	0.011	**<LoD**	
LoD	0.198		0.055		0.391		0.198		0.023		0.531		0.391		0.037		0.031		0.031		0.055	
LoQ	0.475		0.146		0.897		0.475		0.057		1.597		0.897		0.102		0.078		0.078		0.146	

Table A3. 143: Vanadium concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**0.686**	0.038	**0.591**	0.028	**1.635**	0.113	**2.016**	0.152	**1.783**	0.119	**0.915**	0.053	**14.435**	0.564	**1.914**	0.035	**0.309**	0.033	**3.401**	0.314	**0.478**	0.033
2	**0.630**	0.027	**0.575**	0.030	**0.797**	0.071	**1.829**	0.092	**1.521**	0.103	0.722	0.051	**0.937**	0.054	**2.367**	0.062	**0.225**	0.014	**2.602**	0.183	**0.499**	0.027
3	**0.759**	0.032	**0.577**	0.027	**0.221**	0.017	**0.149**	0.012	**0.410**	0.028	**<LoD**		**2.383**	0.171	**3.166**	0.064	**0.337**	0.032	**3.272**	0.104	**0.627**	0.036
4	**0.772**	0.031	**0.547**	0.025	**0.231**	0.016	**0.153**	0.013	**0.306**	0.022	**<LoD**		**2.342**	0.106	**2.255**	0.038	**0.324**	0.020	**2.096**	0.131	**0.626**	0.053
5	**1.412**	0.073	**1.563**	0.104	**0.308**	0.023	**0.157**	0.009	**0.372**	0.030	**<LoD**		**<LoD**		**3.059**	0.114	**2.041**	0.115	**2.736**	0.064	**1.931**	0.079
6	**1.572**	0.051	**1.630**	0.085	**0.462**	0.034	**0.187**	0.009	**0.365**	0.028	**<LoD**		**1.892**	0.090	**2.672**	0.091	**1.867**	0.127	**2.983**	0.271	**1.977**	0.064
7	**1.671**	0.099	**2.070**	0.178	**1.008**	0.088	**0.206**	0.004	**0.504**	0.029	0.302	0.008	**<LoD**		**2.576**	0.074	**1.501**	0.118	**4.286**	0.293	**2.228**	0.224
8	**2.214**	0.038	**2.094**	0.076	**1.161**	0.082	**0.210**	0.017	**0.530**	0.028	0.305	0.006	**2.769**	0.096	**2.351**	0.029	**1.246**	0.109	**4.112**	0.364	**2.422**	0.208
LoD	0.004		0.077		0.009		0.004		0.090		0.265		0.009		0.012		0.054		0.054		0.077	
LoQ	0.011		0.204		0.020		0.011		0.259		0.749		0.020		0.026		0.158		0.158		0.204	

Table A3. 144: Zinc concentrations (<0.45 µm) during the mesocosm experiments and LoDs and LoQs. Values <LoD were removed from the data set. Values >LoQ are bold. All values in µg/L.

	Sampling Site 1						Sampling Site 2						Sampling Site 3						Sampling Site 4			
Sample	Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2		Mesocosm 3		Mesocosm 1		Mesocosm 2	
	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD	Conc.	SD
1	**57.03**	1.21	**11.85**	0.43	**83.43**	0.75	**10.09**	0.45	**8.83**	0.11	**10.62**	0.74	**134.36**	1.92	**13.18**	0.60	**3.45**	0.15	**43.60**	0.62	**3.74**	0.16
2	**39.58**	2.23	**15.46**	1.25	**69.77**	1.40	**8.76**	0.52	**3.29**	0.22	**5.06**	0.32	**28.89**	0.55	**19.56**	0.34	**8.03**	0.20	**10.64**	0.16	**2.79**	0.22
3	**44.75**	1.68	**13.16**	0.42	**11.59**	0.35	**12.94**	0.52	**11.18**	0.18	**15.26**	0.23	**250.27**	3.50	**134.01**	1.84	**5.52**	0.23	**5.26**	0.49	**8.93**	0.19
4	**26.36**	1.24	**10.02**	0.27	**11.78**	0.38	**11.55**	0.76	**2.81**	0.20	**14.58**	0.45	**243.53**	5.79	**68.04**	0.87	**4.31**	0.41	**5.49**	0.15	**13.54**	0.32
5	**24.64**	0.90	**16.91**	0.78	**8.77**	0.24	**17.68**	0.70	**11.33**	4.82	**12.10**	0.52	**336.04**	1.73	**428.21**	15.20	**408.17**	6.40	**8.14**	0.37	**16.66**	0.72
6	**22.90**	0.63	**34.59**	0.65	**10.33**	0.34	**17.27**	0.64	**84.02**	1.64	**12.35**	0.68	**211.56**	2.72	**393.07**	8.01	**438.83**	7.35	**7.07**	0.30	**265.34**	5.18
7	**94.83**	1.87	**201.61**	3.48	**30.96**	0.55	**39.69**	1.07	**801.05**	6.86	**385.55**	5.87	**<LoD**		**513.29**	40.41	**671.98**	14.19	**178.09**	1.53	**462.48**	13.98
8	**122.84**	3.58	**167.94**	6.85	**31.92**	0.28	**37.88**	0.64	**824.16**	12.51	**490.04**	16.55	**<LoD**		**436.95**	22.08	**654.98**	12.63	**178.34**	2.29	**480.84**	25.24
LoD	0.10		0.27		0.10		0.10		0.88		0.21		0.10		0.38		0.22		0.22		0.27	
LoQ	0.25		0.72		0.27		0.25		2.61		0.56		0.27		1.11		0.59		0.59		0.72	

10 References:

[1] D.R. Lide, CRC Handbook of Chemistry and Physics, 84th Edition Edited by David R. Lide (National Institute of Standards and Technology). CRC Press LLC: Boca Raton. 2003. 2616 pp. $139.95. ISBN 0-8493-0484-9, Journal of the American Chemical Society, 126 (2004) 1586-1586.

[2] S. Zhao, C. Feng, Y. Yang, J. Niu, Z. Shen, Risk assessment of sedimentary metals in the Yangtze Estuary: new evidence of the relationships between two typical index methods, J Hazard Mater, 241-242 (2012) 164-172.

[3] C.K. Jain, Metal fractionation study on bed sediments of River Yamuna, India, Water Res, 38 (2004) 569-578.

[4] U.S.EPA, Procedures for the Derivation of Equilibrium Partitioning Sediment Benchmarks (ESBs) for the Protection of Benthic Organisms: Metal Mixtures (Cadmium, Copper, Lead, Nickel, Silver and Zinc), in: EPA-600-R-02-011, Office of Research and Development, Washington, DC 20460, 2005.