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Discussions

Changes in the composition of marine and sea-ice diatoms derived from sedimentary ancient DNA of the eastern Fram Strait over the past 30,000 years

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Abstract. The Fram Strait is an area with a relatively low and irregular distribution of diatom microfossils in surface sediments, and thus microfossil records are underrepresented, rarely exceed the Holocene and contain sparse information about past diversity and taxonomic composition. These attributes make the Fram Strait an ideal study site to test the utility of sedimentary ancient DNA (*sed*aDNA) metabarcoding. By amplifying a short, partial *rbcL* marker, 95.7 % of our sequences are assigned to diatoms across 18 different families with 38.6 % of them being resolved to species and 25.8 % to genus level. Independent replicates show high similarity of PCR products, especially in the oldest samples. Diatom richness is highest in the Late Weichselian and lowest in Mid- and Late-Holocene samples. Taxonomic composition is dominated by cold-water and sea-ice associated diatoms and shows two re-organizations – one after the Last Glacial Maximum and another after the Younger Dryas. Different sequences assigned, amongst others, to *Chaetoceros socialis* indicate the detectability of intra-specific diversity using *sed*aDNA. We detect no clear pattern between our diatom *sed*aDNA record and the previously published IP_{25} record of this core, although proportions of pennate diatoms increase with higher IP_{25} concentrations and proportions of *Nitzschia* cf. *frigida* exceeding 2 % of the assemblage point towards past sea-ice presence.

1 Introduction

The global climate system is strongly coupled with Arctic sea-ice cover (Goosse and Fichefet, 1999): yet Earth system models display large uncertainties in projections of sea ice, which stresses the need for paleo sea-ice reconstructions that can be used to improve the models (de Vernal et al., 2013). Currently, semi-quantitative reconstructions of past sea-ice distribution can be achieved by combining the diatom produced sea-ice proxy IP_{25} (a highly branched isoprenoid alkene with 25 carbon atoms; (Belt et al., 2007)) and phytoplankton biomarkers (e.g. brassicasterol, dinosterol; (Volkman, 1986))

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detected in down-core sediments (Belt, 2018; Belt and Müller, 2013; Müller et al., 2009; Müller and Stein, 2014; Stein et al., 2012). Owing to their sensitive responses to environmental conditions, diatoms are frequently used as indicators for paleoenvironmental reconstructions, to assess, for example, changes in surface water temperatures (Birks and Koç, 2002; Miettinen et al., 2015), paleoproductivity (Fahl and Stein, 1997; Limoges et al., 2018) and sea-ice distribution (Smirnova et al., 2015; Weckström et al., 2013).

Diatoms in northern high-latitudinal regions are less silicified and more prone to silica dissolution (Kohly, 1998; Stabell, 1986) compared to diatoms of the southern polar oceans (Harrison and Cota, 1991). In the Fram Strait – an important area of heat exchange between Arctic and North Atlantic water masses (Untersteiner, 1988) – particularly low and irregular preservation of diatom microfossils prevails in surface sediments (Karpuz and Schrader, 1990; Stabell, 1987). The diatom records are generally underrepresented, contain sparse information about past diversity and taxonomic composition and rarely exceed the Holocene (Jessen et al., 2010; Koç et al., 2002; Stabell, 1986). This makes the Fram Strait an excellent site to test ancient DNA metabarcoding on a sediment core (Müller et al., 2012; Müller and Stein, 2014).

Ancient DNA is a new proxy that can exploit diatoms as indicators of past marine environmental change (Coolen et al., 2007; De Schepper et al., 2019; Kirkpatrick et al., 2016). Deep-sea sediments have been reported to be rich in DNA with up to 70–90 % of the total DNA pool being extracellular DNA (Coolen et al., 2007; Dell'Anno et al., 2002; Lejzerowicz et al., 2013; Morard et al., 2017), and traces of DNA can be detected in sediments even though microfossils are absent or highly degraded (Boere et al., 2009; Coolen et al., 2009, 2013; Lejzerowicz et al., 2013). Therefore, sedimentary ancient DNA (*sed*aDNA) could be advantageous also in areas of biased preservation due to high silica dissolution rates. Beyond morphological or biogeochemical analyses, ancient DNA can distinguish cryptic species that are morphologically similar (Stoof-Leichsenring et al., 2012), trace temporal changes of intra-specific genetic variation (Epp et al., 2018; Parducci et al., 2012; Zimmermann et al., 2017b), and identify genetic relationships and microevolution (Stoof-Leichsenring et al., 2014, 2015).

Paleogenetic analyses with an emphasis on diatoms have been successfully carried out in various limnic settings ranging from the subarctic (Epp et al., 2015; Stoof-Leichsenring et al., 2014, 2015) to the tropics (Stoof-Leichsenring et al., 2012) and Antarctica (Coolen et al., 2004). Yet, it is still a relatively underrepresented branch in the marine realm with only a few published studies targeting phytoplankton ancient DNA (Boere et al., 2009, 2011b, 2011a; Coolen et al., 2006, 2007, 2009, 2013; De Schepper et al., 2019; Giosan et al., 2012; Kirkpatrick et al., 2016).

In this study we examine whether ancient diatom DNA can be retrieved from sediments from the eastern Fram Strait and whether it can be used to analyze temporal changes in the taxonomic composition of diatoms. We have three principal objectives: (1) to assess the quality and replicability of the data obtained by *sed*aDNA metabarcoding, (2) to analyze temporal changes of diatom taxonomic composition and richness, and (3) to evaluate diatom *sed*aDNA as a new proxy for sea-ice reconstruction. DNA was derived from distinct samples of the comprehensively analyzed marine sediment core MSM05/5-712-2, covering the major climatic intervals since the Late Weichselian (i.e. the last ~30 kyr BP). We chose the samples according to high, medium and low concentrations of the diatom produced sea-ice biomarker IP_{25} (Müller et al.,

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2012; Müller and Stein, 2014) as we expect associated changes in the taxonomic composition. We used *sed*aDNA metabarcoding by applying the *rbcL_76* marker (Stoof-Leichsenring et al., 2012) which has already proved successful in low-productivity lakes of northern Siberia (Dulias et al., 2017; Stoof-Leichsenring et al., 2014, 2015). The marker amplifies a short region of the *rbcL* gene, which is located on the chloroplast that is present in diatoms in several copy numbers, thereby increasing the probability of its long-term preservation. The *rbcL* gene has an adequate sequence reference database and was tested as a potential diatom barcode marker with high resolution power (Guo et al., 2015; Kermarrec et al., 2013). Furthermore, it reduces co-amplification of non-photosynthetic bacteria or archaea that are active in subsurface sediments and thus could be preferentially amplified during PCR in comparison to the highly fragmented and damaged ancient DNA.

2 Materials and Methods

2.1 Study site and sample material

The core MSM05/5-712-2 (N 78.915662, E 6.767167, water depth 1487 m) was collected from the western continental slope of Svalbard during the cruise of *Maria S. Merian* (Budéus, 2007) in the eastern Fram Strait in 2007 (Fig. 1). The Fram Strait is located between Greenland and Svalbard and connects the Arctic Ocean with the Atlantic Ocean. The study area is influenced by temperate, saline water masses that are transported northwards via the West Spitzbergen Current, which is a continuation of the North Atlantic Current (Aagaard, 1982). Furthermore, the site is located downslope from Kongsfjorden and is thus influenced by one of the major outlets of western Svalbard meltwater (Werner et al., 2013). Today, the site is in the vicinity of the winter and summer sea-ice margin and is ice-free year round (Fig. 1), but previous work indicates variability in the past sea-ice cover (Falardeau et al., 2018; Müller et al., 2012; Müller and Stein, 2014; Werner et al., 2011, 2013). Age-depth modeling suggests a maximum age of about 30 cal kyr BP for the lowermost core interval (Müller and Stein, 2014). The sampling procedure for ancient DNA analyses followed the protocol for non-frozen sediment cores explained in (Epp et al., 2019) for the 12 samples taken along the core, of which the depth at 8.85 m was sampled twice to check whether different samples from the same level show similar taxonomic composition and diversity, particularly the oldest (Table 1).

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2.2 DNA extraction, PCR and sequencing

The DNA extractions and PCR setups were prepared in a dedicated laboratory for ancient DNA at the Alfred Wegener Institute, Helmholtz Centre for Polar and Marine Research (Potsdam, Germany). Total DNA was extracted from 12 samples of approximately 2 g (wet weight) sediment using the same method as described in (Zimmermann et al., 2017a). Each extraction batch included one negative control. The DNA concentrations were measured with the Qubit dsDNA BR Assay Kit (Invitrogen, Carlsbad, CA, USA) on a Qubit 2.0 fluorometer (Invitrogen, Carlsbad, CA, USA). As DNA concentrations were below the detection limit, we concentrated 600 µl of each sample with the GeneJET PCR Purification KIT (Thermo Scientific, Carlsbad, CA, USA) according to the manufacturer's protocol and eluted twice with 15 µl elution buffer. All DNA extracts were stored at -20°C.

We amplified the marker *rbcl_76* (Stoof-Leichsenring et al., 2012), a 76 bp long fragment of the plastid *rbcL* gene using tagged primers *Diat_rbcL_705F* (AACAGGTGAAGTTAAAGGTTCATAYTT) and *Diat_rbcL_808R* (TGTAACCCATAACTAAATCGATCAT) as described in (Dulias et al., 2017). The PCR reactions were set up in small batches, each including up to 9 samples and the corresponding negative control from the DNA extraction as well as a PCR no template control (NTC). For each sample, extraction negative control and NTC, we performed 3 PCRs with different primer-tag combinations on different days. The PCR reaction mixes and conditions were prepared as described in (Dulias et al., 2017) with the exception that 3 µl DNA (DNA concentration 3 ng/µl) was used as a template. All PCR products were purified with the MinElute purification Kit (Qiagen, Hilden, Germany) according to the manufacturer's recommendations. Elution was carried out twice in 10 µL elution buffer. The purified PCR products were mixed in equal concentrations and sent to Fasteris SA sequencing service (Switzerland) who carried out library preparation and sequencing. The sequencing library was prepared according to the Fasteris Metafast protocol for low complexity amplicon sequencing and checked by qPCR. The library was sequenced (2 x 150 bp, paired-end) on the Illumina NextSeq 500 (Illumina Inc., San Diego, CA, USA). The sequence data are deposited in the Sequence Read Archive (BioProject: PRJxxxx).

2.3 Bioinformatic processing

The sequences were processed, filtered and assigned a taxonomic name according to the NCBI taxonomy using the OBITools package (Boyer et al., 2016) with the same bioinformatics parameter settings as described in (Dulias et al., 2017). We refrained from clustering sequences into operational taxonomic units and used amplicon sequence variants (ASVs) as recommended by Callahan et al. (Callahan et al., 2017). The OBITools program *obiclean* can identify ASVs that likely have arisen due to PCR or sequencing errors. It uses the information of sequence counts and sequence similarities to classify whether a sequence is rather a variant ("internal") of a more abundant ("head") ASV (Boyer et al., 2016). To generate the reference database for the taxonomic assignment of the sequences we downloaded the EMBL release 138 and used *ecopcr* (Ficetola et al., 2010) according to the descriptions of (Dulias et al., 2017; Stoof-Leichsenring et al., 2012). A total of 7,536,449 sequence counts were assigned to samples, 235 sequence counts to extraction negative controls and 201 counts to

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PCR negative controls. Of the 204 different sequence variants detected in extraction and PCR negative controls the majority were singletons and most likely artefacts from tag-jumping during library preparation (Schnell et al., 2015). Using R v. 3.5.0 (R Core Team, 2018), we kept only those ASVs (Suppl. Table 1) that (1) were assigned a taxonomic name based on 90–100 % similarity to an entry in the reference database, (2) were represented with at least 10 read counts in a replicate, (3) were present at least 3 times among the different replicates, (4) showed taxonomic resolution below the phylum level "Bacillariophyta" and (5) were tagged as "internal" by *obiclean* in less than 50 % of the different replicates to reduce PCR and sequencing artefacts.

2.4 Reproducibility of replicates

Diversity estimates depend highly on the sequencing depth. As more taxa, especially rare ones, can be detected with increasing sequencing depth, diversity is only comparable between samples, when it is estimated based on the same number of sequences. Despite efforts to reduce such differences by equimolar pooling of PCR products, the number of sequences generally varies among replicates. Therefore, we analyzed the dissimilarities of PCR replicates. We resampled (https://github.com/StefanKruse/R_Rarefaction (Kruse, 2019)) the dataset 100 times to the minimum number of sequences available (25,601 counts), then, for each replicate, we calculated the mean number of sequence counts for each ASV across the 100 resampling steps. This dataset was used to calculate the proportions of each ASV per replicate. The proportional data were used for the Multiple Response Permutation Procedure (MRPP) using the R function *mrpp* on Bray Curtis Dissimilarities to test if dissimilarities within replicates of the same sample are significant. Furthermore, we applied non-metric multidimensional scaling (NMDS) using *metaMDS* to assess which replicates show high and low replicability.

2.5 Taxonomic composition and richness

For taxonomic composition and richness calculations, we first summed up the sequence counts for each ASV of the replicates belonging to the same sample and then resampled the dataset 100 times based on the new minimum number of sequence counts (300,415 counts) according to descriptions in the preceding paragraph. The resampled dataset was used to calculate the relative abundances of each ASV per sample. Finally, ASVs, which were assigned to the same taxonomic name but had different similarities to an entry in the reference database, were summed up to one entry using the R *aggregate* function. Constrained hierarchical clustering (CONISS) with the R function *chclust* followed by *brokenstick* analysis divided the samples into five significant assemblage zones. Stratigraphic diagrams showing temporal changes in taxonomic composition were generated with *strat.plot*. All statistical analyses and visualizations were prepared with R v. 3.5.0 using the packages "vegan" (Oksanen et al., 2011) and "rioja" (Juggins, 2012).

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3 Marker specificity, taxonomic resolution and taxonomic coverage

The amplification of the short *rbcL_76* marker permitted the retrieval of diatom DNA from all samples and was highly specific for diatom sequence variants (95.7 %). Only 4.3 % of all assigned ASVs were assigned to other organismal groups: 4 % Bolidophyceae (a closely related sister clade of diatoms with unicellular, siliceous, flagellated algae), 0.2 % Phaeophyceae (brown algae) and 0.1 % Eustigmatophyceae (photosynthetic heterokonts). This exceeds the marker specificity found in previous studies focusing on lake sediment cores (84 % (Stoof-Leichsenring et al., 2012), 88 % (Stoof-Leichsenring et al., 2014), 90 % (Stoof-Leichsenring et al., 2015)) as well as specificity of a previous *in silico* PCR (90.4 % (Dulias et al., 2017)). Possibly owing to a much shorter marker size, the *rbcL_76* marker also outperformed the usually amplified 18S rDNA markers (Coolen et al., 2007; De Schepper et al., 2019; Kirkpatrick et al., 2016).

The initial dataset contained 1,398 ASVs that were systematically filtered to a final diatom dataset containing 360 ASVs (6,199,984 counts) which were further grouped into 75 unique taxonomic names. The majority of diatom sequences are assigned to polar centric Mediophyceae (79.7 %), followed by pennate Bacillariophyceae (14.5 %), while radial centric Conscinodiscophyceae (1.1 %) make up only a small proportion of the dataset. The majority of ASVs are assigned as low as species level (38.6 %) or genus level (25.8 %) (Fig. 2a). Yet, the taxonomic resolution (i.e. the taxonomic assignment of ASVs) is limited by the incompleteness of the sequence reference database as indicated by the striking proportion of ASVs (4.8%) for which assignment is restricted to phylum level (Bacillariophyta).

In total 18 different diatom families are represented in the final dataset which is dominated by ASVs assigned to the families Thalassiosiraceae (35 %), Bacillariaceae (15.8 %) and Chaetoceraceae (9.2 %) (Fig. 2b). Particularly dominant ASVs are assigned to *Thalassiosira* (21.2 %) and *Porosira* (10.9 %) (resolution only possible on genus level) and to *Chaetoceros* cf. *contortus* 1SEH-2013 (6.6 %) – all centric diatoms belonging to the class Mediophyceae. Their dominance is likely the result of high paleoproductivity or of differential overrepresentation caused by preservation and/or technical biases. Indeed, in the Fram Strait especially *Chaetoceros* and *Thalassiosira* species have high productivity in different hydrographical regimes (Gradinger and Baumann, 1991; Lalande et al., 2013) as well as at Kongsfjorden, a major outlet of western Svalbard potentially influencing the coring site (Hodal et al., 2012), and even in micropaleontological studies they are often dominant (Birks and Koç, 2002; Bylinskaya et al., 2016; Oksman et al., 2017, 2019). Next to high paleo-productivity, the preservation of *sed*aDNA could be biased by differential degradation. Heavily silicified and/or spore forming diatoms such as some *Thalassiosira* and *Chaetoceros* species may be less sensitive to dissolution, which might also improve the preservation of DNA over long time periods. Furthermore, the enrichment of centric diatoms in the *sed*aDNA record could be the result of copy number variation of the *rbcL* gene between different species, as centric diatoms are known to have multiple chloroplasts while pennate diatoms are restricted to either one or a few (Bedoshvili et al., 2009; Round et al., 1990). Technical biases often arise during PCRs due to mismatches between primer sequences and primer binding sites (Nichols et al., 2018) and the high number of PCR cycles, which is needed to increase the chance of retrieving rare sequences, leads to

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an over-amplification of already abundant template molecules in comparison to rare ones. While the reduction of cycles could reduce this effect, fewer PCR cycles would reduce replicability (Krehenwinkel et al., 2017).

Despite the filtering, several distinct ASVs, (for example, *Chaetoceros socialis*) are assigned the same taxonomic name (Supplementary Table S1). We believe that these represent either different lineages or closely related species so far not included in the database, although we cannot rule out that some ASVs in our filtered dataset might still represent PCR or sequencing artefacts.

Regardless of a few current limitations, *sed*aDNA shows much promise. New reference sequences are added to GenBank on a daily basis, due to numerous phylogenetic studies and barcoding projects aiming to improve our systematic knowledge about taxonomic relationships and to archive the molecular inventory of global biodiversity (Degerlund et al., 2012; Li et al., 2015; Luddington et al., 2016). Taxonomic coverage of the reference database can be increased by subjecting diatom strains to single cell sequencing (Luddington et al., 2016; Sieracki et al., 2019). Most importantly, *sed*aDNA allows tracing ASVs through time and eventually relating them to, for example, environmental change, without relying on the state of taxonomic coverage of the reference database.

4 Quality and replicability of the data obtained by *sed*aDNA metabarcoding

A crucial requirement for the interpretation of ancient DNA records is that replicates show similar signals in biodiversity and taxonomic composition. The recovery of taxa by *sed*aDNA metabarcoding is prone to false presences or absences. As our study lacks a morphological diatom record, false absences cannot be assessed and true presences cannot be confirmed. Hence, it was important to use independent PCR replicates for each sediment sample and stringent criteria to filter the dataset to remove artefacts introduced by ancient DNA damage, PCR and sequencing. The replicates of each sample show some variations (Fig. 3) in the presence and abundance of ASVs, especially for rare ASVs. We tested whether these differences are significant using MRPP ($p = 0.001$, number of permutations 999, observed delta = 0.3683, expected delta = 0.6548), which suggests that PCR replicates of the same sample share significantly lower dissimilarities (average 39.3 %) in comparison to replicates between different samples (67.5 %). The replicates are highly similar in the oldest samples up to 5.8 m depth and in the youngest sample. This indicates that reasons other than sample age and associated DNA degradation controlled replicability in this study. It is possible that higher dissimilarities between some replicates are the result of the low amount of template DNA or due to PCR inhibition by compounds that were not sufficiently removed during the DNA extraction.

5 Temporal change of taxonomic richness and composition

We used *sed*aDNA metabarcoding on samples that, due to the low sample size, represent temporally restricted snapshots of the different climatic intervals since the Late Weichselian. The dataset reveals diatom taxa that have mostly been reported

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from the Fram Strait in modern surveys (Karpuz and Schrader, 1990; Oksman et al., 2019; von Quillfeldt, 2000) and micropaleontological records (Oksman et al., 2017; Stabell, 1986). We detect typical ice-associated (sympagic) and/or cold-water diatoms (e.g. *Nitzschia* cf. *frigida*, *Cylindrotheca closterium*, *Thalassiosira nordenskioeldii*, *T. gravida*, *T. antarctica*, (Hasle, 1976; von Quillfeldt, 1997; von Quillfeldt et al., 2003), the epiphytic *Attheya septentrionalis* (Poulin et al., 2011) and *Pseudo-nitzschia granii* (Lovejoy et al., 2002)) alongside the temperate to warm-water species *Detonula pumila* (Hasle, 1976) and *Thalassiosira angulata* (Krawczyk et al., 2013; Luddington et al., 2016; Weckström et al., 2014) and some cosmopolitans (*Minidiscus trioculatus* and *Cerataulina pelagica* (Hasle, 1976)). Beyond marine diatoms, sequences are also assigned to species preferring fresh to brackish water (e.g. *Skeletonema subsalsum* (Hasle and Evensen, 1975), *Nitzschia palea* and *Nitzschia* cf. *paleaceae* (Husted, 1930)). Taxonomic composition and richness changes with core depth and fits well into the framework reconstructed by other proxy data (biomarkers (Müller et al., 2012; Müller and Stein, 2014); foraminifers (Werner et al., 2011, 2013, 2016; Zamelczyk et al., 2014); dinoflagellates (Falardeau et al., 2018)).

Generally, the richness of both ASVs and unique taxonomic names is slightly higher in samples dated to the Late Weichselian in comparison to those dated to the Holocene (Fig 4). Taxonomic turnover is captured with some ASVs being predominantly abundant in Late Glacial samples (e.g. those assigned to *Thalassiosira gravida*, *Minidiscus trioculatus* and *Nitzschia* cf. *paleacea*) whereas others are mainly present in Holocene samples (e.g. *Chaetoceros* cf. *contortus* 1 SHE-2013 and *Chaetoceros* cf. *pseudobrevis* 1 SHE-2013) (Fig. 5). This turnover is also strongly reflected at the family level (Fig. 6). A general trend that can also be observed at the family level is an inverse relationship of the dominant families Thalassiosiraceae and Chaetoceraceae (Fig 6). Constrained hierarchical clustering (CONISS) followed by brokenstick analysis divided the samples into five significant assemblage zones corresponding to the Late Weichselian (including the last glacial maximum (LGM)), the deglacial (Heinrich Stadial 1, Bølling/Allerød and Younger Dryas) and the Early, Mid and Late Holocene (Fig. 5).

Zone I comprises the samples dated to the Late Weichselian and the LGM and is characterized by highest overall richness with regard to ASVs (Fig.4). The samples contain high proportions of sympagic taxa (*Thalassiosira gravida*, *T. antarctica*, *T. delicata*, *Chaetoceros socialis*, *Nitzschia* cf. *frigida*, *Porosira*) as well as oceanic taxa (*Haslea avium* and *Minidiscus trioculatus*) and freshwater taxa (*Nitzschia* cf. *paleacea*) (Fig. 5). Overall, ASVs assigned to the families Thalassiosiraceae, Bacillariaceae and Naviculaceae (Fig. 6) dominate these samples. High proportions of sympagic taxa, especially of *Nitzschia* cf. *frigida*, in samples dated to the Late Weichselian and LGM (zone I) are in accordance with previously reconstructed cold sea-surface conditions based on high proportions of the polar planktic formanifer *Neogloboquadrina pachyderma* (Zamelczyk et al., 2014), low dinocyst concentrations with a dominance of phototrophic taxa (Falardeau et al., 2018) and moderate concentrations of both, the sea-ice proxy IP_{25} and the phytoplankton biomarker brassicasterol (Müller and Stein, 2014). A heterogeneous and dynamic environment produced by winter sea-ice cover with ice-free conditions during summer probably allowed for diverse diatom communities to develop in the different habitats and over the seasons, which is reflected in the highest numbers overall of ASVs in samples dated to this time span. *Thalassiosira* and *Chaetoceros* are also abundant

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in the LGM microfossil assemblage identified further south at the Knipovich Ridge (eastern Fram Strait), although species of the genera *Rhizosolenia* and *Coscinodiscus* are strongly represented there as well (Bylinskaya et al., 2016).

CONISS assigned samples dated to the deglacial phase to zone II, despite their representation of extremely different climatic intervals. The samples thus show highly variable taxonomic composition. Heinrich Stadial 1 and Bølling/Allerød samples are characterized by high proportions of ASVs assigned to *Thalassiosira*, *T. antarctica* and *T. delicata*, and abundant *Skeletonema subsalsum*, whereas *Porosira* is not detected and proportions of *Thalassiosira gravida*, *Nitzschia* cf. *frigida*, *Haslea avium* and *Minidiscus trioculatus* are lower. The taxonomic composition of the sample dated to Heinrich Stadial 1 suggests a partial re-organization of the diatom *sed*aDNA composition, which took place either gradually or abruptly sometime between 20.5 and 15.1 cal kyr BP. Low proportions of *Nitzschia* cf. *frigida* and other cold-water and sea-ice diatoms in samples corresponding to Heinrich Stadial 1 and Bølling/Allerød correspond well to low IP_{25} and moderate brassicasterol concentrations in these samples, reflecting a reduction of the sea-ice cover (Müller and Stein, 2014). In the Bølling/Allerød sample the relatively high abundance of sequences assigned to the brackish to freshwater preferring diatom *Skeletonema subsalsum* (Hasle and Evensen, 1975) might be explained by elevated meltwater discharge from Svalbard. Low surface-water salinity was inferred previously from the dinocyst record of this core about a century earlier, possibly resulting from melting the Barents Sea ice-sheet (Falardeau et al., 2018).

The Younger Dryas sample exhibits moderate proportions of *Thalassiosira antarctica* and *T. delicata* and is marked by the presence of the sympagic diatom *Cylindrotheca closterium* and relative increases in *Porosira*, *Thalassiosira antarctica* and *Nitzschia* cf. *frigida*. Higher proportions of sympagic diatoms in this sample point towards colder conditions in comparison to the Bølling/Allerød sample and the presence of sea ice. Severe and extended sea-ice cover at the coring site are indicated by heterotrophic species in the dinocyst record (Falardeau et al., 2018), peak concentrations of IP_{25} and very low brassicasterol concentrations (Müller and Stein, 2014). A diatom microfossil record from Hinlopen Strait northwest of Spitzbergen detects first diatom occurrence during the Younger Dryas (10.8 ^{14}C kyr BP) with more than 30 % sea-ice associated species yet with a different taxonomic composition in comparison to our record (Koç et al., 2002).

Zone III encompasses the Early Holocene sample, which is marked by peak proportions of several families such as Skeletonemaceae and Bacillariaceae and considerable increases of Chaetocerotaceae combined with a strong decrease of Thalassiosiraceae and Naviculaceae pointing towards a second partial re-organization of the taxonomic composition between 12.8 and 10.1 cal kyr BP. In particular, the sample is dominated by sequences assigned to *Skeletonema*, *Thalassiosira* and *Pseudo-nitzschia granii*. *Thalassiosira angulata*, a species associated with low sea-ice concentrations (Oksman et al., 2019) and temperate water masses (Weckström et al., 2014), displays peak proportions in this sample. Lower proportions of sympagic diatoms in this sample are in accordance with the sea-ice retreat reconstructed from low IP_{25} and high brassicasterol concentrations (Müller and Stein, 2014) and high proportions of the subpolar planktic foraminifers *Turborotalita quinqueloba* in another core further northwest (Werner et al., 2016). The diatom composition recorded by *sed*aDNA is also quite different to what has been found in microfossil records from the Fram Strait and the Greenland, Iceland and Norwegian Seas, where first diatom microfossils are recorded between 13.4 and 9 cal kyr BP (Koç et al., 1993;

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Schröder-Ritzrau et al., 2001). Southwest of Svalbard, diatom-rich sediments dated to 10.1 and 9.8 cal kyr BP are attributed to the inflow of Atlantic surface water and a retreat of the Polar Front (Jessen et al., 2010; Stabell, 1986) and are composed mostly of *Coscinodiscus* spp., *Rhizosolenia* and *Paralia sulcata* (Jessen et al., 2010; Rigual-Hernández et al., 2017; Stabell, 1986). In concordance with this, sequences assigned to *Paralia* have highest proportions in the Early Holocene sample. *Coscinodiscus* is likely resolved to class level as sequences (Coscinodiscophyceae), and thus are present in our record albeit only sparsely. *Rhizosolenia* was not detected in this sample, which could be explained by poor DNA preservation or regional differences of the past diatom communities between the two coring sites.

Zone IV comprises the sample dated to the Mid Holocene, which is marked by a low diatom richness and by peak proportions of the families Chaetoceraceae and Anomoeneidaceae. It is dominated by sequences assigned to *Chaetoceros* cf. *contortus* 1SEH-2013, *Thalassiosira* and *T. antarctica*, accompanied by abundant *Porosira* and *Skeletonema*. The relatively low richness suggests a loss of diversity between the Early and Mid Holocene. The Mid-Holocene sample is characterized by a diatom composition that cannot be clearly related to sea ice, yet the low richness is supported by low diatom concentrations in a sediment core from Mohn Ridge (Koç et al., 1993) and low phytoplankton productivity (Müller et al., 2012). The near absence of *Nitzschia* cf. *frigida*, however, does not match with the reconstructed strong sea-surface cooling and sea-ice growth from lower proportions of *Turborotalita quinqueloba* (Werner et al., 2011, 2013), low concentrations of $CaCO_3$ and high concentrations of IP_{25} and ice-rafted detritus (Müller et al., 2012).

Zone V includes the samples dated to the Roman Warm Period and the Little Ice Age. Richness in this sample is on a similar level to that of the Mid-Holocene sample. It is characterized by cold-water and ice-associated taxa with peak proportions of *Porosira* accompanied by significant proportions of *Chaetoceros* cf. *contortus* 1SEH-2013, *Attheya*, *Thalassiosira antarctica*, *T. delicata* and *Chaetoceros socialis*. Richness is lowest in the youngest investigated sample which was dated to the Little Ice Age. The sample is characterized by a peak of *Chaetoceros* cf. *pseudobrevis* 1SEH-2013, *Attheya*, and the sympagic diatoms *Porosira*, *Thalassiosira nordenskioeldii* and *Nitzschia* cf. *frigida*. The Late-Holocene samples are characterized by elevated proportions of sympagic taxa in comparison to the Mid-Holocene sample which is in agreement with Neoglacial cooling (increasing IP_{25} concentrations and moderate to high concentrations of brassicasterol (Müller et al., 2012), increases in ice-rafted detritus and the dominance of polar planktic foraminifers (Werner et al., 2011)). Diatom microfossil records located southwest of Svalbard display an increase in diatom abundance since approximately 1.5 cal kyr BP (Rigual-Hernández et al., 2017; Stabell, 1986). The microfossil record of Rigual-Hernández et al. (2017) is mostly composed of *Chaetoceros* resting spores which matches the increase of Chaetocerotaceae in our *sed*aDNA data. The composition of the record published by Stabell (1986) is more similar to Rigual-Hernández et al.'s Early Holocene diatom maximum with *Coscinodiscus* spp., *Rhizosolenia* and *Paralia sulcata*. Differences between composition and diversity of our samples and the records of Rigual-Hernández et al. (2017) and Stabell (1986) suggest either regional differences or differential preservation of microfossils and *sed*aDNA between the sites.

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6 Potential of diatom sedaDNA as proxy for sea-ice distribution

The sea-ice proxy IP_{25} is produced only by a few known ice-associated diatoms: *Haslea kjellmanii* (Cleve) Simonsen, *Haslea crucigeroides* (Hustedt) Simonsen and/or *Haslea spicula* (Hickie) Lange-Bertalot, *Pleurosigma stuxbergii* var. *rhomboides* (Cleve in Cleve and Grunow) Cleve (Brown et al., 2014). We detected none of the known producers, as either the marker did not allow for this resolution due to the incompleteness of the reference database (for the species of *Haslea*) or because the DNA of these species was not preserved in sufficient quantities as these species are low in abundance (Brown et al., 2014). Nevertheless, the *sed*aDNA record generally contains a high proportion of sequences assigned to sea-ice associated and cold-water diatoms and displays an increase in pennate diatoms, which often dominate bottom ice layers (Van Leeuwe et al., 2018), with increasing IP_{25} concentrations (Fig. 6). Our data, in combination with other proxy data from this core, suggest that sequences assigned to *Nitzschia* cf. *frigida* could be a useful indicator of past sea-ice distribution in *sed*aDNA records. Samples with low concentrations of the sea-ice proxy IP_{25} exhibit less than 2 % of sequences assigned to *Nitzschia* cf. *frigida* whereas samples characterized by moderate to high concentrations of IP_{25} display highly variable proportions without a clear relationship. Recently, De Schepper et al. (2019) used *sed*aDNA metabarcoding on a core from the East Greenland Sea and identified the Mediophyceae OTU_5051 which was significantly correlated to the IP_{25} concentrations. The class Mediophyceae is the most diverse and dominant group in our dataset and contains several sea-ice associated taxa, such as, for example, *Thalassiosira antarctica*, *T. nordenskioeldii* and *Porosira glacialis*. Yet their tendency to prevail in both sea ice and open water might be responsible for the indistinct patterns observed in our record, especially in comparison to biomarker signals. This is supported by Weckström et al. (2013) who find no specific response of sea-ice diatom microfossil composition to either IP_{25} concentrations or observational sea-ice data in the Labrador Sea.

7 Conclusions

For the first time in a marine environment, our study targets high-resolution, diatom-specific sedimentary ancient DNA using a DNA metabarcoding approach. We show that diatom DNA is preserved with substantial taxonomic richness in the eastern Fram Strait over the past 30,000 years even though diatom microfossils are recorded in the Svalbard region only since the Younger Dryas. This highlights the advantage of our approach for paleoenvironmental reconstructions aiming to identify drivers of community-level taxonomic composition and diversity, especially in regions known for their irregular and poor diatom microfossil preservation, such as Fram Strait. The *rbcL_76* marker is highly diatom specific and provides highly detailed taxonomic resolution, mostly at genus and species level. The shortness of this marker is a strong advantage that leads to adequate replicability and high quality as diversity patterns do not show conspicuous signs of bias by age-associated DNA fragmentation. The *sed*aDNA record captures substantial temporal change of diatom taxonomic composition and richness with two compositional re-organizations: the first between the LGM and Heinrich Stadial 1 and the second between the Younger Dryas and the Early Holocene. Our record extends diatom compositional and diversity information back to the Late Weichselian as microfossil records in the Fram Strait are rare and extend only as far as the Younger Dryas due to poor

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preservation. Increasing proportions of pennate diatoms are associated with increased IP_{25} concentrations, sympagic diatoms are present, but with no clear pattern with regard to biomarker signals.

Supplement

Supplementary Table S1: Processed and taxonomically assigned sequencing output containing 1,398 amplicon sequence variants, their taxonomic information and their read counts for each PCR replicate.

Code/Data availability

The sequence data are deposited in the Sequence Read Archive (BioProject XXX). The rarefaction script is available at https://github.com/StefanKruse/R_Rarefaction (Kruse, 2019).

Author contributions

H.H.Z., K.R.S.L., and U.H. conceived and designed the study; H.H.Z. performed experiments and data analysis; K.S.L. sampled the core and provided laboratory equipment; S.K. wrote resampling R script; R.S., R.T., J.M. and U.H. provided the framework for the study (samples, funding); H.H.Z. wrote the paper that all co-authors commented on.

Competing interests

The authors declare that they have no conflict of interest.

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Table 1: List of samples of core MSM05/5-712-2 with corresponding age (Müller et al., 2012; Müller and Stein, 2014), covered time interval and the reconstructed paleoenvironmental conditions including references.

Depth (m)	Age (cal kyr BP)	Time interval	Paleoenvironmental conditions
0.12	0.4	Late Holocene, Little Ice Age (LIA)	Sea-ice margin (Müller et al., 2012; Werner et al., 2011)
0.3	1.6	Late Holocene, Roman Warm Period	Sea-ice margin (Müller et al., 2012; Werner et al., 2011)
0.9	5	Mid Holocene	Sea-surface cooling and sea-ice extension (Müller et al., 2012; Werner et al., 2016)
3.1	10.1	Early Holocene	Sea-ice retreat (Falardeau et al., 2018; Müller and Stein, 2014; Werner et al., 2016)
3.71	12.8	Younger Dryas (YD)	Severe and extended sea-ice cover (Falardeau et al., 2018; Müller and Stein, 2014)
5.8	14.3	Bølling/Allerød (B/A)	Sea-ice retreat (Falardeau et al., 2018; Müller and Stein, 2014)
6.68	15.1	Heinrich Stadial 1 (H1)	Sea-ice retreat (Falardeau et al., 2018; Müller and Stein, 2014)
7.27	20.5	Last Glacial Maximum (LGM)	Sea-ice cover allowing spring sea-ice algal productivity (Falardeau et al., 2018; Müller and Stein, 2014; Zamelczyk et al., 2014)
7.85	23.1	LGM	Reduced sea-ice cover allowing spring sea-ice algal and summer phytoplankton productivity (Falardeau et al., 2018; Müller and Stein, 2014; Zamelczyk et al., 2014)
8.56	25.4	LGM	Reduced sea-ice cover allowing spring sea-ice algal and summer phytoplankton productivity (Falardeau et al., 2018; Müller and Stein, 2014; Zamelczyk et al., 2014)
8.85	29.14	Late Weichselian	Significant drop from previously high sea-ice concentration (Müller and Stein, 2014; Zamelczyk et al., 2014)

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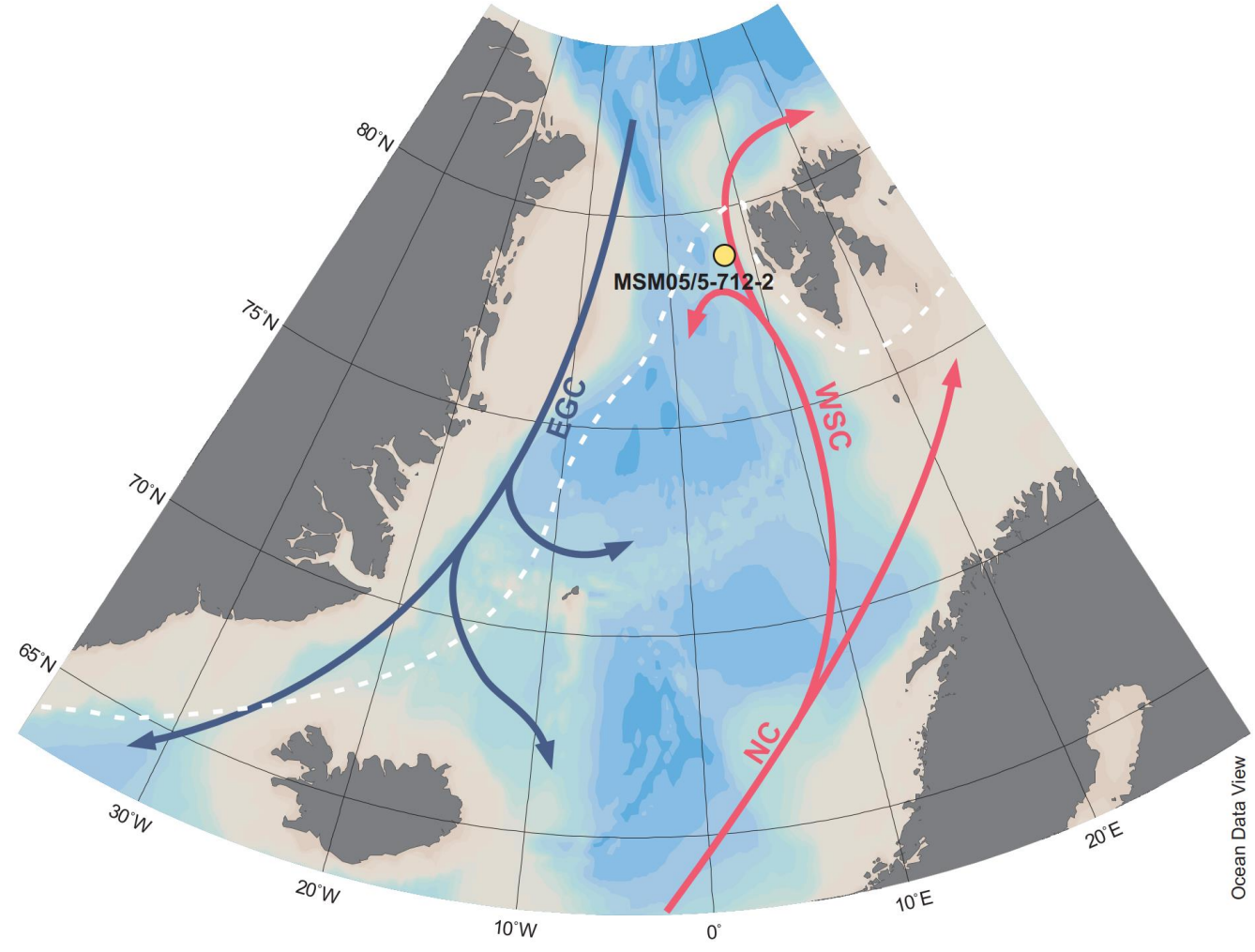

Figure 1: Map showing the coring site of MSM05/5-712-2 with bathymetric data derived from Ocean Data View (Schlitzer, 2002) and median March sea-ice extent from 1981-2010 (white, dashed line; https://nsidc.org/data/seaice_index/archives [accessed 06.08.2019] (Fetterer et al., 2017)).

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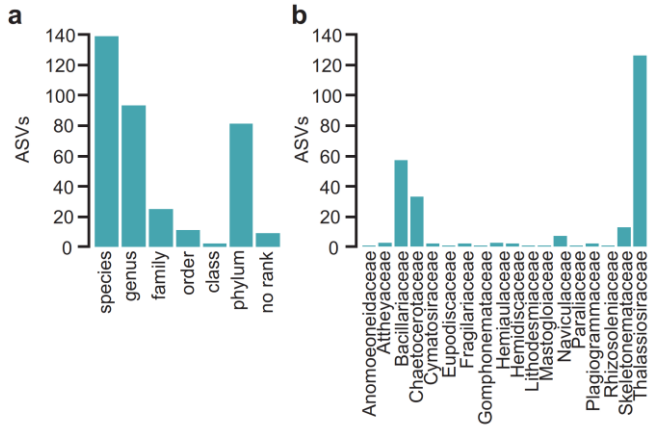

630 **Figure 2: Number of diatom amplicon sequence variants (ASVs) assigned (a) to different taxonomic levels and (b) to different families.**

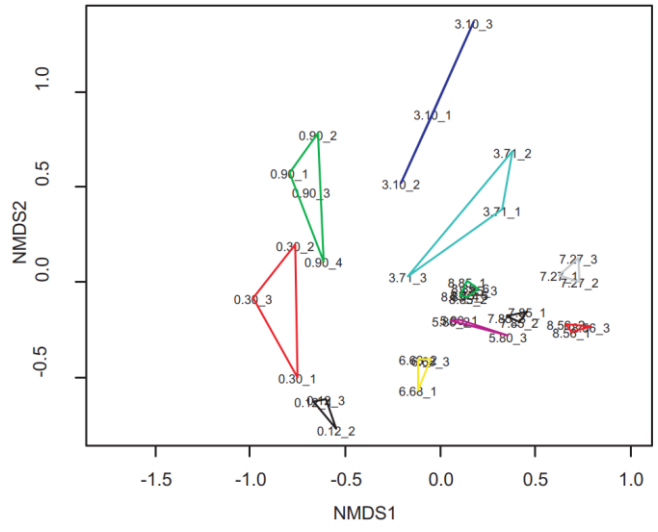

Figure 3: Non-metric multidimensional scaling plot based on the filtered and resampled diatom dataset with the replicates (indicated by an underscore with a number) of a sample (depth in m) linked in a polygon of sample-specific colour.

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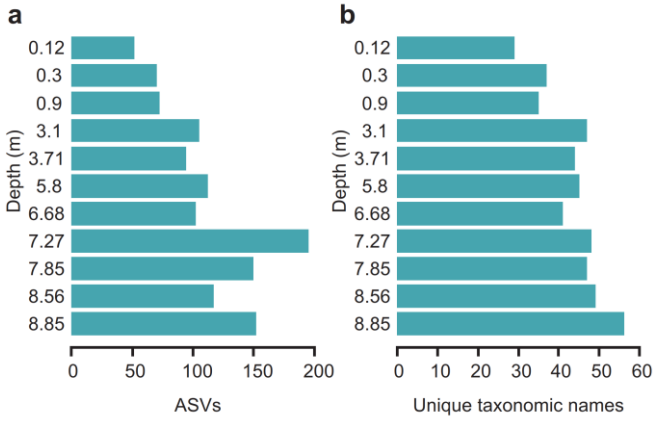

Figure 4: Barplots showing the rarefied (a) number of amplicon sequence variants (ASVs) per sample and (b) number of unique taxonomic names for each sample with depth (m) of the sediment core MSM05/5-712-2.

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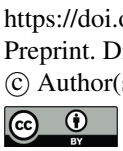

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Figure 5: Taxonomic composition with relative proportions (%) of the 360 detected sequence variants grouped into 75 unique taxonomic names of sediment core MSM05/5-712-2. Gray, dashed lines indicate zones recommended by CONISS. Taxonomic names are sorted by according to the weighted average with depth.

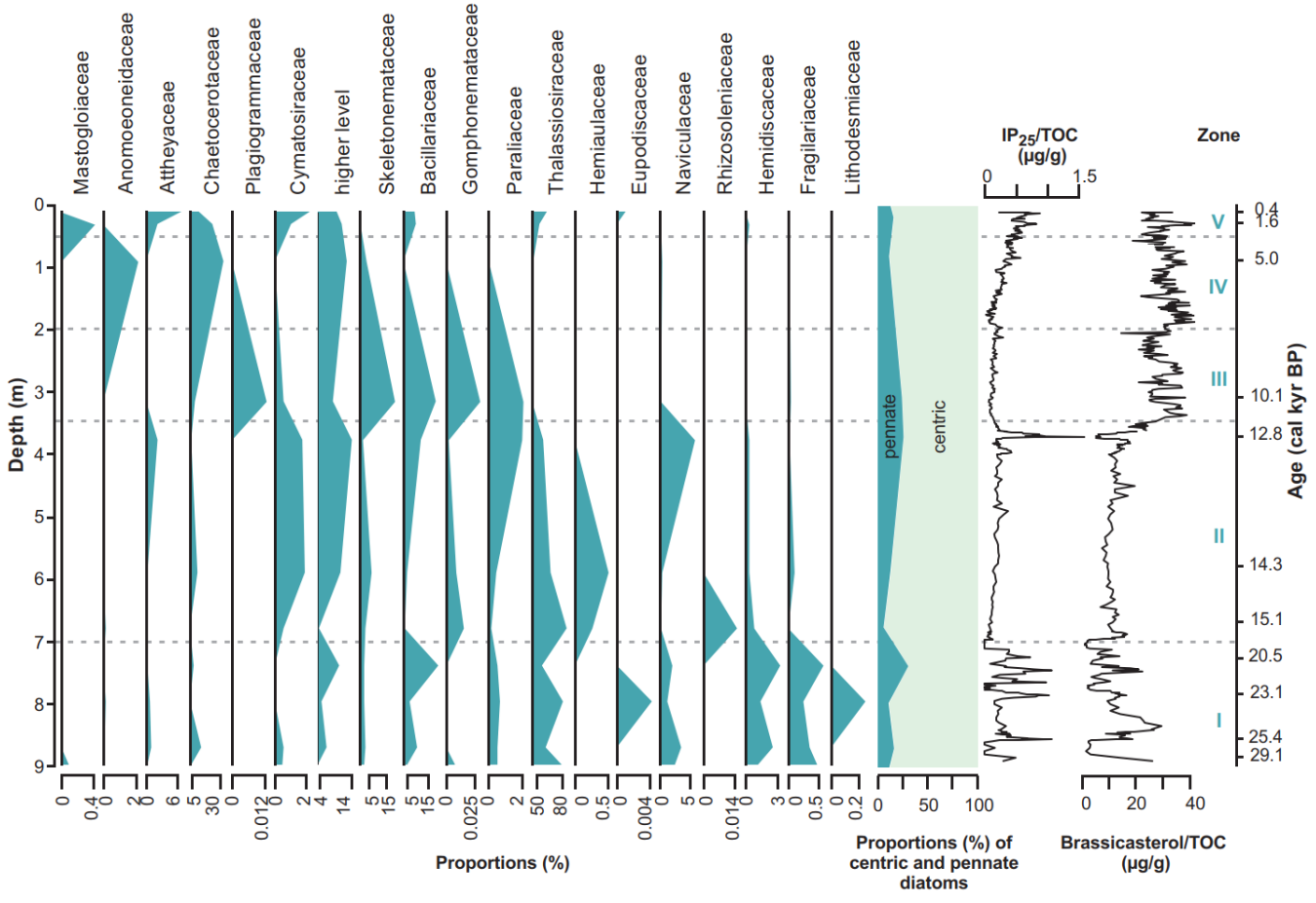

Figure 6: Proportions of sequences assigned to diatoms grouped on family level and down-core proportions of centric and pennate diatoms as well as concentrations of the sea-ice biomarker IP_{25} (Müller et al., 2012; Müller and Stein, 2014) and the phytoplankton biomarker brassicasterol (Müller et al., 2012; Müller and Stein, 2014). Horizontal gray, dashed lines indicate CONISS zone boundaries. TOC = total organic carbon.