

Biochemical remodelling of phytoplankton cell composition under climate change

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Supplementary Methods

Dataset

We compiled a dataset of in situ measurements of proteins, carbohydrates, and lipids in particulate organic matter or living phytoplankton, from several sources; we used photic zone measurements from 38 studies, which sampled at different locations between 1978 and 2018. Data was extracted from tables or images using WebPlotDigitizer (<https://automeris.io/WebPlotDigitizer/>).

For model-data comparison, we formed dimensionless ratios Protein–C:C, Carb–C:C, and Lipid–C:C, from the bulk macromolecular measurements (mostly reported as $\mu\text{g L}^{-1}$) and the average stoichiometric composition of these macromolecules¹⁰⁸, by dividing each macromolecule by the sum of proteins, carbohydrates, and lipids. If all major macromolecules were not available but particulate organic carbon (POC) was reported, values were normalized to the sum of POC.

Another data source is field samples of protein, RNA, and DNA collected from 7 research cruises conducted by the Bedford Institute of Oceanography, Canada, starting in September 1978 and ending in July 1981 (Table S1)^{45–48,100–102}. Samples were taken from different locations with Niskin bottles, filtered (membrane or glass fiber filters depending on station), stored at -20°C , and analyzed fluorometrically to quantify RNA, DNA, and proteins. The methodology remained largely consistent across these 12 reports. In order to match these values with our study, we converted the measurements to Protein–C:C, RNA–C:C, and DNA–C:C, and estimated Carb–C:C and Lipid–C:C using the relationship:

$$\text{Carb–C:C} + \text{Lipid–C:C} = 1 - [\text{Protein–C:C} + \text{RNA–C:C} + \text{DNA–C:C}].$$

We excluded outliers that were outside of ± 2 std of the mean ($n_{\text{outliers}}=10$), and defined the Arctic as all regions north of 66°N . After the removal of outliers, there were 298 observations of Protein–C:C, and Carb–C:C plus Lipid–C:C from the Bedford Institute of Oceanography.

Data distributions, data sources, and further information on sampling date and geographic locations are summarised in Table S1.

Statistical analyses

To examine macromolecular changes over time, we applied linear regressions of the macromolecules vs. time in the Arctic and the Antarctic (Figure 3c–f, Extended Data Fig. 8). These regressions were obtained by the following procedure: Carb–C and Lipid–C were summed. After $\log_{10}$ transforming the

ratios, we removed the outliers (values that were farther than 1.5 times the interquartile range from the median). We did this on log scale, as the data were non-negative and right skewed. We fitted linear regression to the data and recorded the p-value and R^2 . For linear regression data obtained only with colorimetric methods, see Table S5. For data obtained with isotope labelling and colorimetric methods, see Table S6.

Comparison of modeled macromolecular allocation with observations

Most of the data in the compiled data is from polar regions, the Japan Sea, or other restricted basins or coastal environments (Table S1). This challenges a point-by-point comparison to our coarse-resolution model, which does not resolve restricted basins, coastal environments or riverine sources. Within the data compilation we identified three studies across open-ocean gradients^{27,29,30} and compare modeled and observed trends along these transects. We extracted the data from Liefer et al., 2024 from Supplementary Table S3. We divided the values of protein, carbohydrates, and lipids by macromolecular carbon. To compare with the model, we retrieved the simulated cellular allocation to protein, carbohydrates, lipids, chlorophyll, nucleic acids (DNA+RNA), at each location where a measurement was made (10 m depth-integrated mean) at model output average (years 2010–2020) and plotted against latitude (Extended Data Figure 2). In the case of Handa et al., 1973 numeric values were unavailable in tables, and we extracted euphotic zone data from Figures 1, 6b, and 7b using WebPlotDigitizer. We extracted the model output of Protein–C:C, Carb–C:C, and temperature from the pre-industrial simulation at each longitude and latitude, and a measurement (0–115m depth-integrated value) was made and plotted against SST for comparison. To compare the model output with the Handa and Tanoue 1988 we extracted the data on Protein–C:C, Carb–C:C and Lipid–C:C from Table 1 (only data from the upper 100m). We conducted a point-by-point comparison to the depth-integrated (0–115m) preindustrial values.

Comparison of modeled C:N:P_{org} with observations

Dataset of in situ elemental composition of organic matter from 1974–2020^{31–33} were analyzed to assess the distribution of particulate organic matter C:N_{org}, C:P_{org} and N:P_{org} ratios across 17 ecological provinces defined by SST, chlorophyll a concentrations, ice fraction, and maximum mixed layer depth³⁴ (Extended Data Figure 3). We included only samples from the surface (0–170 m) in the analysis and excluded samples where POP was lower than 5 nM, as this was the reported practical detection limit³¹.

Furthermore, we included only open ocean samples, where the bathymetric depth was deeper than 1 km, and ecoprovinces, where observations exceeded 15. This screening yielded 15,012, 5,442, and 5,658 observational data points of C:N_{org}, C:P_{org}, and N:P_{org}, respectively. Modeled C:N_{org}, C:P_{org}, and N:P_{org} values (pre-industrial equilibrium conditions) were extracted for grid cells corresponding to each ecological region, integrated over sampling depth. The observational and modeled data's 25th, 50th (median), and 75th percentiles were recorded (Fig. S2–Fig. S4, Table S2–Table S4).

To compare the model and observations, data at each ecoprovince were log-transformed (base-10). A normal distribution was fitted to the log-transformed observed and modeled data, and the mean (μ) was extracted (Table S4). To quantify the relative differences between observed and modeled distributions, the percentage difference between the means of the distributions was calculated for each province using the following formula:

$$\sigma = \frac{|(C:P)_j' - (C:P)_j|}{(C:P)_j} \cdot 100, \quad \text{Eq. S1}$$

where $(C:P)_j'$ is the modeled value and $(C:P)_j$ is the observed value in ecoprovince j . A Kolmogorov-Smirnov (KS) test was performed to evaluate the similarity between the cumulative distribution functions of the observed and modeled data, with the KS statistic representing the maximum difference recorded (Table S4).

Calculation of the caloric content of organic matter

Following the widely used method for estimating the energy contents in human food²⁶, the caloric energy content can be determined by the composition of the major macromolecules in the cell, mainly proteins, carbohydrates, and lipids, which account for >95% of cellular carbon⁶. Lipids contain 9.50 kcal/g, while proteins and carbohydrates contain 4.20 and 4.19 kcal/g, respectively²⁶. Using these values and model estimates of macromolecular mass in phytoplankton under different environmental conditions, we estimate the global energy content in phytoplankton.

The caloric content of organic matter (Q_{cal}^C ; kcal/gC) was estimated using the following equation:

$$Q_{cal}^C = Q_{cal}^{Pro} + Q_{cal}^{Carb} + Q_{cal}^{Lip} \quad \text{Eq. S2}$$

where:

$$Q_{\text{Cal}}^{\text{Pro}} = \frac{Q_{\text{C}}^{\text{Pro}} \text{ mol C in proteins}}{\text{mol C}} \cdot \frac{100 \text{ g proteins}}{4.43 \text{ mol C proteins}} \cdot \frac{\text{mol C}}{12 \text{ g C}} \cdot \frac{4.19 \text{ kcal}}{\text{g proteins}} \quad \text{Eq. S3}$$

$$Q_{\text{Cal}}^{\text{Carb}} = \frac{Q_{\text{C}}^{\text{Carb}} \text{ mol C in carbs}}{\text{mol C}} \cdot \frac{180 \text{ g carbs}}{6.0 \text{ mol C carbs}} \cdot \frac{\text{mol C}}{12 \text{ g C}} \cdot \frac{4.20 \text{ kcal}}{\text{g carbs}} \quad \text{Eq. S4}$$

$$Q_{\text{Cal}}^{\text{Lip}} = \frac{Q_{\text{C}}^{\text{Lip}} \text{ mol C in lipids}}{\text{mol C}} \cdot \frac{634 \text{ g lipids}}{40 \text{ mol C lipids}} \cdot \frac{\text{mol C}}{12 \text{ g C}} \cdot \frac{9.50 \text{ kcal}}{\text{g lipids}} \quad \text{Eq. S5}$$

Here $Q_{\text{C}}^{\text{Pro}}$, $Q_{\text{C}}^{\text{Carb}}$, and $Q_{\text{C}}^{\text{Lip}}$ are cellular allocations of carbon to proteins, carbohydrates, and lipids, respectively, derived from model simulations averaged over depth (0–170 m) in preindustrial simulations. 100, 180, 634 are the molecular weights (g/mol) of proteins, carbohydrates, and lipids for 4.43, 6.0, and 40 mol C in these molecules respectively¹⁰⁸. 4.19, 4.20, and 9.50 kcal/g are conversion factors from kcal/g for proteins, carbohydrates, and lipids, respectively.

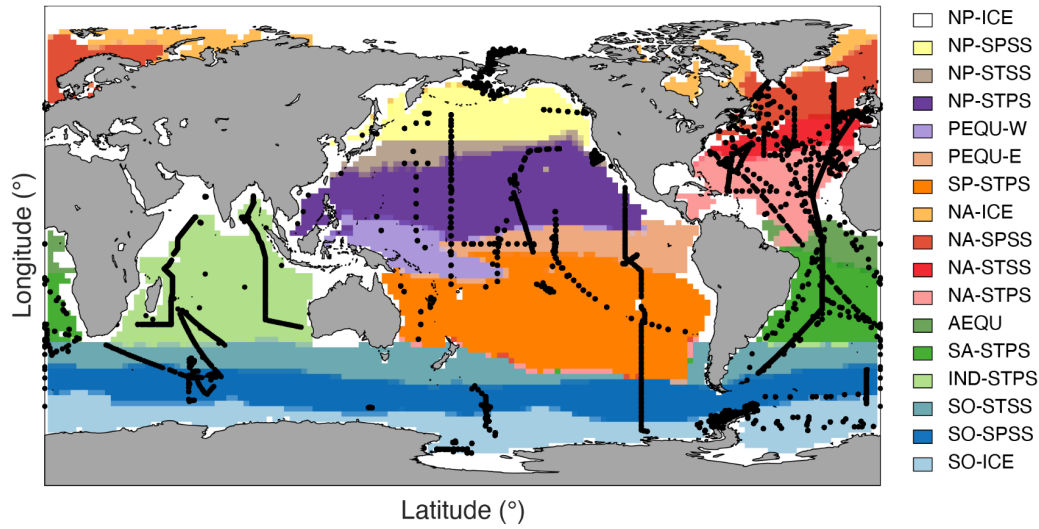


Fig. S1: Sampling locations of particulate organic matter $C:N_{org}$, $C:P_{org}$, and $N:P_{org}$ across global ecoprovinces. Sampling locations^{31,33} of $C:N_{org}$, $C:P_{org}$, and $N:P_{org}$ plotted against ecoprovinces defined by SST, chlorophyll a concentrations, ice fraction, and maximum mixed layer depth³⁴. Only locations meeting two criteria are included: (1) bathymetric depth greater than 1 km (open ocean) and (2) sampling conducted within the upper 170 m, corresponding to the mixed layer. Regions: NP-ICE: North Pacific Ice, NP-SPSS: North Pacific Subpolar Seasonally Stratified, NP-STSS: North Pacific Subtropical Seasonally Stratified, NP-STPS: North Pacific Subtropical Permanent Stratified, PEQU-W: West Pacific Equatorial, PEQU-E: East Pacific Equatorial, SP-STPS: South Pacific Subtropical Permanent Stratified, NA-ICE: North Atlantic Ice, NA-SPSS: North Atlantic Subpolar Seasonally Stratified, NA-STSS: North Atlantic Subtropical Seasonally Stratified, NA-STPS: North Atlantic Subtropical Permanent Stratified, AEQU: Atlantic Equatorial, SA-STPS: South Atlantic Subtropical Permanent Stratified, IND-STPS: Indian Ocean Subtropical Permanent Stratified, SO-STSS: Southern Ocean Subtropical Seasonally Stratified, SO-SPSS: Southern Ocean Subpolar Seasonally Stratified, SO-ICE: Southern Ocean Ice.

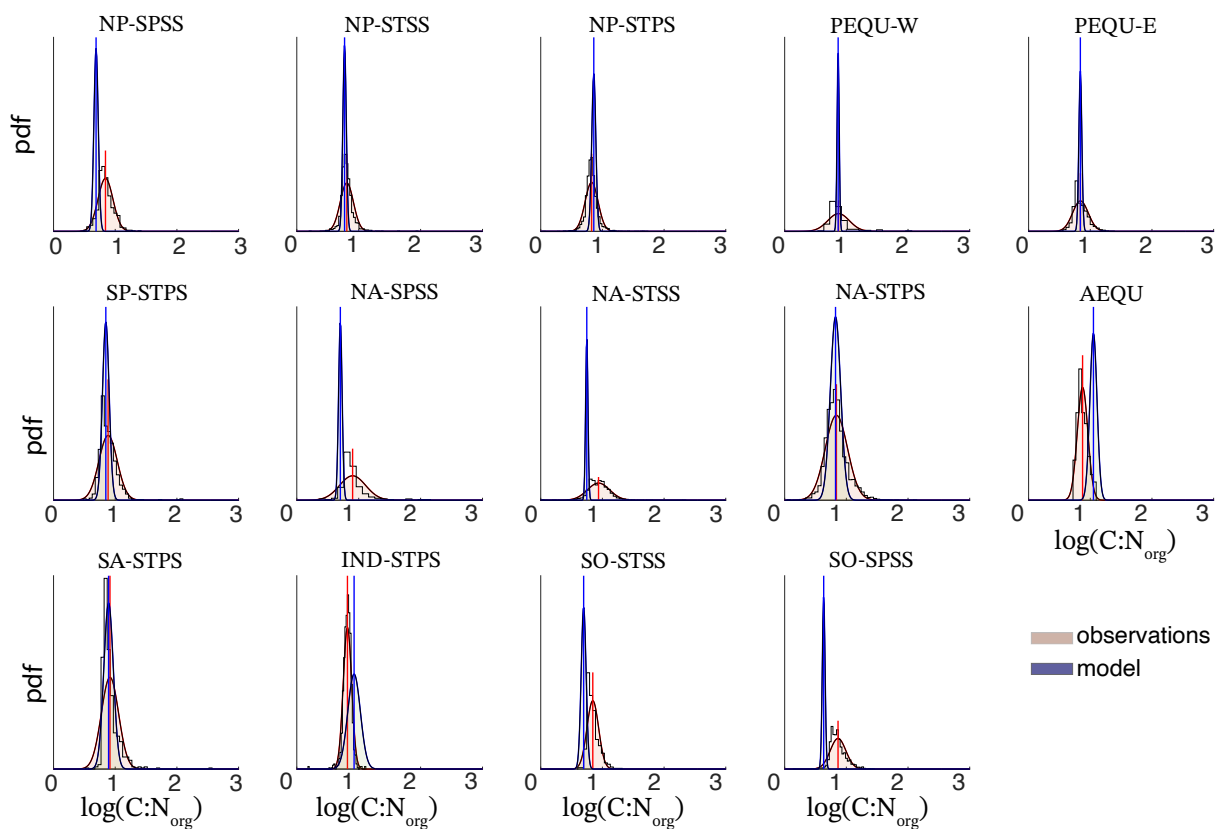


Fig. S2: Comparison between modeled and observed $C:N_{org}$ distributions. The orange Probability Density Functions (PDFs) represent the observed log-transformed $C:N_{org}$ ratios, while the blue pdfs represent the log-transformed modeled $C:N_{org}$ ratios calculated from the macromolecular model (molar ratios). The vertical lines represent the means of the distributions. All data were clustered according to oceanographic regions defined in Fig. S1.

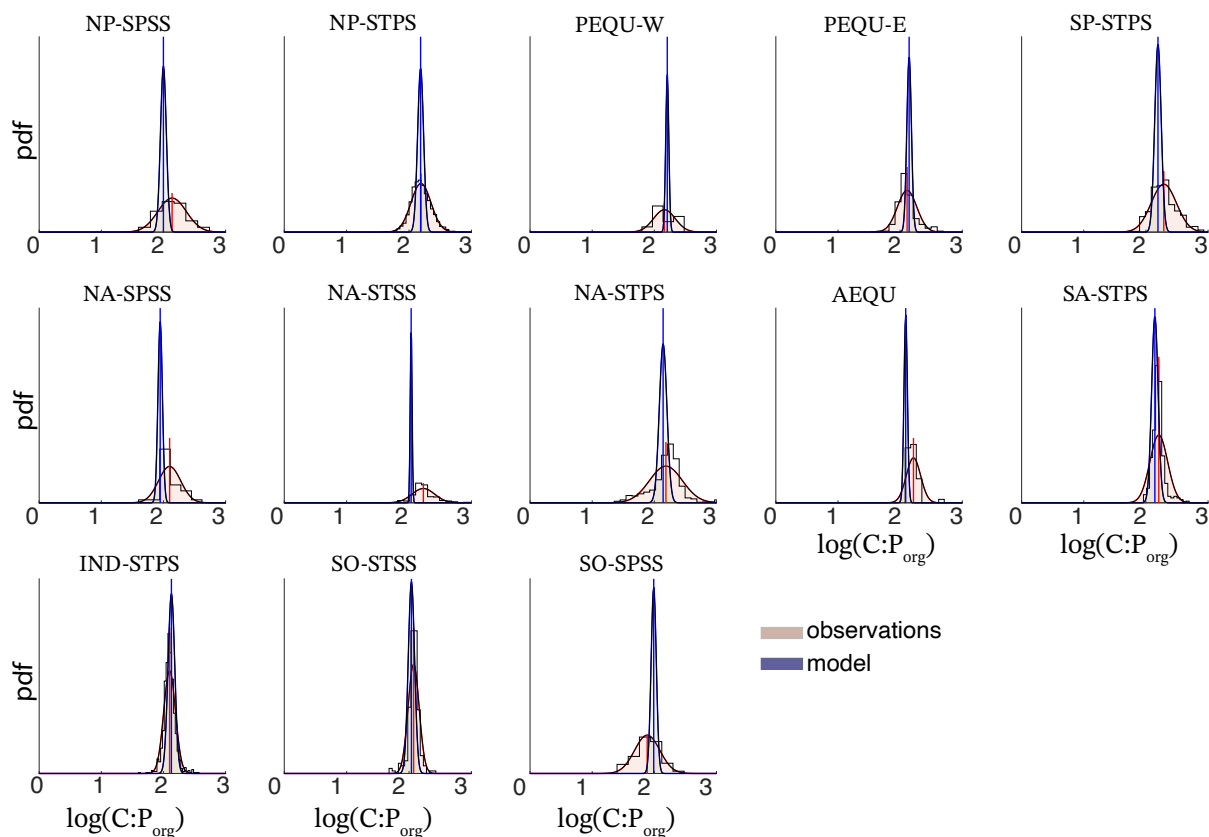


Fig. S3: Comparison between modeled and observed $C:P_{org}$ distributions. The orange Probability Density Functions (PDFs) represent the observed log-transformed $C:P_{org}$ ratios, while the blue pdfs represent the log-transformed modeled $C:P_{org}$ ratios calculated from the macromolecular model (molar ratios). The vertical lines represent the means of the distributions. All data were clustered according to oceanographic regions defined in Fig. S1.

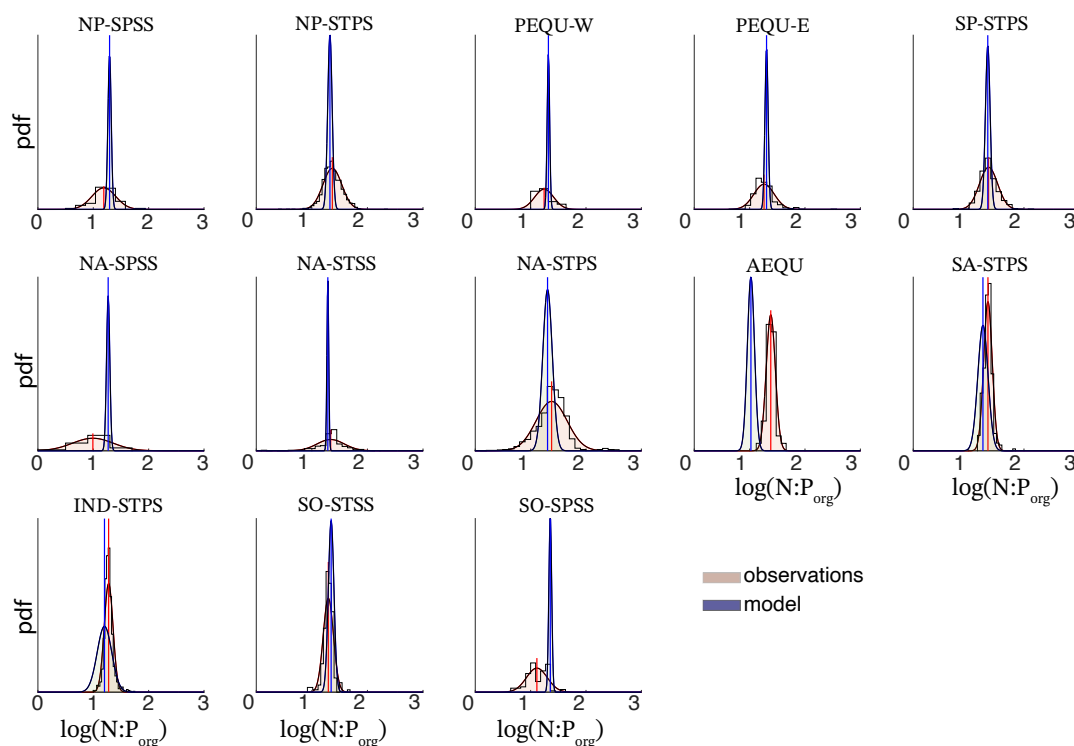


Fig. S4: Comparison between modeled and observed $N:P_{org}$ distributions. The orange Probability Density Functions (PDFs) represent the observed log-transformed $N:P_{org}$ ratios, while the blue pdfs represent the log-transformed modeled $N:P_{org}$ ratios calculated from the macromolecular model (molar ratios). The vertical lines represent the means of the distributions. All data were clustered according to oceanographic regions defined in Fig. S1.

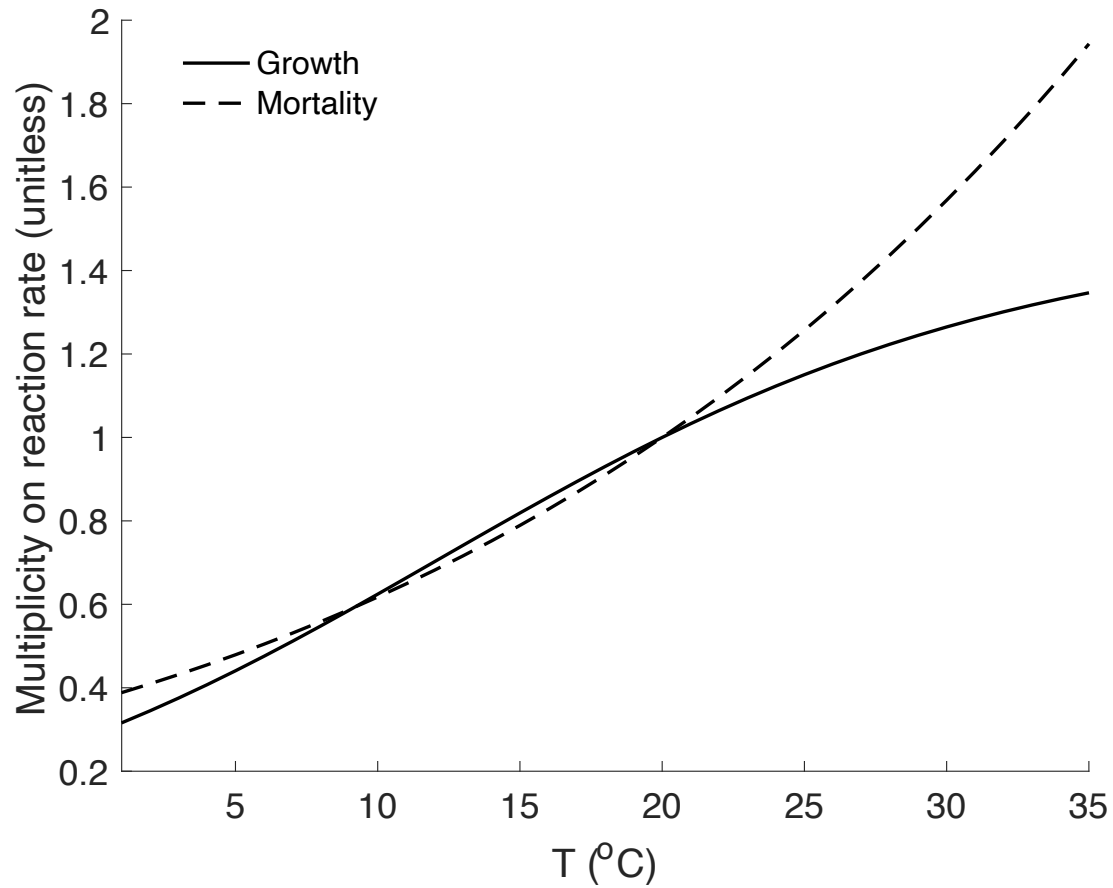


Fig. S5: The effect of temperature on phytoplankton growth and mortality rates. We calculated the temperature response on growth from the carbon mass balance (Eq. 1). Mortality follows an Arrhenius relationship with an activation energy of 34,000 J/mol⁷⁶.

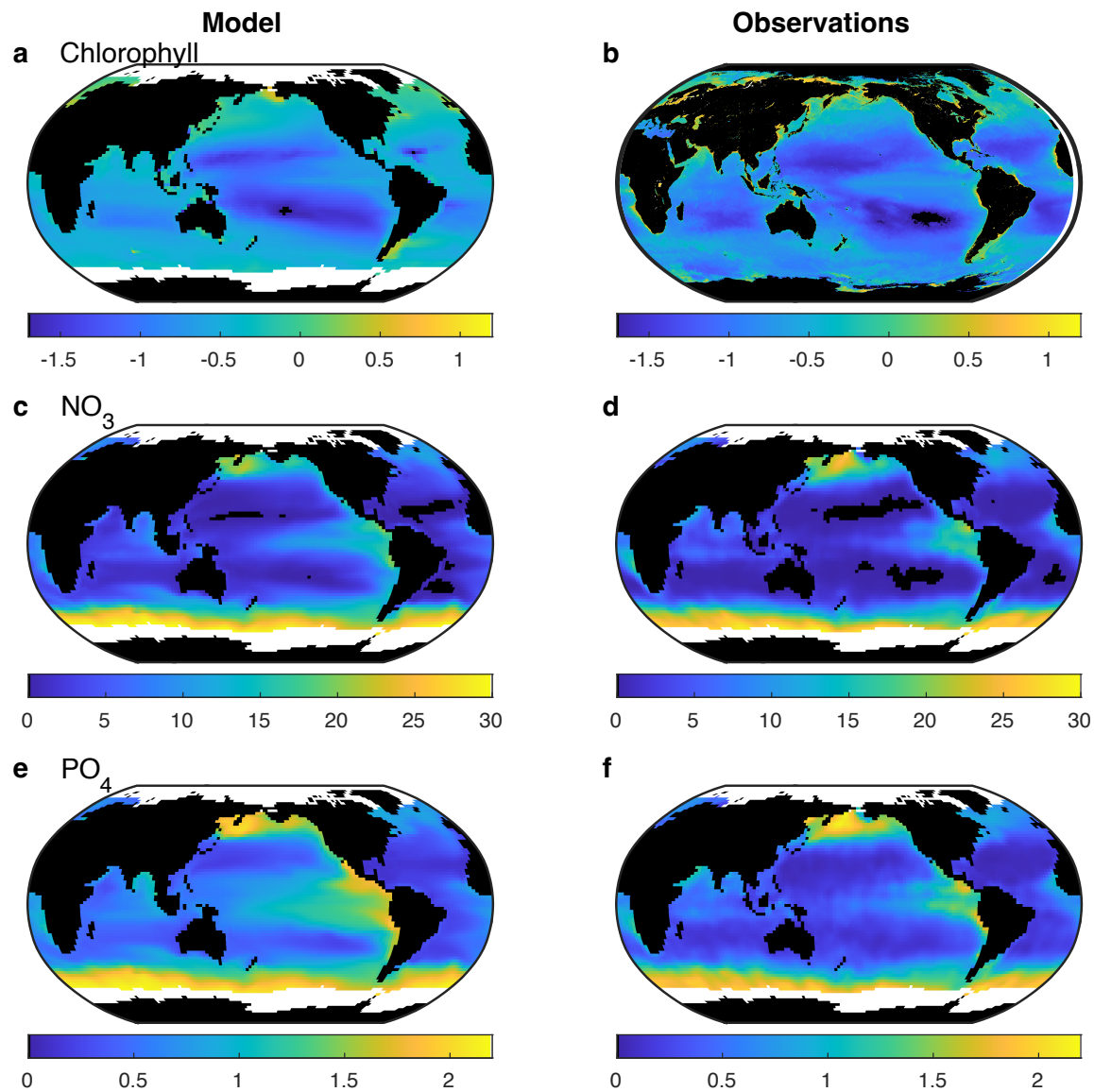


Fig. S6: Comparison between observed and modeled biogeochemical tracers. Depth-integrated (0–115 m), annual means of (a, b) chlorophyll concentration (mg Chl m^{-3}) (c, d) nitrate (mmol m^{-3}), and (e, f) phosphate (mmol m^{-3}). Observed chlorophyll data are derived from ocean colour products¹⁰⁹, while dissolved nutrient observations are from the World Ocean Atlas¹¹⁰. The left column shows model results, and the right column shows observational data. The model results represent a 10-year mean of the model output for the preindustrial simulation (Phase 1).

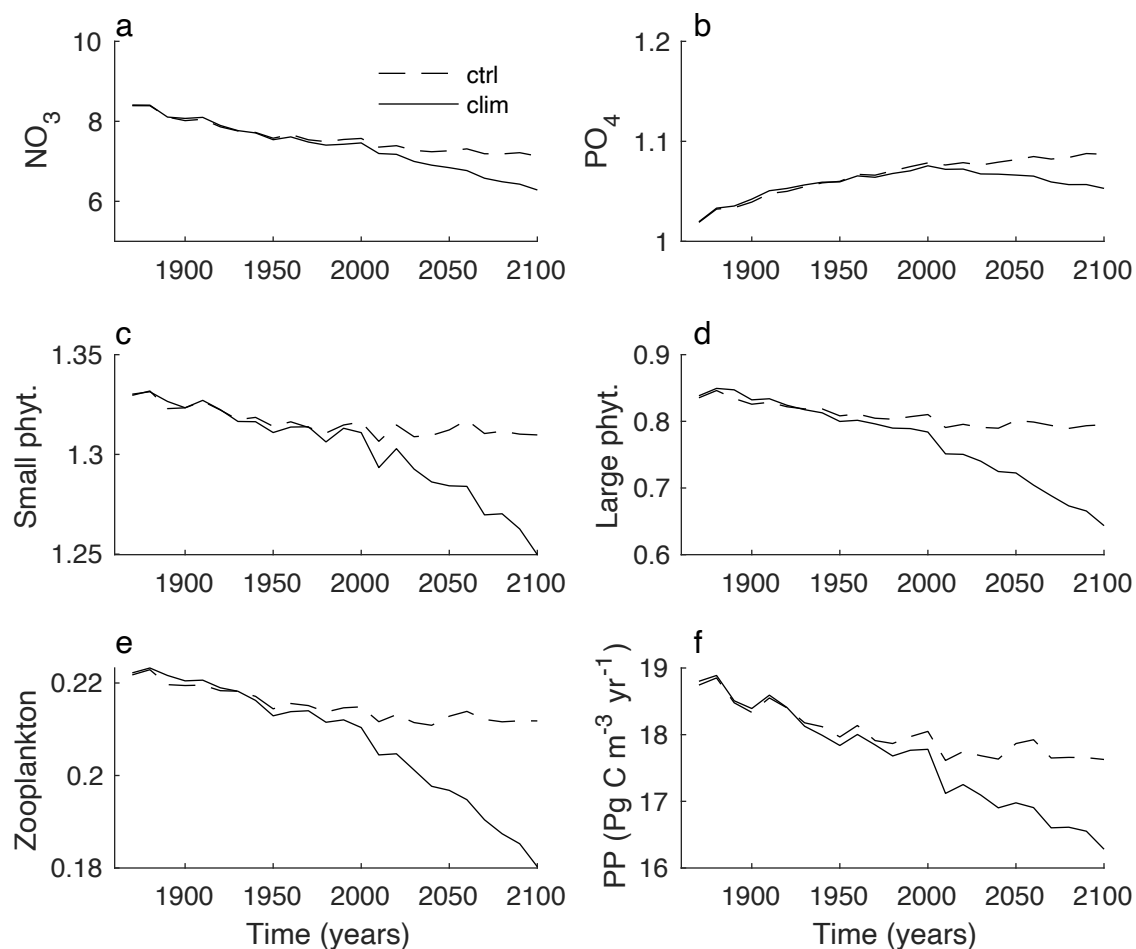


Fig. S7: Modeled marine biogeochemical tracers. Global mean concentrations of (a) dissolved nitrate (NO_3), (b) dissolved phosphate (PO_4), (c) small phytoplankton organic carbon, (d) large phytoplankton organic carbon, (e) zooplankton organic carbon, and (f) primary productivity (PP; $\text{Pg C m}^{-3} \text{ yr}^{-1}$). All tracers, except PP, are reported in mmol m^{-3} . Dashed and solid lines show control simulation (Phase 2; Methods) and high emission scenarios (Phases 3–4), respectively.

Table S1. Literature compilation of in situ measurements of carbohydrates, proteins and lipids collected from the photic zone. The values in the table represent 5th–95th percentiles (median) of the samples collected in the photic zone. For ratios with fewer than three observations, raw values are displayed. *n* is the number of individual sampling points.

	#	Sampling Location	Sampling Time	Carb-C:C	Protein-C:C	Lipid-C:C	<i>n</i>	Refs.
Arctic Ocean	1	Labrador Sea	Sep 1978	0.28–0.46(0.42)	0.06–0.37(0.13)	0.28–0.46(0.42)	27	Irwin et al., 1980 ⁴⁵
	2	Can. Arctic	July-Oct, 1979	0.16–0.39(0.30)	0.20–0.61(0.37)	0.16–0.39(0.30)	82	Irwin et al., 1984 ⁴⁶
	3	Can. Arctic	July-Aug, 1980	0.11–0.42(0.20)	0.14–0.74(0.57)	0.11–0.42(0.20)	16	Irwin et al., 1983a ⁴⁷
	4	Can. Arctic	Aug-Sep, 1981	0.18–0.42(0.33)	0.13–0.62(0.32)	0.18–0.42(0.33)	11	Irwin et al., 1983b ⁴⁸
	5	N. Atlantic	July-Aug, 1980	0.16–0.48(0.30)	0.22–0.52(0.38)	0.11–0.26(0.18)	35	Li and Platt, 1982⁴⁴
	6	N.E. Greenland	May-July, 1993	0.36, 0.39	0.34, 0.42	0.11, 0.11	2	Smith et al., 1997⁴⁹
	7	Chukchi Sea	Aug, 2004	0.05–0.20(0.05)	0.21–0.85(0.60)	0.02–0.08(0.04)	15	Lee et al., 2009⁵⁰
	8	Chukchi Sea	July-Aug, 2011	0.12–0.43(0.21)	0.01–0.35(0.10)	0.46–0.79(0.62)	42	Kim et al., 2015 ⁵¹
	9	Chukchi sea	Aug-Sep, 2012	0.11–0.23(0.16)	0.07–0.25(0.12)	0.60–0.78(0.71)	25	Yun et al., 2015 ¹¹
	10	Laptev Sea	Aug-Sep, 2013	0.16–0.48(0.35)	0.19–0.53(0.41)	0.20–0.36(0.27)	37	Ahn et al., 2019 ⁷²
	11	Chukchi sea	July-Aug, 2014	0.19–0.67(0.37)	0.03–0.36(0.17)	0.22–0.71(0.38)	63	Choe et al., 2021 ⁵²
	12	Chukchi Sea	Aug, 2017	0.06–0.16(0.12)	0.16–0.44(0.25)	0.45–0.73(0.65)	12	Kim et al., 2020 ⁵³
Antarctic Ocean	13	S. Ocean	Sep-Oct, 1987	0.08–0.84(0.49)	0.03–0.27(0.11)	0.04–0.89(0.37)	8	Smith and Morris, 1980⁴³
	14	S. Pacific	1980–1981	0.11–0.13(0.12)	0.34–0.40(0.37)	0.22–0.31(0.23)	3	Handa and Tanoue 1983 ³⁰
	15	Ross Sea	Nov 1989 – Jan 1990	0.18–0.54(0.27)	0.35–0.71(0.59)	0.08–0.16(0.11)	10	Fabiano et al., 1993 ⁵⁴
	16	Ross Sea	Jan-Feb, 1990	0.17, 0.20	0.60, 0.64	0.16, 0.22	2	Fabiano et al., 1996 ⁵⁵
	17	Ross Sea	Jan-Feb, 1995	0.20–0.25(0.24)	0.46–0.59(0.52)	0.18–0.29(0.25)	6	Fabiano and Pusceddu 1998 ⁵⁶
	18	Ross Sea*	Jan, 1995	0.03–0.12(0.08)	0.34–0.56(0.43)	0.34–0.57(0.45)	15	Pusceddu et al., 1999 ⁵⁷
	19	Amundsen Sea	Feb-March, 2012	0.09–0.26(0.17)	0.52–0.77(0.68)	0.08–0.32(0.13)	14	Kim et al., 2016 ⁵⁸
	20	Amundsen Sea	March-Nov, 2014	0.20–0.54(0.36)	0.25–0.48(0.37)	0.12–0.41(0.26)	21	Kim et al., 2018 ¹⁰
	21	Ross Sea	Jan-Feb 2017	0.26–0.39(0.35)	0.43–0.55(0.50)	0.13–0.19(0.17)	4	Misic et al., 2024 ⁵⁹
	22	Ross Sea	Feb, 2018	0.23–0.52(0.43)	0.05–0.26(0.15)	0.36–0.55(0.41)	18	Jo et al., 2021 ⁶⁰
Japan Sea	23	Japan Sea	Oct, Apr, 2012	0.16–0.49(0.30)	0.20–0.36(0.26)	0.24–0.60(0.44)	21	Kang et al., 2017 ⁸⁹
	24	Japan Sea	Apr-Nov, 2014	0.27–0.59(0.41)	0.10–0.49(0.18)	0.18–0.62(0.34)	8	Jo et al., 2017 ⁹⁰
	25	Japan Sea	May-Oct, 2015	0.28–0.47(0.43)	0.12–0.22(0.13)	0.35–0.58(0.40)	5	Jo et al., 2018 ⁹¹
	26	Japan Sea	Apr, 2016	0.05–0.46(0.30)	0.05–0.34(0.16)	0.29–0.82(0.54)	38	Kang et al., 2020 ⁹²
Other Regions	27	S. Korea	Jun 2012 -Apr 2013	0.10–0.31(0.18)	0.11–0.69(0.33)	0.22–0.71(0.48)	45	Lee et al., 2017 ⁹³
	28	S. Korea	Jan-Dec 2015	0.21–0.48(0.36)	0.15–0.37(0.30)	0.25–0.52(0.34)	12	Kim et al., 2018b ⁹⁴
	29	Yellow Sea	Apr 2015-Nov 2016	0.32–0.64(0.49)	0.06–0.33(0.21)	0.19–0.53(0.31)	54	Lee et al., 2020 ⁹⁵
	30	Mediterranean	Aug 1994-Sep 1995	0.20–0.54(0.33)	0.23–0.51(0.34)	0.16–0.52(0.32)	102	Danovaro et al., 2000 ⁹⁶
	31	Mediterranean	May, July, 2001	0.05–0.29(0.21)	0.36–0.57(0.47)	0.21–0.83(0.52)	8	Modica et al., 2006 ⁹⁷
	32	Baltic Sea	Apr-Sep, 1988	0.15–0.46(0.27)	0.18–0.62(0.39)	0.09–0.38(0.14)	24	Lindqvist and Lingell 1997⁹⁸
	33	N. Atlantic	Apr, 1969	0.17–0.73(0.47)	0.31–0.57(0.40)	0.14–0.42(0.35)	10	Platt and Irwin, 1973⁴²
	34	N. Atlantic	June-Oct, 1976	0.20–0.31(0.23)	0.56–0.68(0.62)	0.11–0.17(0.13)	8	Mayzaud and Taguchi 1979 ⁹⁹
	36	N. Atlantic	Apr-May, 1979	0.23–0.45(0.40)	0.08–0.48(0.16)	0.23–0.45(0.40)	53	Irwin et al., 1983c ¹⁰⁰
	37	N. Atlantic	Jul-Oct, 1979	0.23–0.44(0.38)	0.09–0.51(0.21)	0.23–0.44(0.38)	54	Irwin et al., 1984 ⁴⁶
	38	N. Atlantic	July, 1980	0.14–0.35(0.23)	0.27–0.68(0.50)	0.14–0.35(0.23)	6	Irwin et al., 1983a ⁴⁷
	39	N. Atlantic	May, 1981	0.37–0.48(0.44)	0.03–0.24(0.10)	0.37–0.48(0.44)	23	Irwin et al., 1983d ¹⁰¹
	40	N. Atlantic	July, 1982	0.22–0.44(0.36)	0.10–0.54(0.25)	0.22–0.44(0.36)	26	Irwin et al., 1983e ¹⁰²
	41	N.E. Atlantic	July 2010-May 2011	0.15–0.20(0.16)	0.48–0.55(0.52)	0.28–0.36(0.30)	8	Fernández-Reiriz, 2017 ¹⁰³
	42	N.E. Atlantic	Apr-July, 2000	0.03–0.13(0.06)	0.40–0.88(0.68)	0.06–0.57(0.24)	18	Diaz et al 2007 ¹⁰⁴
	43	N. Pacific	June, 2017	0.18–0.38(0.25)	0.24–0.50(0.40)	0.23–0.35(0.26)	12	**Liefer et al., 2024 ²⁷
	44	Pacific	1968	0.16–0.33(0.21)	0.21–0.55(0.36)	-	22	**Handa 1973 ²⁹
	45	E. Eq. Pacific	Jan-Feb, 2006	0.19–0.31(0.28)	0.17–0.37(0.21)	0.33–0.63(0.51)	8	Isla et al., 2010 ¹⁰⁵
	46	E. Eq. Pacific	Feb, July 2006, 2007	0.08–0.32(0.18)	0.17–0.53(0.39)	0.37–0.51(0.44)	4	Isla et al., 2012 ¹⁰⁶
	47	Magellan Strt.	Feb-March, 1991	0.12–0.17(0.15)	0.35–0.55(0.46)	0.21–0.51(0.31)	7	Fabiano et al., 1999 ¹⁰⁷

*Sea ice samples⁵⁷.

**Open ocean samples.

Bold references used isotope labelling techniques, which measure photosynthetic carbon allocation in living phytoplankton.

Table S2. Statistical analyses of the observations at the different ecoprovinces.

<i>Region</i>	CN _{nob}	CN _{out}	CN ₂₅	CN ₅₀	CN ₇₅	CP _{nob}	CP _{out}	CP ₂₅	CP ₅₀	CP ₇₅	NP _{nob}	NP _{out}	NP ₂₅	NP ₅₀	NP ₇₅
<i>NP—SPSS</i>	1144	40	5.9	6.7	8.0	64	3	96	139	182	64	1	12	16	19
<i>NP—STPS</i>	1206	18	5.7	6.3	7.1	1342	57	122	152	196	1342	52	18	23	30
<i>NP—STSS</i>	2989	69	5.9	6.6	7.4	-	-	-	-	-	-	-	-	-	-
<i>PEQU—W</i>	158	4	6	6.8	8.1	22	-	102	133	209	21	1	14	15	24
<i>PEQU—E</i>	839	43	5.8	6.6	8.1	349	20	105	123	148	384	8	14	18	22
<i>SP—STPS</i>	718	6	6.1	7.3	9.0	369	18	141	189	259	445	19	18	22	28
<i>NA—SPSS</i>	201	4	6.3	7.2	8.9	32	1	107	120	149	30	2	7	12	14
<i>NA—STSS</i>	1109	9	6.7	8.6	10.9	268	12	137	162	200	264	10	18	23	27
<i>NA—STPS</i>	3100	97	5.3	6.6	8.4	1513	36	121	166	212	1625	30	17	25	34
<i>AEQU</i>	141	9	6.4	7.2	8.5	42	2	139	152	177	42	3	22	24	26
<i>SA—STPS</i>	588	2	6.8	7.5	8.9	307	1	141	155	174	307	7	20	23	25
<i>IND—STPS</i>	948	37	6.0	6.6	7.2	848	28	111	124	140	848	27	17	19	20
<i>SO—STSS</i>	488	21	5.9	6.6	7.7	191	11	109	119	132	191	10	18	20	22
<i>SO—SPSS</i>	1383	69	6.0	6.9	8.4	95	2	58	75	112	95	2	10	12	19

The observations are from the upper 170 m depth. CN_{nob}, CP_{nob}, NP_{nob} represent the number of observations at each ecoprovince. CN_{out}, CP_{out}, NP_{out} are the outliers excluded from the mean (mean $\pm$ 2 standard deviations). CN₂₅, CN₅₀, CP₂₅, CP₅₀, CP₇₅ and NP₂₅, NP₅₀, NP₇₅ are the 25th, 50th, and 75th percentiles of the C:N_{org}, C:P_{org} and N:P_{org} observed data in each ecoprovince, respectively (molar ratios).

Table S3. Modeled C:N_{org}, C:P_{org} and N:P_{org} means from the global macromolecular model.

<i>Region</i>	CN' _{nobs}	CN'25	CN'50	CN'75	CP' _{nobs}	CP'25	CP'50	CP'75	NP' _{nobs}	NP'25	NP'50	NP'75
<i>NP—SPSS</i>	282	4.6	4.8	5.2	284	93	97	105	284	19	20	22
<i>NP—STSS</i>	111	5.6	5.8	6.2	-	-	-	-	-	-	-	-
<i>NP—STPS</i>	667	6.9	7.4	7.6	667	151	160	165	667	21	22	22
<i>PEQU—W</i>	176	7.1	7.3	7.6	176	160	164	167	176	21	21	22
<i>PEQU—E</i>	236	6.6	6.9	7.2	236	137	139	145	236	20	20	21
<i>SP—STPS</i>	938	6.6	7.4	7.7	938	150	166	170	938	21	22	24
<i>NA—SPSS</i>	298	4.8	5.0	5.3	298	84	86	92	298	18	19	20
<i>NA—STSS</i>	98	5.5	5.5	5.7	98	106	108	110	98	19	19	20
<i>NA—STPS</i>	312	5.9	6.7	7.4	312	122	142	158	312	18	19	22
<i>AEQU</i>	101	10.5	11.7	12.4	101	119	122	127	101	10	10	11
<i>SA—STPS</i>	299	6.8	7.5	8.7	299	127	141	157	299	16	19	22
<i>IND—STPS</i>	588	7.1	8.3	10.2	588	126	136	147	588	12	16	21
<i>SO—STSS</i>	564	4.7	4.9	5.2	564	102	110	119	564	22	23	24
<i>SO—SPSS</i>	742	4.1	4.3	4.4	742	91	95	102	742	22	23	23

CN'_{nobs}, CP'_{nobs}, NP'_{nobs} represent the number of modeled values at each ecoprovinces. CN'25th, CN'50th, CN'75th, CN'25th, CN'50th, CP'75th and NP'25th, NP'50th, NP'75th are the 25th, 50th, and 75th percentiles of the C:N_{org}, C:P_{org} and N:P_{org} modeled data in each ecoprovince, respectively (molar ratios).

Table S4. Comparison between the model and observed C:N_{org}, C:P_{org}, and N:P_{org}.

<i>Region</i>	$\mu_{CN,obs}$	$\mu_{CN,model}$	Δ_{CN}	σ_{CN}	$\mu_{CP,obs}$	$\mu_{CP,model}$	Δ_{CP}	σ_{CP}	$\mu_{NP,obs}$	$\mu_{NP,model}$	Δ_{NP}	σ_{NP}
<i>NP—SPSS</i>	6.9	4.9	0.349	30	138	100	0.677	27	15	20	0.718	27
<i>NP—STSS</i>	6.4	5.9	0.308	8	-	-	-	-	-	-	-	-
<i>NP—STPS</i>	6.7	7.3	0.276	8	156	153	0.471	1	23	21	0.504	10
<i>PEQU—W</i>	7.5	7.4	0.628	2	145	161	0.698	11	18	21	0.615	19
<i>PEQU—E</i>	6.9	6.9	0.398	0	129	140	0.527	8	18	20	0.614	11
<i>SP—STPS</i>	7.7	7.0	0.370	8	194	156	0.606	19	23	22	0.475	3
<i>NA—SPSS</i>	8.0	5.1	0.721	37	126	89	0.621	29	10	19	0.853	89
<i>NA—STSS</i>	8.7	5.6	0.642	35	170	108	0.809	34	22	19	0.886	11
<i>NA—STPS</i>	6.9	6.7	0.378	3	154	138	0.639	10	24	20	0.605	16
<i>AEQU</i>	7.5	11.3	0.089	50	164	123	0.454	25	24	11	0.105	56
<i>SA—STPS</i>	8.2	7.8	0.245	5	161	139	0.372	13	22	18	0.048	19
<i>IND—STPS</i>	6.6	8.4	0.140	28	125	134	0.181	7	19	16	0.193	16
<i>SO—STSS</i>	7.0	5.0	0.225	29	119	109	0.179	8	20	22	0.156	12
<i>SO—SPSS</i>	7.3	4.3	0.423	41	77	98	0.648	27	13	23	0.640	75
Σ			5.1898*	284*			6.8831*	221*			6.4136*	364*

$\mu_{CN,obs}$, $\mu_{CP,obs}$ and $\mu_{NP,obs}$ represent the means of the log-transformed distributions of the observed C:N_{org}, C:P_{org} and N:P_{org} ratios, respectively, in each ecoprovince (molar ratios). Similarly, $\mu_{CN,model}$, $\mu_{CP,model}$ and $\mu_{NP,model}$ denote the means of the log-transformed distributions of the modeled C:N_{org}, C:P_{org} and N:P_{org} ratios, respectively, in each ecoprovince. Δ represents the maximum difference between the cumulative distribution functions of the observed and modeled log-transformed C:N_{org}, C:P_{org} and N:P_{org}, as determined by the Kolmogorov-Smirnov test. σ (%) is the relative distance between the modeled and observed distribution means, calculated using Eq. S1. Σ is the sum of the distances in all ecoprovinces.

Table S5. Linear regression results for temporal trends in polar phytoplankton macromolecules. Temporal trends in protein and carbohydrate + lipid concentrations were evaluated using ordinary least squares linear regression against time. Statistical significance was assessed using a two-sided test of the regression slope against zero. The table reports the number of observations, number of excluded outliers, slope estimates, P values and R^2 . Only data obtained with colorimetric methods are included.

<i>Region</i>	<i>Regression</i>	<i>#Observations</i>	<i>#Outliers</i>	<i>Slope</i>	<i>p-value</i>	<i>R²</i>
<i>Arctic</i>	Protein vs. year	307	5	−0.0038	1.68×10^{-12}	0.156
<i>Arctic</i>	Carb + lipid vs. year	302	10	0.0041	2.52×10^{-15}	0.189
<i>Antarctic</i>	Protein vs. year	85	8	−0.0037	0.00941	0.078
<i>Antarctic</i>	Carb + lipid vs. year	93	0	0.0076	4.41×10^{-7}	0.246

Table S6. Linear regression results for temporal trends in polar phytoplankton macromolecules. Temporal trends in protein and carbohydrate + lipid concentrations were evaluated using ordinary least squares linear regression against time. Statistical significance was assessed using a two-sided test of the regression slope against zero. The table reports the number of observations, number of excluded outliers, slope estimates, P values and R^2 . All data are included.

<i>Region</i>	<i>Regression</i>	<i>#Observations</i>	<i>#Outliers</i>	<i>Slope</i>	<i>p-value</i>	<i>R²</i>
<i>Arctic</i>	Protein vs. year	359	5	−0.0037	4.2×10^{-12}	0.126
<i>Arctic</i>	Carb + lipid vs. year	342	22	0.0054	1.1×10^{-24}	0.266
<i>Antarctic</i>	Protein vs. year	96	5	−0.0020	0.143	0.022
<i>Antarctic</i>	Carb + lipid vs. year	101	0	0.0018	0.214	0.015

Table S7. Variables in the macromolecular model.

Symbol	Definition	Units
Q_C^{Pro}	Cellular carbon in proteins (all)	mol C (mol C) ⁻¹
$Q_C^{\text{Pro-photo}}$	Cellular carbon in photosynthetic proteins	mol C (mol C) ⁻¹
$Q_C^{\text{Pro-bio}}$	Cellular carbon in biosynthetic proteins	mol C (mol C) ⁻¹
$Q_C^{\text{Pro-other}}$	Cellular carbon in essential proteins	mol C (mol C) ⁻¹
Q_C^{RNA}	Cellular carbon in RNA	mol C (mol C) ⁻¹
Q_C^{DNA}	Cellular carbon in DNA	mol C (mol C) ⁻¹
Q_C^{Chl}	Chlorophyll to carbon ratio	mol C in Chl (mol C) ⁻¹
Q_C^{PLip}	Cellular carbon in thylakoid lipids	mol C (mol C) ⁻¹
Q_C^{Stor}	Carbon stored as carbohydrates and lipids	mol C (mol C) ⁻¹
Q_C^{Other}	Fixed pool of carbon in carbohydrates and lipids	mol C (mol C) ⁻¹
Q_N^{RNA}	Cellular nitrogen allocated to RNA	mol N (mol C) ⁻¹
Q_N^{DNA}	Cellular nitrogen allocated to DNA	mol N (mol C) ⁻¹
Q_N^{Chl}	Cellular nitrogen in chlorophyll	mol N (mol C) ⁻¹
Q_N^{NStor}	Cellular nitrogen storage as cyanophycin	mol N (mol C) ⁻¹
Q_P^{RNA}	Cellular phosphorous in RNA	mol P (mol C) ⁻¹
Q_P^{Thy}	Cellular phosphorus in the thylakoid membrane	mol P (mol C) ⁻¹
Q_P^{Stor}	Cellular phosphorus storage	mol P (mol C) ⁻¹
Q_P^{Other}	Fixed pool of phosphorus	mol P (mol C) ⁻¹
$Q_{\text{Fe}}^{\text{Pho}}$	Cellular iron in photosynthetic proteins	mol Fe (mol C) ⁻¹
$Q_{\text{Fe}}^{\text{Stor}}$	Cellular iron storage	mol Fe (mol C) ⁻¹

Table S8. Allometric relationships between cell volume and parameters.

Parameter	Description (units)
$V_j^{\max, \text{P}} = 0.077V^{-0.27}$	Maximum uptake rate (mmol P/mmol C/day)
$V_j^{\max, \text{N}} = 0.51V^{-0.27}$	Maximum uptake rate (mmol N/mmol C/day)
$V_j^{\max, \text{Fe}} = 14 \times 10^{-6}V^{-0.27}$	Maximum uptake rate (mmol Fe/mmol C/day)
$k_j^{\text{P}} = 0.026V^{0.27}$	Half saturation constant (mmol P/m ³)
$k_j^{\text{N}} = 0.17V^{0.27}$	Half saturation constant (mmol N/m ³)
$k_j^{\text{Fe}} = 80 \times 10^{-6}V^{0.27}$	Half saturation constant (mmol Fe/m ³)
$V_{\text{small}} = 0.41$ and $V_{\text{large}} = 46.0$, where V is phytoplankton cell volume (μm ³).	

Table S9. Stoichiometric parameters and constant that are used in the macromolecular model.

Parameter	Description	Value	Units
$Y_{Pro}^{C:N}$	C:N in proteins	5.3/1.4	mol C (mol N) ⁻¹
$Y_{Nsto}^{C:N}$	C:N in N-storage as cyanophycin	2	mol C (mol N) ⁻¹
$Y_{DNA}^{P:C}$	P:C in DNA	1/9.75	mol P (mol C) ⁻¹
E	Respiratory costs of synthesis	0.774*	unitless
m	Maintenance respiration rate	0.393*	day ⁻¹
V_I^{max}	Per-chlorophyll maximum photosynthesis rate	277*	mol C (mol C in Chl) ⁻¹ day ⁻¹
A_I	Absorption cross-section of the photosyn. unit	8.63×10^{-3} *	m ² s μ mol ⁻¹
A_{Pho}	Proteins : Chl in the photosynthetic machinery	16*	mol C (mol C in Chl) ⁻¹
$A_{Pho}^{P:Chl}$	P in thylakoid : Chl in the photosynthetic machinery	2.8163×10^{-2} *	mol P (mol C in Chl) ⁻¹
$A_{Pho}^{Fe:Chl}$	Fe in thylakoid : Chl in the photosynthetic machinery	5.83×10^{-3} *	mol Fe (mol C in Chl) ⁻¹
A_{bio}	Linear relationship between biosyn. proteins and growth	0.2711*	mol C (mol C) ⁻¹ day
A_P^{RNA}	A constant of proportionality between RNA and proteins	4.23×10^{-3} *	mol P (mol C) ⁻¹ day
$Q_{P,min}^{RNA}$	Minimum RNA in the cell	2.23×10^{-4} *	mol P (mol C) ⁻¹
Q_P^{Other}	Fixed pool of phosphorus	6.5344×10^{-4} *	mol P (mol C) ⁻¹
$Q_C^{Pro-other}$	Cellular carbon in essential proteins	0.24*	mol C (mol C) ⁻¹
Q_C^{Other}	Fixed pool of carbon in carbohydrates and lipids	0.0182*	mol C (mol C) ⁻¹
Q_C^{DNA}	Fixed pool of cellular carbon in DNA	9.41×10^{-4} *	mol C (mol C) ⁻¹
$Q_z^{P,max}$	Maximum grazer phosphorous quota	0.008	mol P (mol C) ⁻¹
$Q_z^{P,min}$	Minimum grazer phosphorous quota	0.010	mol P (mol C) ⁻¹
$Q_z^{N,max}$	Maximum grazer nitrogen quota	0.1	mol N (mol C) ⁻¹
$Q_z^{N,min}$	Minimum grazer nitrogen quota	0.2	mol N (mol C) ⁻¹
$Q_z^{Fe,max}$	Maximum grazer iron quota	2×10^{-5}	mol Fe (mol C) ⁻¹
$Q_z^{Fe,min}$	Minimum grazer iron quota	1×10^{-6}	mol Fe (mol C) ⁻¹

*These constants were originally tuned to simulate stoichiometry and growth of the cyanobacteria *Synechococcus linearis* in the original study that developed the macromolecular model²³, and in the study that embedded the macromolecular model in the Darwin package in the MITgcm²⁵.

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