Phytoplankton pigments, group composition and absorption coefficients:
The following diagnostic pigments were used to identify seven phytoplankton groups:
fucocaroten (Fuco), peridinin (Peri), alloxanthin (Allo), 19´-hexanoyloxyfucoxanthin (19HF),
19´-butanoyloxyfucoxanthin (19BF), zeaxanthin (Zea), and total chlorophyll-b (TChl-b, i.e. the
sum of monovinylchl-b, chl-b, and divinylchl-b (div-b)). According to Hirata et al. (2011) the
weighted relationships of these diagnostic pigments (DPw) were calculated by multiple
regression analysis as follows:

\[
\begin{align*}
\% \text{ pico (<2 µm)} &= 100 \times (0.86 \, \text{Zea})/\text{DPw} \\
\% \text{ nano (2 -20 µm)} &= 100 \times (1.27 \, 19HF +1.01 \, \text{TChl-b} +0.35 \, 19BF +0.6 \, \text{Allo})/\text{DPw} \\
\% \text{ micro (>20 µm)} &= 100 \times (1.41 \, \text{Fuco} +1.41 \, \text{Peri})/\text{DPw} \\
\% \text{ diatoms} &= 100 \times (1.41 \, \text{Fuco})/\text{DPw} \\
\% \text{ dinoflagellates} &= 100 \times (1.41 \, \text{Peri})/\text{DPw} \\
\% \text{ haptophytes} &= 100 \times (1.2719HF)/\text{DPw} \\
\% \text{ chrysophytes} &= 100 \times (0.3519BF)/\text{DPw} \\
\% \text{ cryptophytes} &= 100 \times (0.6 \, \text{Allo})/\text{DPw} \\
\% \text{ chlorophytes} &= 100 \times (1.01 \, \text{TChl-b})/\text{DPw} \\
\% \text{ all cyanobacteria} &= 100 \times (0.86 \, \text{Zea})/\text{DPw}
\end{align*}
\]

where,

\[
\text{DPw} = 0.86 \, \text{Zea} +1.01 \, \text{TChl-b} +1.27 \, 19HF +0.35 \, 19BF +0.6 \, \text{Allo} +1.41 \, \text{Fuco} +1.41 \, \text{Peri}.
\]

By multiplying the total chl-a concentration (TChl-a) (i.e. the sum of monovinylchl-a, chl-a, and
divinylchl-a, div-a) with %-values for each group, the chl-a concentration for each group was
derived. In addition, TChl-a concentration of prochlorophytes, a subgroup of cyanobacteria
which is characterized by very low size (~0.5 µm), and the pigments of div-a and div-b, was
calculated from div-a/(div-a+chl-a). The chl-a concentration of all other cyanobacteria was
calculated by subtracting prochlorophytes chl-a from all cyanobacteria chl-a concentration.
Identifying phytoplankton assemblages with hierarchical cluster analysis:
The HCA clustering based on the hyperspectral phytoplankton absorption coefficients provided a
cluster tree in which the input data set was partitioned into subsets or clusters with no previous
information regarding membership of input data objects to predefined classes. Each cluster tree
was obtained based on a selected linkage algorithm that considers a previously calculated
similarity distance between all samples included in the input data set. Because we focus in this
study on spectral signatures related to the specific pigment composition, when computing the
similarity between pairs of phytoplankton absorption spectra, an angular distance was utilized.
This type of distance reflects better the differences in the spectral shape of optical data. The
cluster partition obtained based on the pigment data served as a reference for partitioning the
entire data set into distinct groups - clusters, each characterized by a different phytoplankton
pigment composition (shown in Fig. 1 in the supplemental material). To minimize variability in
pigment composition associated with changes in phytoplankton biomass, the input to the cluster
analysis was represented by the ratio of individual pigment concentrations to the surface TChl-a.
In that sense, the information regarding the dominance of pigments for each station can be better
assessed. Otherwise, the analysis would be mainly driven by the amount of total pigments
concentration. In addition, a Euclidean distance was utilized to generate the pigment-based
cluster partition in order to indicate differences in magnitude of ratios of concentrations of
individual pigments to TChl-a rather than differences in shape.
The feasibility of using hyperspectral phytoplankton absorption data for identifying
phytoplankton assemblages (see clustering in Fig. 2 in the supplemental material) was tested by
comparison of the clustering based on the pigment data using the cophenetic index (see more
details in Torrecilla et al., 2011). This index is an objective criterion of cluster similarity ranging
from 0 (for no similarity) to 1 (for maximum similarity).

Statistical analysis:
Multiple linear regression models (MLRM) computed with RStudio™ were used. The terms were
added and removed from a MLRM based on their statistical significance. At each step an F-test
was performed to test the regressions with and without certain terms. A term was added to the
model if it contributed significantly at the 95%-confidence level or removed from the model if it
did not contribute at the 95%-confidence level. To identify the simplest MLRM with the best
explanatory power, each model was compared with the previous one using Analysis of Variances (ANOVA) to test if the latest and simpler model showed no significant differences to the former model. The influence of the interaction of two or more parameters on the sulphur compound concentrations was additionally tested with the same procedure as described above.

Different diagnostic tests were performed to determine if the assumptions made to perform the regression model calculations were valid. All response variables were tested for normal distribution with the Shapiro-Wilk normality test or the Anderson-Darling test (for more than 100 data points) and got transformed if necessary. A tree model was used to obtain an overview of the interactions between the predictor variables prior the calculation of the MLRM. After each calculation, the model was tested for multicollinearity by computing the variance inflation factor (VIF). The heteroscedascity of the models as well as the normal distribution of the residuals were examined graphically. A Durbin-Watson Test was used to find auto-correlations in the residuals. Data points that had a strong influence on the models were identified graphically with the Cook’s distance. The model was compared with the next to last simplest model using the Akaike’s Information Criterion to check if the simplest model with the best prediction was selected. The entire outputs for all MLRM are given in Table I between the different sulphur compounds and in Table II between sulphur compounds and phytoplankton marker pigments.

Table I: Significant multiple linear regressions between DMS, DMSP and DMSO (d=dissolved, p=particulate, t=total) for the whole data set and within the cluster 2 and 4. Single coefficients, estimates, standard Errors, t and p values of the different independent variables in each multiple linear regression model as well as $R^2$, F-statistic and p-value of each whole model are given. Under model number is the response variable given. Variable square showed quadratic relationship to response variable. The complete output of all models is given in the supplements.
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<th>model no.</th>
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<th>Estimate</th>
<th>Std. Error</th>
<th>t value</th>
<th>p-value (e.m.)</th>
<th>R², F-st., p-value (e.m.)</th>
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<td>-3.08</td>
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| b        | Intercept           | -0.54    | 0.40       | 1.34    | 0.19           | 0.48                     |
|          | Cluster 2           |          |            |         |                |                          |
|          | DMS                 | 0.10     | 0.05       | 2.00    | 0.005          | 6.01                     |
|          | DMSod               | 0.31     | 0.13       | 2.42    | 0.002          | 5.27E-05                 |
|          | DMSOp               | 0.02     | 0.005      | 3.34    | 0.002          |                          |
|          | DMSPp               | 0.54     | 0.29       | 1.85    | 0.07           |                          |
|          | DMSPP^2             | -0.02    | 0.01       | -1.82   | 0.08           |                          |
|          | DMSPP^3             | -0.18    | 0.10       | -1.78   | 0.08           |                          |
|          | DMSPP,DMSOD,DMSOp  | -0.04    | 0.01       | -3.08   | 0.004          |                          |
|          | DMSPP,DMSOD,DMSOp  | -0.04    | 0.01       | -3.08   | 0.004          |                          |

| c        | Intercept           | -0.60    | 0.78       | -0.78   | 0.45           | 0.58                     |
|          | Cluster 4           |          |            |         |                |                          |
|          | DMS                 | -0.56    | 0.16       | -3.53   | 0.002          | 5.62                     |
|          | DMSOD               | 0.73     | 0.37       | 1.99    | 0.06           | 0.002                    |
|          | DMSPP^2             | -0.14    | 0.24       | -4.34   | 0.0003         |                          |
|          | DMSPP,DMSOD,DMSOp  | 0.08     | 0.19       | 3.63    | 0.002          |                          |

| d        | Intercept           | 0.027    | 0.08       | 0.32    | 0.075          | 0.32                     |
|          | DMSPP^2             | 0.002    | 0.0003     | 5.71    | 1.14E-07       | 0.062                    |
|          | DMSPP,DMSOD,DMSOp  | 0.01     | 0.003      | 2.32    | 0.02           | 1.084E-08                |

| e        | Intercept           | 0.65     | 0.18       | 3.53    | 0.98E-04       | 0.47                     |
|          | Cluster 2           |          |            |         |                |                          |
|          | DMSPP^2             | 0.23     | 0.08       | 2.99    | 0.005          | 5.01                     |
|          | DMSPP,DMSOD,DMSOp  | 0.06     | 0.02       | 2.55    | 0.014          | 1.77E-04                 |
|          | DMSPP,DMSOD,DMSOP  | -0.04    | 0.01       | -3.12   | 0.003          |                          |
|          | DMSPP,DMSOD,DMSOP  | -0.04    | 0.01       | -3.12   | 0.003          |                          |

| f        | Intercept           | -7.51    | 2.3        | -3.26   | 0.004          | 0.52                     |
|          | DMSPP^2             | 4.5      | 1.77       | 2.55    | 0.019          | 3.54                     |
|          | DMSPP,DMSOD,DMSOP  | 3.39     | 0.98       | 3.46    | 0.002          | 0.015                    |
|          | DMSPP,DMSOD,DMSOP  | -0.24    | 0.11       | -2.25   | 0.04           |                          |
|          | DMSPP,DMSOD,DMSOP  | 0.4      | 0.09       | 4.48    | 2.3E-04        |                          |
|          | DMSPP,DMSOD,DMSOP  | -1.28    | 0.43       | -2.94   | 0.008          |                          |

| g        | Intercept           | 1.49     | 0.21       | 7.11    | 3.92E-10       | 0.4                      |
|          | DMSPP^2             | -1.19    | 0.05       | -2.35   | 0.02           | 7.92                     |
|          | DMSPP,DMSOD,DMSOp  | 0.02     | 0.01       | 4.57    | 1.73E-05       | 2.57E-07                 |
|          | DMSPP,DMSOD,DMSOp  | 0.53     | 0.30       | 1.79    | 0.08           |                          |

| h        | Intercept           | 1.82     | 0.31       | 5.94    | 2.7E-09        | 0.38                     |

| i        | Intercept           | 2.93     | 0.42       | 6.91    | 4.28E-10       | 0.19                     |
|          | DMSPP^2             | 0.72     | 0.36       | 2.04    | 0.04           | 8.05                     |

| j        | Intercept           | 2.66     | 0.82       | 3.24    | 0.002          | 0.28                     |

| k        | Intercept           | 6.31     | 0.63       | 10.05   | 1.91E-10       | 0.35                     |

| l        | Intercept           | 1.57     | 0.10       | 16.34   | 2.00E-16       | 0.43                     |

| m        | Intercept           | 1.29     | 0.24       | 5.01    | 0.614          | 0.56                     |

| n        | Intercept           | 0.40     | 0.23       | 0.18    | 0.86           | 0.46                     |

**Abbr.:** st.: statistic; e. m.: entire model; e. d. s.: entire data set; a – n: number of models
Tabel II: Significant multiple linear regressions between DMS, DMSP and DMSO (d=dissolved, p=particulate, t=total) and phytoplankton marker pigments for the whole data set and within the cluster 2 and 4. Single coefficients, estimates, standard errors, t values and p values of the different independent variables in each multiple linear regression model as well as $R^2$, F-statistic and p-value of each whole model are given. Under model number is the response variable given. Variable square showed quadratic relationship to response variable.

<table>
<thead>
<tr>
<th>model no.</th>
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<th>Estimate</th>
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<th>t value</th>
<th>p-value</th>
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Abbr.: st.: statistic; e. m.: entire model; e. d. s.: entire data set; a – n: number of models, fuco: fucoxanthin, hex: 19'-hexanoyloxyfucoxanthin, pero: peridinin, diato: diatoxanthin, dia: diadinoxanthin, diato: diatoxanthin, but: 19'-butanoyloxyfucoxanthin, zeax: zeaxanthin, ant: anthraeoxanthin, viol: violaxanthin
Figure 1: HCA cluster tree based on pigment data obtained during TransBrom Sonne (stations are labeled with consecutive numbers increasing with latitude). Different clusters are identified with different colors: cluster 1 (yellow), cluster 2 (green), cluster 3 (blue) and cluster 4 (red). It is noted that clusters 2, 3 and 4 have as dominant pigments Chla, Zea and Diva. Nevertheless, for cluster 4 Zea contributes the largest, for cluster 3 Chla and for cluster 2 all pigments equally.
Figure 2: HCA cluster tree based on hyperspectral phytoplankton absorption coefficients measured at different stations during TransBrom Sonne. Stations are labeled with consecutive numbers increasing with latitude and identified with different colors in accordance with the pigment-based clusters shown in Fig. 1.