1014   Supplement A:

1015   Absolute masses of IPLS detected in this study including for GDGTs, OH-GDGTs, and
1016   diOH-GDGTs with either MH, DH, or HPH head.

Monohexose (MH)

	H+	NH4+	Na+
GDGT-0	1464.375493	1481.402042	1486.357437
GDGT-1	1462.359843	1479.386392	1484.341787
GDGT-2	1460.344193	1477.370742	1482.326137
GDGT-3	1458.328542	1475.355092	1480.310487
GDGT-Cren	1454.297242	1471.323791	1476.279187
OH-GDGT-0	1480.370407	1497.396956	1502.352352
diOH-GDGT0	1496.365322	1513.391871	1518.347267

Dihexose (DH)

	H+	NH4+	Na+
GDGT-0	1626.428316	1643.454865	1648.410261
GDGT-1	1624.412666	1641.439215	1646.394611
GDGT-2	1622.397016	1639.423565	1644.378961
GDGT-3	1620.381366	1637.407915	1642.363310
GDGT-Cren	1616.350066	1633.376615	1638.332010
OH-GDGT-0	1642.423231	1659.449780	1664.405175
diOH-GDGT0	1658.418145	1675.444694	1680.400090

Hexosephosphohexose (HPH)

|	H+	NH4+	Na+
GDGT-0	1706.394646	1723.421195	1728.376591
GDGT-1	1704.378996	1721.405545	1726.360941
GDGT-2	1702.363346	1719.389895	1724.345291
GDGT-3	1700.347696	1717.374245	1722.329641
GDGT-Cren	1696.316396	1713.342945	1718.298341
OH-GDGT-0	1722.389561	1739.416110	1744.371506
diOH-GDGT0	1738.384476	1755.411025	1760.366420

1017

1018   Supplement B:

1019   S1: CTD matrix showing temperature (°C), salinity (PSU), Fluorescence (mg/m^3), Oxygen
1020   (ml/L) for CTD stations PS104/003 (A), PS104/007 (B), PS104/017 (C), PS104/022 (D),
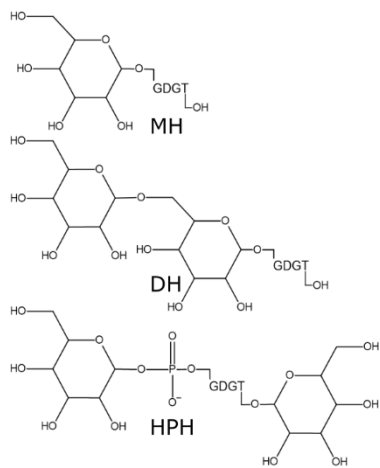1021   PS104/043 (E), with sample depths indicated by a triangle.
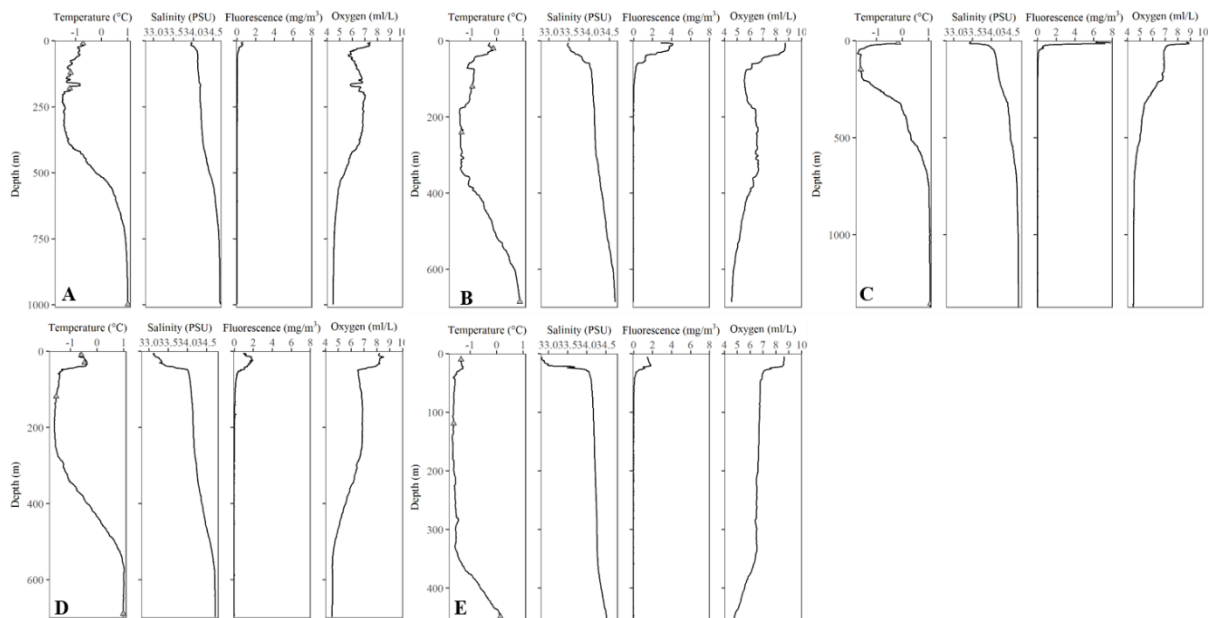
1022

1023   S2: Intact GDGT structures showing GDGT cores where, GDGT: R & R' = H; OH-GDGT:
1024   R=OH, R'=H; diOH-GDGT: R & R' = OH. Monohexose (MH), dihexose (DH), and hexose-
1025   phosphohexose (HPH) polar head groups structures shown.
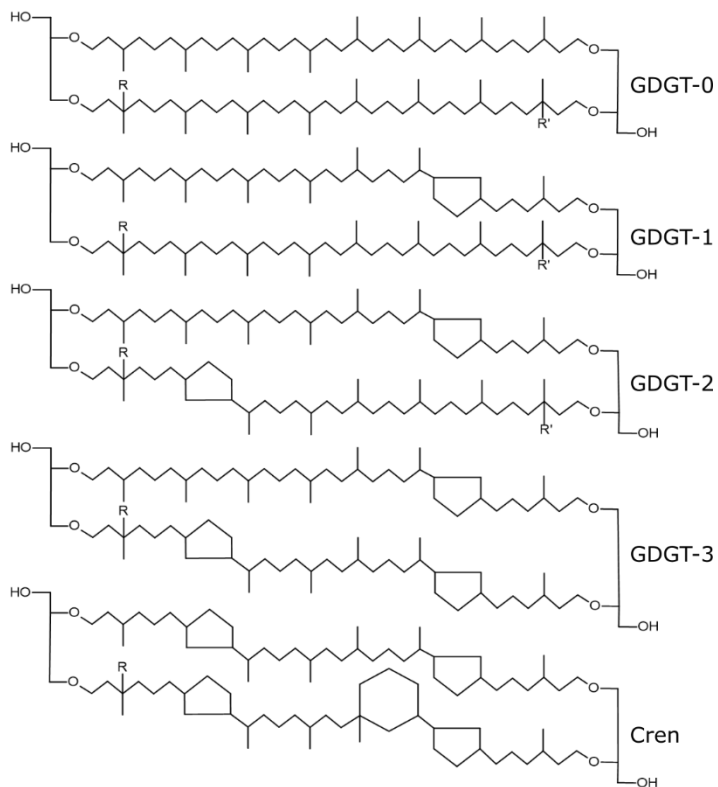
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1028   Supplement C: Redundancy analysis (RDA) raw outputs.

1029   Table 1: Variance inflation factors (VIF) for explanatory variables

Explanatory variable	Temperature	Salinity	Oxygen concentration	Fluorescence
VIF	7.8	10.2	11.4	3.5

1030   Table 2: RDA – partitioning of correlations

	Inertia	Proportion
Total	7	1.00
Constrained	4.46	0.64
Unconstrained	2.54	0.36

1031   Table 3: RDA - Eigenvalues and their contribution to the correlations.

	RDA1	RDA2	RDA3	RDA4	PC1	PC2	PC3	PC4	PC5	PC6	PC7
Eigenvalue	3.65	0.75	0.05	0.01	1.71	0.43	0.25	0.11	0.03	0.01	0.00
Proportion Explained	0.52	0.11	0.01	0.00	0.24	0.06	0.04	0.02	0.00	0.00	0.00
Cumulative Proportion	0.52	0.63	0.64	0.64	0.88	0.94	0.98	0.99	1.00	1.00	1.00

1032   Table 4: Accumulated constrained eigenvalues and importance of components.

	RDA1	RDA2	RDA3	RDA4
Eigenvalue	3.65	0.75	0.05	0.01
Proportion Explained	0.82	0.17	0.01	0.00
Cumulative Proportion	0.82	0.99	1.00	1.00

1033   Table 5: RDA Species scores.

	RDA1	RDA2	RDA3	RDA4	PC1	PC2
gdgt_mh_0	-0.89	0.51	-0.01	0.04	0.10	0.46
gdgt_mh_cren	-0.87	0.50	0.12	-0.02	0.07	0.53
gdgt_hph_0	0.32	-0.29	0.17	-0.02	-1.02	-0.06
gdgt_hph_cren	0.44	-0.08	0.10	0.08	-1.03	0.17
ohgdgt_mh_0	-1.03	-0.20	0.01	-0.04	0.00	0.20
ohgdgt_dh_0	-0.97	-0.40	0.06	0.02	-0.30	-0.06
diohgdgt_mh_0	-0.97	-0.43	-0.07	0.04	-0.18	-0.07

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1035   Table 6: Site scores (weighted sums of species scores).

	RDA1	RDA2	RDA3	RDA4	PC1	PC2
23_100m	-0.32	1.37	-1.88	-0.40	0.23	-0.72
24_80m	-0.88	2.86	1.47	0.25	0.30	1.85
22_110m	-0.82	0.27	-1.06	-4.77	0.39	0.65
21_110m	-2.01	-1.61	-0.81	5.34	-0.15	-0.01
20_110m	-0.85	-0.41	1.26	-3.09	-0.09	-0.03
19_80m	0.08	-1.01	2.75	-0.61	-0.47	-1.38
18_90m	0.43	-0.67	4.57	7.95	-1.50	-0.77
16_70m	0.55	-0.04	-3.74	-4.30	0.59	0.08
13_65m	0.67	0.42	-2.57	-0.01	0.20	-0.14
10_80m	0.77	-0.13	-2.24	-4.25	0.36	-0.90
7_75m	0.51	-0.09	-3.85	-6.24	0.91	0.17
5_70m	1.06	-1.39	10.65	11.95	-1.93	1.20
3_60m	0.80	0.44	-4.55	-1.83	1.14	0.00

1036   Table 7: Site constraints (linear combinations of constraining variables).

	RDA1	RDA2	RDA3	RDA4	PC1	PC2
23_100m	-0.35	1.73	0.89	-0.71	0.23	-0.72
24_80m	-0.73	1.27	-0.07	0.31	0.30	1.85
22_110m	-0.54	0.03	0.22	-0.07	0.39	0.65
21_110m	-1.89	-1.36	-0.46	0.28	-0.15	-0.01
20_110m	-0.84	-0.30	0.03	-0.30	-0.09	-0.03
19_80m	-0.31	-0.13	1.47	-0.48	-0.47	-1.38
18_90m	0.23	0.92	-1.21	1.56	-1.50	-0.77
16_70m	0.77	-0.26	-0.93	-1.50	0.59	0.08
13_65m	0.71	0.39	-1.23	-0.78	0.20	-0.14
10_80m	0.24	-0.57	-0.63	0.02	0.36	-0.90
7_75m	0.58	-0.76	0.08	0.72	0.91	0.17
5_70m	1.08	-0.77	0.85	-0.50	-1.93	1.20
3_60m	1.06	-0.19	0.99	1.44	1.14	0.00

1037   Table 8: Biplot scores for constraining variables.

	RDA1	RDA2	RDA3	RDA4	PC1	PC2
temperature	-0.84	0.41	0.30	-0.18	0.00	0.00
salinity	0.21	-0.94	0.21	0.20	0.00	0.00
oxygen	0.78	0.61	-0.16	-0.02	0.00	0.00
fluorescence	0.77	0.08	0.11	0.62	0.00	0.00

1038   Table 9: ANOVA for RDA

	Df	Variance	F	Pr(>F)
Model	4	4.46	3.50	0.01
Residual	8	2.54		

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1040   Table 10: ANOVA by axis.

	Df	Variance	F	Pr(>F)
RDA1	1	3.65	11.48	0.00
RDA2	1	0.75	2.35	0.42
RDA3	1	0.05	0.15	1.00
RDA4	1	0.01	0.03	1.00
Residual	8	2.54		

1041   Table 11: ANOVA by terms.

	Df	Variance	F	Pr(>F)
temperature	1	2.72	8.56	0.00
salinity	1	0.83	2.61	0.07
oxygen	1	0.82	2.58	0.09
fluorescence	1	0.08	0.26	0.87
Residual	8	2.54		

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