# Supplement

Supplement S1

Table S1: Sea-ice stations >80°N where vertical profiles were obtained

| Station | Date/Time (UTC) | Latitude | Longitude | Sampling depths (m) |
|---|---|---|---|---|
| PS92/19_05 | 28/05/2015 06:28 | 81° 10.43' N | 19° 08.07' E | 0.5-10-20-30-40-50 |
| PS92/27_03 | 31/05/2015 06:52 | 81° 23.13' N | 17° 35.13' E | 0.5-10-20-30-40-50 |
| PS92/31_03 | 03/06/2015 11:44 | 81° 37.20' N | 19° 25.64' E | 0.5-10-25-30-40-50 |
| PS92/32_05 | 06/06/2015 20:04 | 81° 13.76' N | 19° 26.63' E | 0.5-10-25-30-40-50 |
| PS92/39_08 | 11/06/2015 15:05 | 81° 55.04' N | 13° 27.55' E | 0.5-10-30-35-40-50 |
| PS92/43_05 | 15/06/2015 04:45 | 82° 12.67' N | 07° 35.30' E | 0.5-10-20-30-40-50 |
| PS92/46_02 | 15/06/2015 04:45 | 82° 12.67' N | 07° 35.30' E | 0.5-10-20-30-40-50 |
| PS92/47_04 | 19/06/2015 12:03 | 81° 20.80' N | 13° 36.56' E | 0.5-10-20-30-40-50 |

Supplement S2

Biological measurements

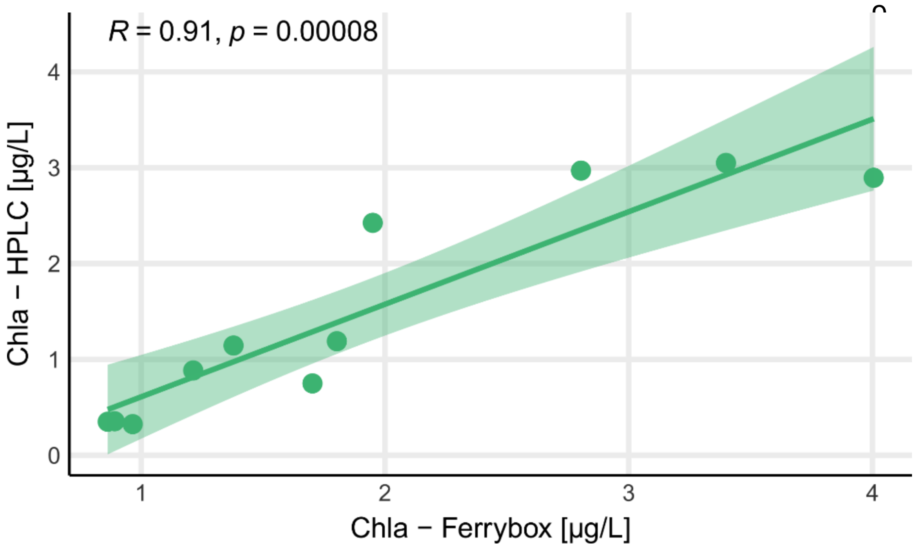


Figure S1: Relationship between chlorophyll a concentrations obtained from HPLC and Ferrybox.

Bacterial community analyses

16S rRNA gene amplicon libraries were prepared according to the standard instructions of the 16S Metagenomic Sequencing Library Preparation protocol (Illumina, San Diego, CA). The hypervariable V4–V5 region was amplified using primers 515F (GTGYCAGCMGCCGCGGTAA) and 926R (CCGYCAATTYMTTTRAGTTT). Sequences were obtained on an Illumina MiSeq platform in 2x300 bp paired-end runs at CeBiTec (Bielefeld, Germany). Primer were clipped using cutadapt, and reads processed into amplicon sequence variants (ASVs) following the standard DADA2 workflow at https://benjjneb.github.io/dada2/tutorial.html. Filtering settings were truncLen=c(230,195), maxN=0, minQ=2, maxEE=c(3,3) and truncQ=0, followed by merging using minOverlap=10, chimera removal and taxonomic classificaton using the Silva v138 database. Data was processed in RStudio using R v4.1.1 and packages phyloseq, vegan, iNEXT, tidyverse, psych and scico, with aesthetic modifications of figures using Inkscape (https://inkscape.org). We obtained on average 85,000 quality-controlled, chimera-filtered reads per sample (Table S2) sufficiently covering community composition (Fig. S2). The complete amplicon workflow is available under https://github.com/matthiaswietz/transsiz.

Table S2: Amplicon-sequenced samples, showing read counts at each step of the DADA2 pipeline.

| sample_title | Date | Lat | Lon | input | filtered | denoised | merged | nochim | tabled |
|---|---|---|---|---|---|---|---|---|---|
| PS92 Auto2 | 2015-05-21 | 60.35920 | 3.29927 | 118097 | 98967 | 98357 | 82764 | 82764 | 80333 |
| PS92 Auto3 | 2015-05-21 | 62.38333 | 3.35833 | 92223 | 78393 | 78082 | 70022 | 70022 | 67872 |
| PS92 Auto4 | 2015-05-22 | 64.52022 | 3.55040 | 131377 | 110858 | 110483 | 93018 | 93018 | 90123 |
| PS92 Auto5 | 2015-05-22 | 64.94027 | 3.58943 | 129259 | 109748 | 109459 | 104074 | 104074 | 98374 |
| PS92 Auto6 | 2015-05-22 | 65.90325 | 3.64348 | 159876 | 139180 | 138735 | 126581 | 126581 | 122124 |
| PS92 Auto7 | 2015-05-22 | 66.35847 | 3.72702 | 94039 | 79638 | 79452 | 66107 | 66107 | 64204 |
| PS92 Auto8 | 2015-05-22 | 66.76948 | 3.76842 | 147626 | 123900 | 123608 | 98729 | 98729 | 94205 |
| PS92 Auto9 | 2015-05-23 | 67.31610 | 3.82471 | 88694 | 75721 | 75541 | 64079 | 64079 | 61492 |
| PS92 Auto10 | 2015-05-23 | 67.89882 | 3.88550 | 103359 | 83813 | 83655 | 69791 | 69791 | 66430 |
| PS92 Auto11 | 2015-05-23 | 68.33135 | 3.91565 | 85213 | 72459 | 72343 | 59608 | 59608 | 57793 |
| PS92 Auto12 | 2015-05-23 | 68.68500 | 3.97063 | 130307 | 108826 | 108595 | 95159 | 95159 | 91516 |
| PS92 Auto13 | 2015-05-23 | 69.28850 | 4.01345 | 80729 | 67543 | 67404 | 55925 | 55925 | 54072 |
| PS92 Auto14 | 2015-05-23 | 69.49642 | 4.01595 | 121385 | 104120 | 103898 | 93522 | 93522 | 89969 |
| PS92 Auto15 | 2015-05-24 | 70.00000 | 10.00000 | 102120 | 86176 | 85987 | 77672 | 77672 | 74763 |
| PS92 Auto16 | 2015-05-24 | 70.22695 | 13.14900 | 114758 | 98526 | 98230 | 87839 | 87839 | 83624 |
| PS92 Auto17 | 2015-05-25 | 73.25000 | 12.25000 | 128590 | 108477 | 108250 | 91623 | 91623 | 88079 |
| PS92 Auto18 | 2015-05-25 | 74.13037 | 11.69167 | 138591 | 116132 | 115847 | 104990 | 104990 | 100890 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PS92 Auto19 | 2015-05-25 | 74.84322 | 11.20822 | 108687 | 91919 | 91697 | 87735 | 87735 | 82825 |
| PS92 Auto20 | 2015-05-26 | 75.51768 | 10.72912 | 179367 | 152923 | 152479 | 146291 | 146291 | 137753 |
| PS92 Auto21 | 2015-05-26 | 76.76033 | 9.78639 | 137058 | 115973 | 115657 | 109506 | 109506 | 104299 |
| PS92 Auto22 | 2015-05-26 | 77.27977 | 9.35135 | 164814 | 141216 | 140814 | 129011 | 129011 | 124403 |
| PS92 Auto23 | 2015-05-27 | 80.87068 | 18.44780 | 123060 | 102837 | 102585 | 96182 | 96182 | 91236 |
| PS92 Auto24 | 2015-05-27 | 81.01718 | 19.84131 | 111661 | 93595 | 93043 | 84908 | 84908 | 79382 |
| PS92 Auto25 | 2015-05-28 | 81.17000 | 19.13450 | 133543 | 112984 | 112116 | 103696 | 103696 | 97757 |
| PS92 Auto26 | 2015-05-28 | 81.19041 | 19.09177 | 143276 | 122930 | 122362 | 107995 | 107995 | 102390 |
| PS92 Auto27 | 2015-05-29 | 81.20624 | 18.69745 | 87506 | 74860 | 74472 | 61118 | 61118 | 58023 |
| PS92 Auto28 | 2015-05-29 | 81.22513 | 18.58100 | 158441 | 138134 | 137782 | 129089 | 129089 | 121849 |
| PS92 Auto31 | 2015-05-30 | 81.23292 | 18.76116 | 107153 | 91266 | 91018 | 81765 | 81765 | 77238 |
| PS92 Auto33 | 2015-06-01 | 81.32160 | 17.30839 | 146149 | 124768 | 124324 | 111819 | 111819 | 107371 |
| PS92 Auto34 | 2015-06-02 | 81.52571 | 19.44756 | 122832 | 105891 | 105552 | 95344 | 95344 | 89608 |
| PS92 Auto35 | 2015-06-03 | 81.55412 | 19.51593 | 89976 | 73560 | 73331 | 57493 | 57493 | 55347 |
| PS92 Auto36 | 2015-06-04 | 81.52757 | 18.65566 | 81157 | 68831 | 68620 | 62260 | 62260 | 58519 |
| PS92 Auto38 | 2015-06-11 | 81.90915 | 13.40468 | 72012 | 59645 | 59380 | 49796 | 49796 | 48994 |
| PS92 Auto39 | 2015-06-15 | 82.20975 | 7.38825 | 97048 | 82690 | 82426 | 70980 | 70980 | 69627 |

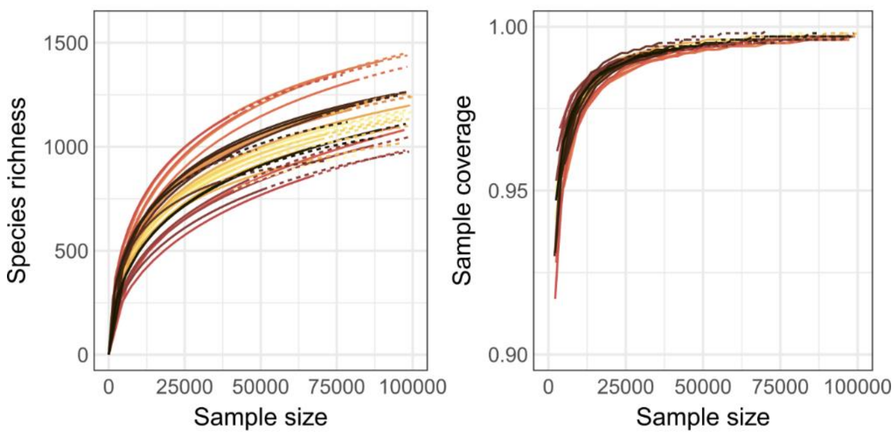


Figure S2: Rarefaction and coverage analyses of amplicon sequence variants, showing that community composition was sufficiently covered. Each coloured line corresponds to an individual sample.

Supplement S3: Extraction system

Dissolved gases in seawater were quantified in the headspace of a glass cell, where gases were extracted by stripping with zero air at a flow rate of 100 mL/min. Three mini-water liquid diaphragm pumps KNF (type FEM 1.02.KT.18S. KNF (KNF Neuberger, IncTrenton, New Jersey USA), were used for the injection and circulation of seawater in the cell at 20 mL/min.  Before entering the extraction cell, the water went through a mixing cell which was used for injection of a calibrated solution. For calibration, secondary standard liquid solutions were injected at a flow rate of 250 µL/min by mean of a fine metering pump (World Precision Instruments; Hitchin, Hertfordshire, UK), and diluted in an identical flow of 20 mL/min of pure distilled water. Figure S3 shows a schematic view of the extraction device.

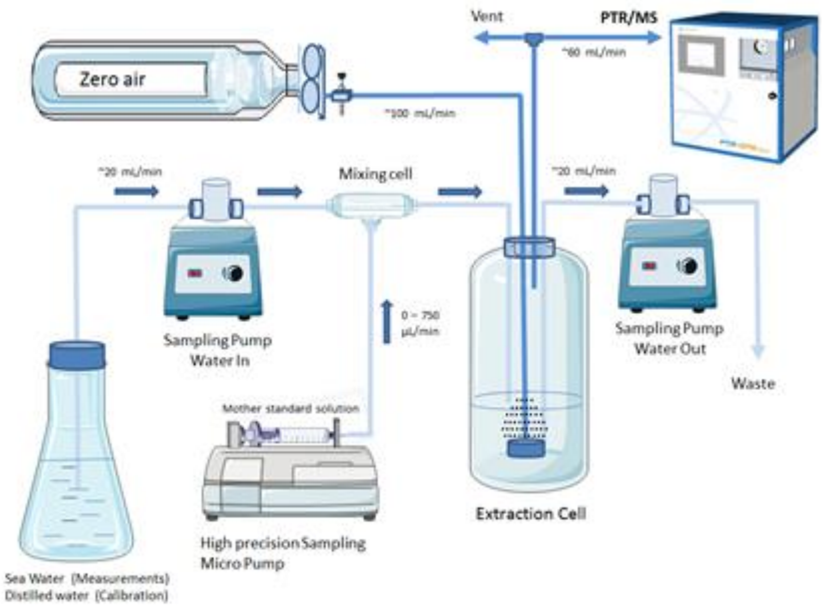


Figure S3: Schematic view of the extraction system

## Supplement S4: Calibration procedure

For the calibration, stock solutions were prepared from pure substances (Sigma Aldrich) diluted in distilled water: isoprene (1.0 x$10^{-4}$ M), dimethylsulphide (2.7 x $10^{-3}$ M), acetaldehyde (8.95 x $10^{-3}$ M), acetone (2.73 x $10^{-2}$ M), acetonitrile (7.67 x $10^{-3}$ M), and methanol (1.24 x $10^{-1}$ M), all stored at 4°C. Secondary standard liquid solutions were prepared immediately before the calibrations from a dilution of 2 x$10^{-4}$ (0.2 mL/L) in distilled water. The injection of liquid standard was achieved by dilution of stock solution in distilled water by a high precision micro pump. The calibration factor was expressed as the ratio of the concentration of a given VOC in the water (nmol/L or pmol/L) to the concentration in the head space (ppbv) measured by PTR/MS. An example is given for the calibration for acetone (Fig. S4), with excellent linearity between the PPB measured in the headspace by PTRMS and the concentration in water. Experimentally this calibration factor is very close to the Henry's law constant (expressed in mol/L per atmosphere) whatever the solubility of the compound over 4 to 5 orders of magnitude (Fig. S5). Therefore, knowing the Henry's law constant, measurements can be reasonably extrapolated to new compounds detected in water which have not been previously calibrated (such as methanethiol).

Concerning the gas-phase calibration, a complete calibration had been done one month before the campaign in the laboratory using a calibration unit (Ionicon Analytik) and by injecting different amounts of a calibration gas mixture from Ionicon, allowing to derive sensitivity ncps/ppb for all compounds contained in the standard (methanol, acetaldehyde, acetonitrile, acetone and isoprene for the compounds of interest for this study). On the same day, a gas cylinder has been measured and brought on-board in order to check the stability of the detection (at the beginning and in the middle of the campaign). As lab- and ship-based results (in ncps) were congruent, the lab-determined calibration coefficients were used for the campaign.  As DMS was not included in the standard, the calibration was done directly on water measurements by using the relation between ncps and concentration in the water of the injected standard.

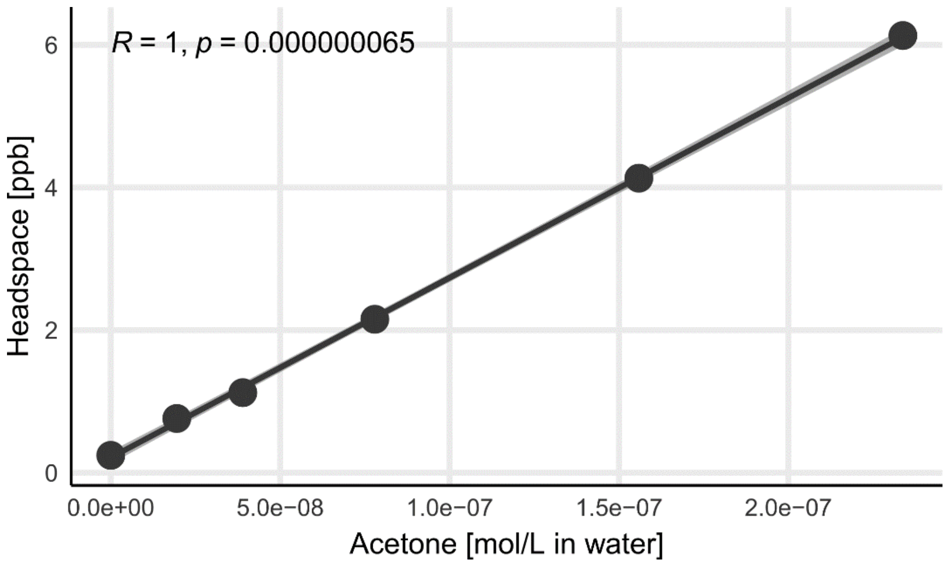


Figure S4: Calibration of acetone performed on-board

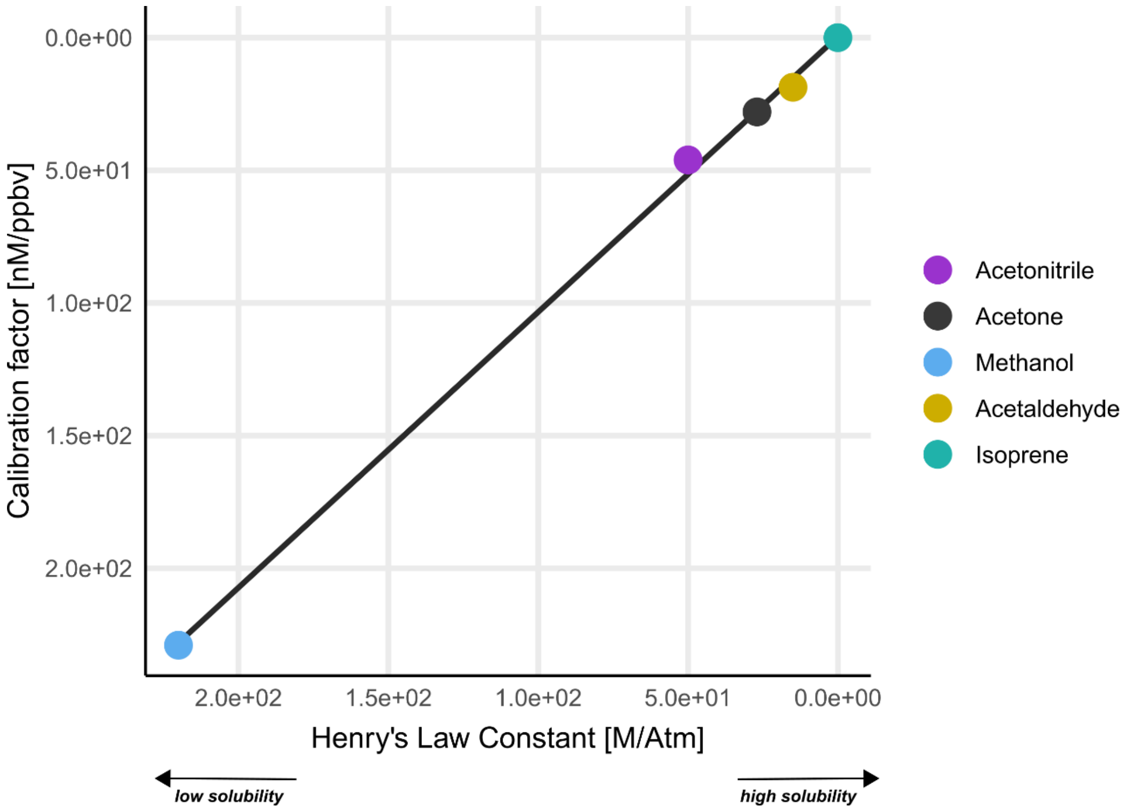


Figure S5: Calibration factor against Henry's law constant

Supplement S5: Water masses during the transect

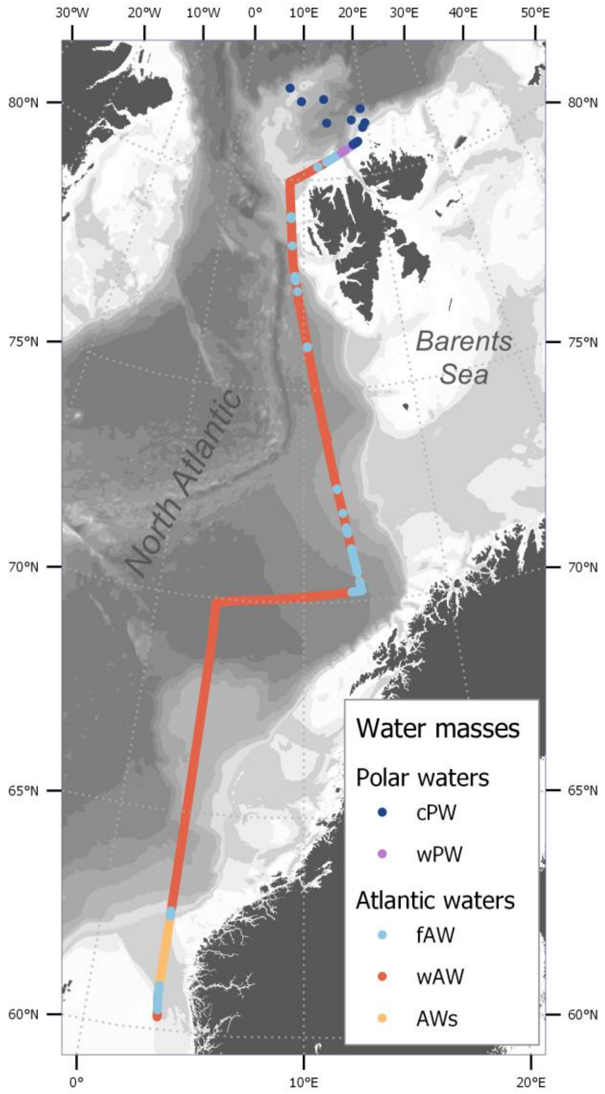


Figure S6: The sampled transect and sea-ice stations colour-coded by water mass: coastal influenced Atlantic water with low salinity (AWs), 'regular' warm Atlantic Water (wAW), fresh Atlantic Water (fAW), cold Polar Water (cPW) and warm Polar Water (wPW), see temperature and salinity criteria in Table 1.

Supplement S6: Vertical profiles of selected phytoplankton groups

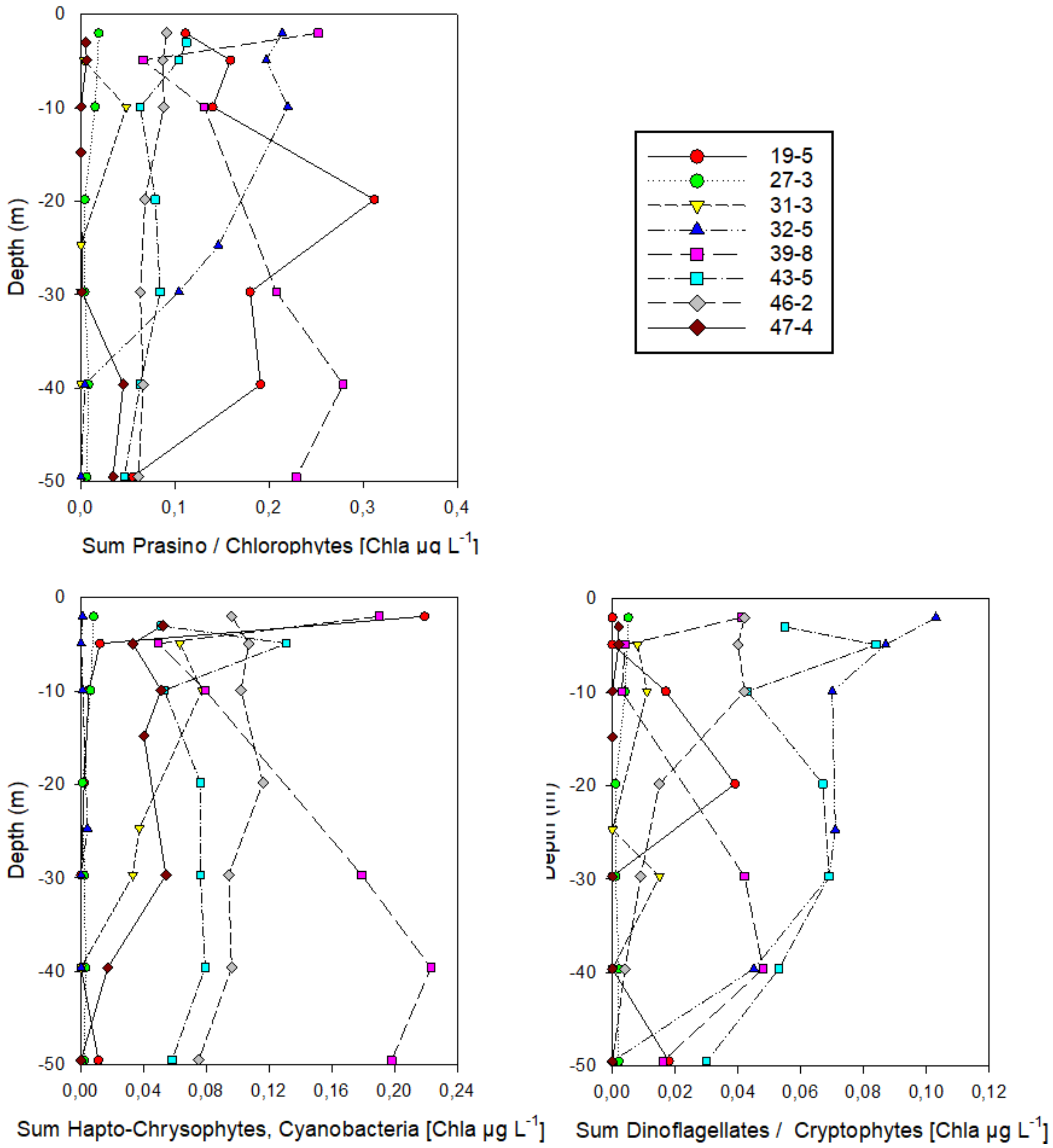


Figure S7: Depth profiles of selected phytoplankton groups, summarizing various types. Colors indicate stations.

Supplement S7 :Correlation between selected trace gases and Chl a

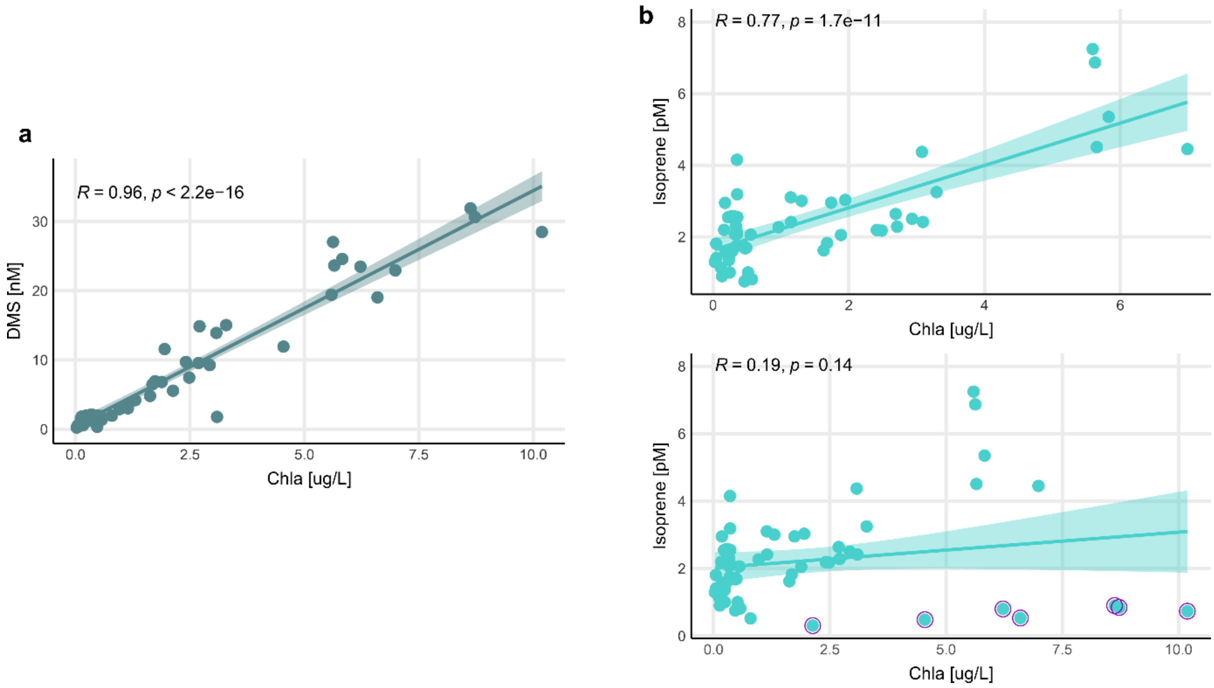


Figure S8: Correlations of DMS (a) and isoprene (b) with Chl a at sea-ice stations >80°N. Correlations with isoprene were only significant when excluding station 19 (upper panel; see explanation in the main text). The lower panel includes all data points >80°N. Data from station 19 are indicated by a purple circle.

## <u>Supplementary references</u>


- Callahan et al. DADA2: High-resolution sample inference from Illumina amplicon data. Nature Methods 13:581-583.
- Hsieh et al. (2019). iNEXT: an R package for rarefaction and extrapolation of species diversity (Hill numbers). Methods in Ecology and Evolution 7:1451-1456.
- Crameri (2018). Scientific colour maps (Version 3.0.1). doi: 10.5281/zenodo.1243909
- Crameri (2018). Geodynamic diagnostics, scientific visualisation and StagLab 3.0. Geosci. Model Dev. Discuss. doi: 10.5194/gmd-2017-328
- McMurdie and Holmes (2013). phyloseq: An R Package for Reproducible Interactive Analysis and Graphics of Microbiome Census Data. PLoS ONE 8:e61217.
- Oksanen et al. (2020). vegan: community ecology package; R package version 2.5-7; https://CRAN.R-project.org/package=vegan
- Revelle et al. (2021). psych: Procedures for Psychological, Psychometric, and Personality Research. R package version 2.1.9; https://CRAN.R-project.org/package=psych
- Wickham et al., (2019). Welcome to the Tidyverse. Journal of Open Source Software, 4:1686.