Diversity of intact polar lipids in the oxygen minimum zone of the Eastern Tropical North Pacific: Biogeochemical implications of non-phosphorus lipids

Florence Schubotz [1*], Sitan Xie [1,¶], Julius S. Lipp [1], Kai-Uwe Hinrichs [1], Stuart G. Wakeham[2]

[1]MARUM Center for Marine Environmental Sciences and Department of Geosciences, University of Bremen, 28359 Bremen, Germany

[2]Skidaway Institute of Oceanography, Savannah, GA 31411, USA

[¶]Current address: Wai Gao Qiao Free Trade Zone, 200131 Shanghai, China

[*]Corresponding author. MARUM, University of Bremen, Leobener Str. 13, Room 1070, 28359 Bremen, Germany. Tel: +49-421-218-65724. Fax: +49-421-218-65715. E-mail: schubotz@uni-bremen.

Suppl. Table 1. Absolute concentrations of pigments detected in surface waters of the Eastern Tropical North Pacific at stations 1, 5 and 8.

		Conc (ng/L)																													
Station	Depth (m)	MgDVP	Chl c2	Chl c1	Per	19-But	Fuco	Neo	Prasino	Viola	19-Hex	DD	Cis-fuco	Allo	DT	Zeax	Lutein	Lutein Late	8-Apo	Croco	DV Chl a	Chl a	Chl c2 Like	a-Car	b-Car	Chl c3	Chl b	c-MVP	Sum Ph-ide	Ph-ide 2	Ph-ide 3	Ph-tin
1	3	2.64	7.55	0.00	0.00	4.77	4.74	0.00	0.00	0.00	14.60	3.24	0.00	0.00	0.00	109.7	1.53	0.00	18.46	0.00	69.51	125.76	0.00	10.94	4.02	7.91	30.08	0.00	0.00	0.00	0.00	5.35
1	9	4.07	3.91	0.00	0.00	5.69	4.95	0.00	0.00	0.00	15.94	3.79	0.00	0.00	0.00	136.6	1.05	3.97	15.21	0.00	74.43	123.91	0.00	13.97	6.14	4.08	28.25	0.00	0.00	0.00	0.00	6.61
1	16	4.84	15.00	0.00	2.49	8.66	6.83	0.75	0.00	0.00	23.91	3.31	0.00	0.00	0.00	90.62	0.00	9.54	14.95	0.00	87.95	148.73	2.24	14.79	4.19	12.87	36.40	0.91	0.38	0.00	0.38	9.29
1	29	8.08	32.27	0.00	1.75	16.59	38.92	1.17	1.58	0.53	42.64	4.18	0.00	1.47	0.00	60.07	0.00	1.59	17.28	3.23	91.55	293.10	2.80	47.24	3.23	43.08	136.8	0.00	55.53	10.81	44.72	23.40
1	51	25.23	20.58	11.20	0.00	6.46	8.73	0.85	3.49	0.00	15.57	1.14	0.00	1.41	0.00	37.65	0.00	0.00	17.22	4.03	132.9	148.47	6.44	105.9	0.00	14.95	238.3	2.70	68.71	14.21	54.50	35.86
1	71	17.78	102.6	0.00	0.00	15.65	246.1	0.00	0.00	63.51	63.10	14.01	10.36	0.00	0.00	19.87	0.00	0.00	18.67	4.29	21.58	931.31	16.29	103.0	17.00	276.1	79.45	15.18	333.2	79.38	253.8	101.6
5	0	0.00	192.1	0.00	12.99	187.8	270.1	6.43	0.00	0.00	240.8	51.14	0.00	5.60	3.52	62.41	0.00	8.06	15.56	0.00	8.76	1352.2	15.66	5.56	14.05	152.7	100.1	14.63	52.93	10.79	42.14	33.16
5	25	6.79	181.5	0.00	23.55	156.3	279.2	0.00	9.86	0.00	224.5	33.02	0.00	5.25	0.00	38.49	0.00	7.04	15.96	0.00	0.00	1319.5	9.27	0.00	12.44	184.3	81.11	17.59	73.68	0.00	73.68	54.97
5	30	5.13	148.8	0.00	20.79	97.17	230.6	2.41	21.46	0.00	253.4	21.60	0.00	7.45	0.00	16.37	0.00	7.06	15.74	15.57	0.00	1234.4	7.25	8.25	9.26	206.5	95.88	26.30	128.5	35.16	93.40	58.44
5	50	4.82	39.66	0.00	0.00	4.68	19.93	0.00	0.00	0.00	48.81	0.00	0.00	0.00	0.00	6.07	0.00	0.00	16.28	0.00	17.57	229.27	0.00	0.00	16.58	59.42	85.63	7.91	0.00	0.00	0.00	5.26
8	3	3.66	10.30	0.00	3.92	14.61	13.04	1.97	0.00	0.00	48.72	10.54	0.00	0.00	0.36	78.80	1.56	1.97	12.95	0.03	39.71	229.12	3.18	10.15	6.56	8.44	42.99	1.70	11.39	10.84	0.55	8.17
8	8	3.63	16.05	0.00	4.67	17.55	14.94	2.50	0.00	0.00	59.27	12.54	0.00	0.00	0.00	83.38	1.92	2.35	14.36	0.00	43.07	256.61	3.82	10.76	5.78	12.57	50.16	0.00	14.53	14.25	0.29	14.02
8	15	4.40	18.75	0.00	4.43	18.17	15.02	2.45	0.00	0.00	59.63	11.33	0.00	0.00	0.05	82.00	1.91	2.28	15.11	0.00	45.50	249.58	3.88	10.53	4.98	16.99	51.01	2.54	14.66	12.49	2.17	10.26
8	22	3.55	21.55	0.00	4.87	26.04	12.62	3.15	0.00	0.00	62.91	8.31	0.00	0.00	0.00	55.30	1.80	2.31	14.78	0.00	40.34	239.20	3.83	12.16	3.06	24.03	62.93	3.13	16.03	13.40	2.63	10.65
8	28	8.16	34.03	1.20	6.15	39.75	15.38	4.55	1.98	0.00	81.30	7.41	0.00	8.13	0.00	132.0	3.21	2.78	15.05	3.23	104.3	325.87	3.53	40.16	3.58	36.93	135.7	4.95	23.00	16.64	6.36	20.17
8	36	9.75	46.13	0.00	9.39	46.60	19.96	5.58	3.74	0.00	85.55	7.43	0.00	6.35	0.00	179.4	2.51	3.07	16.39	5.07	171.8	410.98	3.59	73.91	5.26	52.45	213.1	6.05	29.87	18.78	11.09	34.61
8	51	15.21	27.88	0.00	11.44	24.12	34.07	5.41	5.15	0.00	55.41	6.82	0.00	3.44	0.00	92.29	0.00	1.98	16.50	5.72	157.3	316.46	9.21	114.1	6.78	34.50	250.4	5.53	56.84	30.00	26.84	44.70
8	70	4.90	9.97	0.00	2.89	6.10	7.30	0.80	0.37	0.00	26.00	1.61	0.00	1.69	0.00	7.67	0.00	0.96	15.45	1.48	18.44	117.73	0.00	18.98	0.00	13.62	61.13	3.72	7.39	3.96	3.43	6.78
8	0	10.84	37.93	0.00	8.34	19.02	10.52	2.97	0.00	0.00	70.72	9.44	0.00	0.00	0.00	115.4	3.21	2.95	14.47	0.00	68.20	280.17	4.31	19.80	7.23	62.74	66.98	2.75	13.96	3.60	10.35	6.93
8	8	8.71	26.02	0.00	9.92	26.58	11.05	4.33	0.00	0.00	91.62	12.79	0.00	0.00	0.00	145.1	3.84	3.63	15.33	17.41	85.10	337.85	5.44	19.81	6.96	29.75	82.22	3.53	16.36	10.98	5.38	13.84
8	15	3.91	16.41	0.00	6.50	23.06	9.86	3.50	0.00	0.00	77.40	10.31	0.00	1.00	0.00	92.79	1.66	3.03	15.80	0.36	59.86	277.69	4.32	15.46	5.37	17.11	70.49	2.77	18.44	18.44	0.00	13.64
8	22	4.94	37.27	0.00	7.67	47.25	12.27	4.76	0.00	0.00	94.68	7.68	0.00	4.44	0.00	49.99	2.10	3.49	15.42	0.00	19.44	359.89	5.32	8.21	3.48	45.18	100.2	5.54	4.38	3.93	0.45	12.13
8	36	9.30	31.81	0.00	6.37	60.45	32.80	4.85	2.32	0.00	62.93	6.48	0.00	2.79	0.00	47.77	0.00	2.61	14.82	0.14	59.68	365.47	3.08	27.08	2.72	43.56	131.7	5.68	7.47	5.87	1.60	16.81
8	51	11.20	28.60	0.00	2.88	23.59	38.55	4.25	4.48	0.00	37.61	4.76	0.00	2.40	0.00	71.85	0.00	1.53	17.44	4.84	147.4	278.60	8.48	138.1	0.00	34.34	270.8	4.81	45.38	16.85	28.53	45.95

Suppl. Table 2. Relative abundance of detected intact polar lipids at all four stations (1, 2, 5 and 8) in the Easter Tropical North Pacific.

			Relative Abundance (%)																							
Station	Depth (m)	Total IPL (ng/L)	1G-DAG	2G-DAG	SQ-DAG	DGTS	PE+PC-AEG	PE	PC	PG	DPG	3G-DAG	SQ-DEG	1G-Cer	DGCC	2nd DGCC	OL	PME	PDME	PI	1G-OH-DAG	1G-OH-Cer	OH-DGTS	1G-GDGT	2G-GDGT	HPH-GDGT
1	3	882.25	17.42	9.76	51.22	1.34	1.41	2.82	3.51	9.03	0.00	0.18	1.27	0.28	0.01	0.93	0.00	0.00	0.00	0.53	0.07	0.23	0.00	0.00	0.00	0.00
1	25	1357.81	18.44	9.58	34.31	5.26	4.89	3.19	5.04	13.52	0.01	0.17	1.68	0.56	0.07	1.90	0.00	0.00	0.00	0.34	0.26	0.78	0.00	0.00	0.00	0.00
1	35	361.55	15.03	13.55	16.68	2.43	29.83	2.99	8.53	3.97	0.07	0.47	0.31	0.80	0.34	2.16	0.00	0.00	0.00	1.81	0.37	0.66	0.00	0.00	0.00	0.00
1	75	303.98	28.54	8.71	39.77	0.92	4.24	1.53	3.66	7.70	0.23	0.22	0.00	0.44	0.16	1.91	0.00	0.00	0.00	0.35	0.34	0.50	0.00	0.24	0.12	0.40
1	120	22.26	22.94	4.47	8.65	5.51	11.84	4.20	10.66	14.38	1.10	0.08	0.00	1.39	0.23	2.90	0.00	0.12	0.41	0.27	0.00	0.53	0.00	3.28	2.55	4.50
1	200	8.38	23.18	0.98	0.68	14.04	11.89	3.81	10.88	5.69	0.79	0.00	0.00	1.15	0.43	2.87	0.00	1.07	2.34	0.00	0.00	0.34	0.00	16.41	3.22	0.25
1	300	2.88	21.42	2.87	4.02	7.79	4.46	4.10	4.95	18.54	4.79	0.00	0.00	1.18	1.24	3.21	0.00	2.85	0.00	0.00	0.00	1.16	0.00	14.85	2.58	0.00
1	400	56.4	3.10	2.93	11.30	2.73	0.00	8.78	8.08	50.56	3.14	0.00	0.37	0.36	1.48	2.27	0.00	1.98	0.61	0.07	0.00	0.00	0.00	1.45	0.78	0.00
1	600	11.42	5.58	0.88	2.83	3.54	3.94	15.05	7.98	33.89	3.11	0.00	0.00	0.00	1.30	0.22	0.00	4.33	0.14	0.00	0.10	0.00	0.00	13.32	3.81	0.00
1	725	9.67	9.79	1.01	1.89	9.58	8.73	6.10	13.25	16.22	1.46	0.00	0.00	0.31	0.32	2.11	0.00	0.00	0.00	0.18	0.00	0.53	0.00	14.95	10.41	3.16
1	820	3.25	12.34	1.98	1.06	8.36	11.40	7.31	15.11	16.81	1.76	0.00	0.00	0.34	0.21	2.97	0.00	0.00	0.00	0.07	0.00	0.46	0.00	9.31	9.38	1.15
1	1250	0.82	32.36	1.28	1.91	14.91	1.95	0.85	1.64	12.96	1.39	0.00	0.00	0.60	0.31	1.59	0.00	0.00	0.00	0.00	0.20	0.47	0.00	20.97	6.31	0.31
2	3	266.21	9.31	18.86	35.71	6.82	4.85	1.43	8.63	6.16	0.11	0.23	1.43	0.85	0.15	2.50	0.03	0.00	0.26	0.39	0.04	0.50	1.73	0.00	0.00	0.00
2	6	349.59	30.10	14.90	20.28	7.18	5.91	0.85	3.52	8.96	0.08	0.03	5.02	0.12	0.04	1.00	0.00	0.12	0.00	0.37	0.11	1.40	0.01	0.00	0.00	0.00
2	55	21.85	18.14	17.51	12.45	3.74	26.53	2.78	8.86	3.63	0.05	0.20	0.36	0.26	0.26	3.35	0.02	0.05	0.00	0.44	0.10	1.02	0.00	0.25	0.00	0.00
2	85	160.03	24.27	7.49	33.48	3.45	7.25	2.72	7.05	4.70	0.90	0.02	0.36	0.76	0.08	4.15	0.05	0.62	0.59	0.33	0.54	0.29	0.00	0.64	0.20	0.04
2	115	50.04	7.00	6.60	18.20	4.97	7.41	5.81	9.06	21.86	2.01	1.61	0.91	1.80	0.28	6.16	0.13	1.51	0.32	0.26	0.00	1.07	0.00	2.05	0.98	0.00
2	200	5.96	79.95	0.00	0.40	10.83	0.23	0.19	0.33	0.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.51	0.00	0.00	6.82	0.00	0.00
2	400	12.59	4.18	2.78	4.82	5.37	4.07	13.00	17.18	31.18	4.67	0.49	0.00	0.88	0.00	1.55	0.54	3.91	1.85	0.13	0.00	0.00	0.00	1.71	0.71	0.95
2	600	11.76	2.37	0.00	12.47	2.11	1.94	0.05	1.94	34.06	11.26	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.06	0.00	0.00	0.00	0.00	6.48	13.81	7.50
2	830	7.24	6.24	3.45	6.81	7.74	12.55	8.69	11.48	14.99	1.56	0.99	0.51	1.22	0.18	5.07	0.01	2.94	1.74	0.65	0.00	1.14	0.00	5.10	1.81	5.10
5	3	244.4	23.11	16.14	18.40	24.59	3.77	0.79	4.12	4.64	0.14	0.00	1.21	1.08	0.02	0.42	0.00	0.00	0.00	0.12	0.85	0.53	0.07	0.00	0.00	0.00
5	25	1187.57	66.08	1.03	4.14	22.93	0.00	0.21	0.44	4.47	0.00	0.00	0.00	0.00	0.17	0.19	0.00	0.00	0.00	0.06	0.29	0.00	0.00	0.00	0.00	0.00
5	35	38.14	67.72	0.74	4.03	14.54	2.78	0.42	1.66	3.30	0.03	0.00	0.00	0.59	0.00	0.19	0.00	0.05	0.00	0.03	0.76	0.00	1.00	2.16	0.00	0.00
5	75	174.78	20.48	11.04	49.35	2.91	0.21	0.33	0.87	8.61	1.81	0.01	0.25	0.18	0.02	0.33	0.01	0.09	0.18	0.18	0.42	0.00	0.02	1.06	0.85	0.80

5	125	2.32	3.91	6.66	35.32	5.65	9.32	3.58	2.80	3.57	0.77	0.24	0.17	1.77	0.22	5.59	0.00	11.94	0.40	0.14	0.07	0.00	0.03	7.06	0.00	0.79
5	250	1.05	41.71	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	58.29	0.00	0.00
5	400	11.22	5.42	2.83	4.97	7.65	3.42	11.79	11.26	33.04	3.35	0.36	0.00	0.40	0.09	2.12	0.48	5.11	1.29	0.14	0.00	0.35	0.00	4.01	0.79	1.12
5	600	21.35	3.87	4.16	6.35	5.83	2.06	17.10	15.09	21.99	5.47	1.30	0.44	2.18	0.30	4.06	0.66	5.38	2.75	0.35	0.00	0.67	0.00	0.00	0.00	0.00
5	830	12.36	5.68	3.63	7.17	7.71	12.82	8.60	11.57	15.35	1.59	1.05	0.54	1.29	0.18	5.27	0.11	3.14	1.96	0.68	0.00	1.20	0.00	4.13	1.25	5.07
8	3	955.41	11.21	16.19	14.89	9.00	5.75	3.99	13.62	8.61	0.49	0.01	2.40	1.13	0.05	3.47	0.35	0.50	0.22	0.69	0.21	0.25	6.92	0.03	0.00	0.03
8	10	1458.79	8.55	18.50	19.24	6.02	12.12	3.23	11.57	8.26	0.15	0.08	2.45	1.40	0.10	3.82	0.13	0.05	0.07	1.10	0.00	0.15	2.99	0.00	0.00	0.00
8	25	348.72	13.22	22.19	11.63	6.76	12.91	3.92	9.53	8.16	0.04	0.08	1.38	0.99	0.59	3.72	0.07	0.09	0.00	0.03	0.14	1.34	3.21	0.00	0.00	0.00
8	50	474.36	18.03	18.29	18.36	5.69	10.18	5.30	11.27	3.07	0.22	0.07	0.27	1.13	0.58	3.25	0.00	0.00	0.00	0.34	0.53	0.74	0.88	0.84	0.24	0.74
8	125	54.21	9.82	1.91	1.67	4.36	14.11	8.51	15.81	6.48	0.90	0.03	0.10	1.30	0.36	3.48	0.02	1.86	0.84	0.19	0.00	0.41	1.00	9.07	6.71	11.05
8	200	3.78	41.10	0.23	0.31	14.47	0.00	0.05	0.29	1.75	0.98	0.00	0.00	0.14	0.29	0.73	0.00	0.00	0.00	0.53	0.00	0.31	1.11	22.28	0.42	15.04
8	350	19.54	6.68	1.35	1.12	10.54	8.51	7.51	12.56	11.34	5.65	0.12	0.00	2.30	0.54	7.20	0.20	6.04	4.29	0.08	0.00	0.99	1.79	6.52	1.01	3.65
8	450	1.47	24.18	0.00	0.00	22.57	2.09	1.17	2.40	1.45	0.45	0.00	0.00	0.48	0.78	1.08	0.00	1.06	3.21	0.00	0.00	0.34	2.39	22.79	0.87	12.67
8	550	17.19	9.40	1.43	3.49	8.68	9.44	11.39	15.51	15.13	1.86	0.22	0.00	0.00	0.37	5.75	0.10	5.27	2.87	0.15	0.00	0.73	0.60	4.02	1.44	2.13
8	650	5.07	32.44	0.00	0.00	30.37	1.24	0.05	0.63	1.22	0.04	0.00	0.00	0.00	1.31	1.03	0.00	0.00	0.00	0.00	0.00	0.00	1.59	19.45	0.14	10.53
8	750	0.1	14.54	0.00	0.00	0.36	0.00	0.05	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	61.21	0.00	23.85
8	1000	0.1	37.87	0.00	0.00	1.59	0.00	0.05	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	40.69	0.00	19.77
8	1250	0.12	47.27	0.00	0.00	0.61	0.00	0.05	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00	0.12	0.00	0.79	36.26	0.00	14.85

Suppl. Table 3. Fatty acyl combinations (chain lengths and double bonds) of the major groups of intact polar lipids and their relative abundance at different depths within the water column of the Eastern Tropical North Pacific.

					Rel. Abundance (%)							
					Oxic		Upper OMZ		Core OMZ		Deep Oxycline	
IPL	*m/z* (pos mode)	Chain length	Double bonds	FA combination	Mean	SD	Mean	SD	Mean	SD	Mean	SD
1G-DAG	788.531	36	8		1.86	1.03	3.55	4.15	0.74	0.50	1.10	0.24
	786.515	36	9	18:4/18:4	6.05	7.89	1.72	1.67	0.84	0.87	1.52	0.31
	774.609	34	1		2.69	1.99	1.48	1.36	2.59	1.93	2.96	1.06
	766.546	34	5		1.17	0.82	1.74	1.31	1.11	0.47	3.43	3.63
	762.515	34	7	18:3/16:4	5.07	3.61	1.59	1.00	2.20	1.52	2.70	0.61
	746.578	32	1		3.82	5.24	3.59	2.09	4.53	1.78	4.54	0.71
	732.562	31	1		2.09	2.55	2.02	1.51	2.96	1.93	2.43	1.72
	720.562	30	0	16:0/14:0	6.98	10.09	5.76	2.92	7.15	3.49	6.99	0.86
	718.546	30	1	16:1/14:0	27.91	10.70	40.79	11.46	49.59	5.41	39.07	3.42
	716.531	30	2	16:2/14:0	10.59	7.40	11.90	5.88	7.93	2.21	7.74	2.53
	692.531	28	0		4.79	2.82	2.97	1.30	4.48	1.18	3.71	1.20
	690.515	28	1		3.83	2.61	4.54	2.48	3.18	1.18	2.45	1.35
2G-DAG	948.568	36	9		2.11	1.62	1.18	1.35	0.41	0.50	4.10	6.60
	936.662	34	1	18:1/16:0	5.27	2.43	4.50	4.54	13.94	1.86	11.00	5.92
	934.646	34	2	18:2/16:0	6.68	2.86	2.87	2.77	7.43	3.02	9.11	4.42
	932.631	34	3	18:3/16:0	4.94	1.71	2.45	1.91	2.95	1.75	4.93	1.89
	930.615	34	4		3.15	1.65	1.66	1.62	1.54	0.89	3.37	1.14
	928.599	34	5	18:3/16:2	4.11	1.86	1.64	1.22	1.43	0.93	6.93	9.29
	926.584	34	6		3.12	1.66	1.61	1.56	1.36	0.91	2.28	1.57
	924.568	34	7	18:3/16:4	4.90	2.40	1.73	1.78	1.20	0.80	2.75	0.39
	908.631	32	1	18:1/14:0 ;	5.03	2.49	13.67	12.27	23.54	5.07	15.29	4.20
	906.615	32	2		2.20	0.92	3.52	4.42	2.89	1.71	3.42	0.84
	902.584	32	4	18:4/14:0	5.45	2.91	1.14	2.07	0.78	0.68	0.76	0.94
	900.568	32	5	18:5/14:0	4.76	2.10	4.25	13.38	0.17	0.49	0.63	1.27
	898.552	32	6		4.19	7.62	0.27	0.42	0.00	0.00	0.00	0.00
	882.615	30	0	16:0/14:0	13.49	6.98	17.20	7.58	15.68	1.76	9.10	7.37
	880.599	30	1	16:1/14:0	9.95	3.90	24.46	11.88	16.88	2.52	9.50	6.58
	878.584	30	2	16:2/14:0	2.71	2.54	5.21	4.96	0.09	0.26	0.00	0.00
	854.584	28	0		3.82	2.91	3.17	3.47	2.73	4.45	1.72	3.44
SQ-DAG	838.571	34	1	18:1/16:0	1.97	1.08	2.83	3.36	4.98	4.57	8.52	7.97
	836.555	34	2		4.02	2.38	1.70	1.63	1.02	1.23	1.64	1.90
	834.540	34	3		3.22	1.71	0.56	0.72	0.44	0.87	1.24	1.43

	812.555	32	0	16:0/16:0 ;	9.15	3.10	4.46	3.78	9.29	4.07	12.60	3.12
	810.540	32	1	16:1/16:0	7.29	2.63	11.61	6.09	12.53	2.50	10.36	4.74
	808.524	32	2	16:1/16:1	5.23	3.07	11.49	7.09	6.69	3.79	5.43	4.34
	784.524	30	0	16:0/14:0	26.72	5.24	24.93	16.07	30.45	3.33	30.89	3.33
	782.508	30	1	16:1/14:0	15.90	6.46	31.16	11.93	13.75	4.21	12.69	4.69
	780.493	30	2	16:2/14:0	4.95	3.47	2.81	4.28	7.29	11.51	0.47	0.54
	756.493	28	0	14:0/14:0	16.24	6.46	6.84	5.26	13.57	11.15	13.66	9.59
PG	806.591	37	2		1.59	2.88	1.88	2.51	3.07	1.23	2.63	1.39
	792.575	36	2	18:1/18:1	9.81	5.61	7.12	3.44	9.78	3.67	7.69	0.25
	780.575	35	1		1.55	2.32	3.48	2.67	4.22	1.57	3.26	0.62
	778.559	35	2	18:1/17:1 ;	3.26	2.46	10.69	6.95	13.26	2.11	11.05	0.62
	766.559	34	1	18:1/16:0	12.32	2.78	8.63	8.75	7.21	2.63	7.00	0.45
	764.544	34	2	18:2/16:0	21.87	10.62	18.84	8.87	19.50	4.17	25.57	4.49
	762.528	34	3	18:3/16:0	15.03	9.19	2.67	3.22	3.78	1.34	3.78	0.32
	752.544	33	1	17:1/15:0	7.52	4.63	13.03	5.80	16.60	2.27	14.65	3.77
	738.528	32	1	16:1/16:0	11.41	4.41	11.43	5.08	10.84	3.29	10.11	1.45
	736.512	32	2	16:1/16:1	13.19	3.79	19.08	12.58	9.77	2.20	10.42	0.80
	710.497	30	1		2.31	1.41	3.09	1.76	1.76	1.22	3.84	0.17
PE	730.538	32	2	18:1/17:1	12.02	9.37	19.53	13.16	23.32	7.97	19.51	11.03
	718.538	34	1	18:1/16:0	7.28	6.14	6.44	7.72	11.29	5.49	9.85	6.57
	716.522	34	2	18:1/16:1 ;	3.78	3.64	2.91	2.90	9.97	8.36	3.83	2.93
	704.522	33	1	17:1/16:0	22.14	14.88	16.16	8.54	13.55	2.63	10.32	6.89
	702.507	33	2		1.32	1.33	1.79	2.25	2.05	1.35	4.12	5.50
	690.507	32	1	16:1/16:0	6.93	10.80	5.53	7.05	7.11	4.76	8.29	10.09
	688.491	32	2		2.26	4.02	3.14	10.46	3.16	3.63	0.48	0.97
	678.507	31	0	16:0/15:0	33.48	20.83	23.89	15.41	10.07	4.24	15.60	11.12
	676.491	31	1		3.82	3.31	2.83	2.43	3.07	1.10	1.66	1.85
	674.476	31	2		0.09	0.30	0.02	0.07	0.04	0.11	0.00	0.00
	664.491	30	0	16:0/14:0	1.54	2.69	8.02	8.30	6.76	2.37	11.74	4.36
	662.476	30	1		1.57	1.44	2.74	5.83	1.92	1.77	2.72	4.35
	650.476	29	0	15:0/14:0	2.61	2.09	6.66	5.43	6.50	3.55	10.94	8.75
	648.460	29	1		0.08	0.19	0.14	0.34	0.04	0.11	0.00	0.00
	636.460	28	0		1.08	1.54	0.21	0.49	1.17	0.88	0.95	1.44
PC	878.575	44	12	22:6/22:6	3.87	3.27	6.12	11.60	3.83	7.70	2.29	3.39
	852.560	42	9	22:6/20:5	1.87	1.60	2.90	3.11	3.55	6.04	4.79	5.74
	822.601	39	5		1.59	1.12	1.50	1.49	0.67	0.93	1.47	1.35
	806.569	38	6	22:6/16:0	20.28	7.02	19.69	16.84	13.97	11.29	36.10	36.79
	788.616	36	1		1.74	1.20	1.76	1.63	2.28	4.20	0.74	0.68
	780.554	36	5	20:5/16:0	12.14	7.79	9.03	6.74	4.58	3.79	8.41	6.72
	776.616	35	0		0.49	0.66	1.09	1.23	0.59	0.58	0.71	0.77
	774.601	35	1		1.69	0.98	1.68	1.58	1.53	1.07	2.12	3.00
	760.585	34	1	18:1/16:0	6.68	4.39	5.27	3.65	8.01	8.70	2.70	3.23
	754.538	34	4		2.73	1.57	1.86	2.02	0.76	0.66	1.15	1.10

	748.585	33	0		1.21	1.18	1.93	1.89	1.59	1.36	1.24	1.20
	746.569	33	1		1.85	3.95	3.18	3.63	3.88	2.12	2.66	2.43
	744.554	33	2	17:1/16:1	0.91	1.03	1.97	1.68	5.96	6.54	2.33	1.39
	734.569	32	0	16:0/16:0 ;	6.20	3.84	4.16	3.36	4.78	4.00	3.09	2.34
	732.554	32	1	16:0/16:1	4.83	2.98	5.96	3.69	7.15	3.92	6.15	3.68
	730.538	32	2	16:1/16:1	2.19	1.51	4.96	4.91	7.57	4.32	4.47	3.08
	720.554	31	0		1.86	1.32	2.86	3.45	2.09	1.43	1.61	1.59
	718.538	31	1		1.65	1.61	1.91	3.22	3.86	2.53	2.63	2.51
	716.522	31	2		0.91	1.01	0.87	1.10	4.55	5.76	0.97	0.89
	706.538	30	0	16:0/14:0	9.35	2.79	5.68	4.00	3.29	1.87	2.53	2.65
	704.522	30	1	16:1/14:0	4.89	4.78	3.71	2.41	4.62	2.79	2.75	2.62
	702.507	30	2		0.25	0.27	0.48	0.66	0.87	0.90	1.19	1.98
	692.522	29	0		2.13	1.68	3.21	2.35	2.26	1.52	1.67	1.99
	690.507	29	1		2.01	3.26	1.57	1.99	3.08	3.45	2.38	3.68
	688.491	29	2		0.45	0.64	0.76	2.63	1.57	2.59	0.10	0.21
	678.507	28	0	14:0/14:0	6.22	3.39	5.89	4.62	3.09	1.68	3.76	3.82
DGTS	764.640	36	2	18:1/18:1	6.72	3.20	8.70	4.81	14.23	4.45	7.86	2.68
	762.624	36	3		3.66	1.56	2.53	0.76	1.43	0.64	3.14	0.91
	760.609	36	4	18:2/18:2 ;	7.36	2.99	4.41	2.02	1.57	0.80	5.41	2.37
	758.593	36	5	18:2/18:3	5.12	2.44	2.89	1.46	1.45	0.80	3.96	1.22
	740.640	34	0		1.11	0.39	2.65	1.48	4.93	1.81	1.98	1.10
	738.624	34	1	18:1/16:0	3.90	1.70	14.87	13.30	32.49	12.73	14.69	2.83
	736.609	34	2	18:2/16:0	7.44	3.95	6.57	1.85	8.60	0.91	8.33	2.26
	734.593	34	3	18:3/16:0	5.04	2.11	2.84	1.05	1.14	0.59	3.33	0.85
	732.577	34	4		4.34	1.23	2.15	1.12	0.58	0.48	1.30	1.08
	710.593	32	1	18:1/14:0	3.94	1.25	6.92	2.50	9.60	4.41	10.54	2.56
	708.577	32	2	18:2/14:0	3.85	1.31	3.80	1.46	2.89	2.26	5.61	1.86
	706.562	32	3		2.65	0.83	2.07	1.25	0.74	0.41	3.05	2.00
	698.593	31	0		1.40	0.47	2.90	2.18	2.26	2.04	3.24	1.44
	684.577	30	0	16:0/14:0	3.90	1.45	3.69	1.69	2.18	1.75	3.45	0.77
	682.562	30	1	16:1/14:0	3.58	3.14	8.92	4.80	4.13	4.52	7.75	0.96
	670.562	29	0		3.60	1.39	3.47	1.93	2.14	1.62	2.34	0.76
	656.546	28	0	14:0/14:0	9.56	4.74	6.54	3.47	4.44	2.18	4.81	0.46

Suppl. Table 4. Goodness of fit statistics for the NMDS analyses of normalized intact polar lipid (IPL) composition and quantitative microbial data (FISH), number of double bonds in the IPL and chain length of IPL.

	IPL (relative abundance)			
FISH Probe	NMDS1	NMDS2	r2	p
Alphaproteobacteria	-0.56	-0.83	0.02	0.613
Betaproteobacteria	-0.60	-0.80	0.10	0.133
Gammaproteobacteria	-0.66	-0.76	0.24	0.004
SRB	-0.42	-0.91	0.33	0.002
Epsilonproteobacteria	-0.88	-0.47	0.18	0.022
Nso	-0.94	-0.33	0.18	0.023
Anammox	-0.04	-1.00	0.25	0.006
Planctomycetes	-0.87	-0.50	0.13	0.730

	Number of double bonds			
Environmental parameter	NMDS1	NMDS2	r2	p
Depth	-0.80	0.59	0.12	0.081
POC	0.93	-0.35	0.19	0.019
TN	0.95	-0.30	0.20	0.012
Phosphate	-0.90	0.44	0.12	0.740
Nitrate	-0.51	0.86	0.07	0.250
Nitrite	-0.57	-0.82	0.14	0.043
Ammonium	0.67	-0.75	0.06	0.311
Salinity	0.96	0.29	0.00	0.909
Temperature	0.66	-0.76	0.02	0.686
Fluorescence	0.97	-0.26	0.27	0.003
Oxygen	0.83	-0.55	0.26	0.002
Chl-a	0.96	-0.27	0.28	0.002

	Chain length (carbon atoms)			
Environmental parameter	NMDS1	NMDS2	r2	p
Depth	0.48	0.88	0.00	0.944
POC	-0.14	0.99	0.05	0.340
TN	-0.10	1.00	0.56	0.324
Phosphate	0.06	-1.00	0.03	0.531
Nitrate	0.65	-0.76	0.34	0.472
Nitrite	-0.54	-0.84	0.15	0.052
Ammonium	-0.15	0.99	0.05	0.339
Salinity	0.94	1.00	0.01	0.713
Temperature	-0.23	-0.97	0.01	0.882
Fluorescence	0.04	1.00	0.05	0.374
Oxygen	-0.12	0.99	0.09	0.138
Chl-a	-0.01	1.00	0.16	0.042

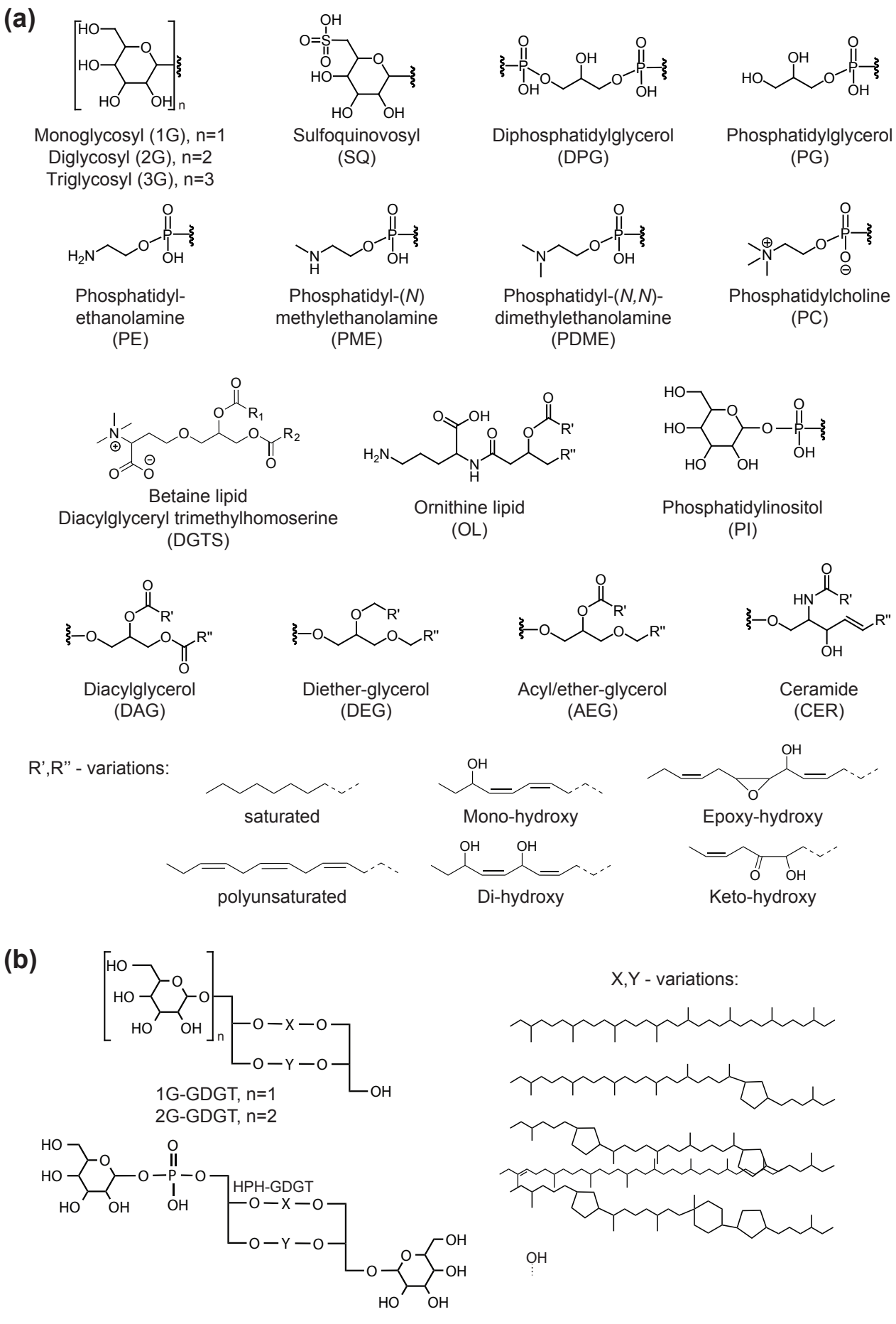
Suppl. Figure 1. Structures of (a) bacterial/eukaryotic and (b) archaeal IPLs observed in the ETNP. The position of the double bonds and the OH-, epoxy- and keto-groups of the R' and R'' side chains were not determined.

Suppl. Fig 2. Section plots of (a) total particulate nitrogen and (b) phaeophytin concentrations, absolute abundance of (c) archaeal and (d) unclassified cells and (e) absolute and (f) relative abundance of archaeal intact polar lipids (IPL) along a northwest-southeast transect of the study area in the ETNP. Numbers across the top panels denote station, black dots are individual samples.

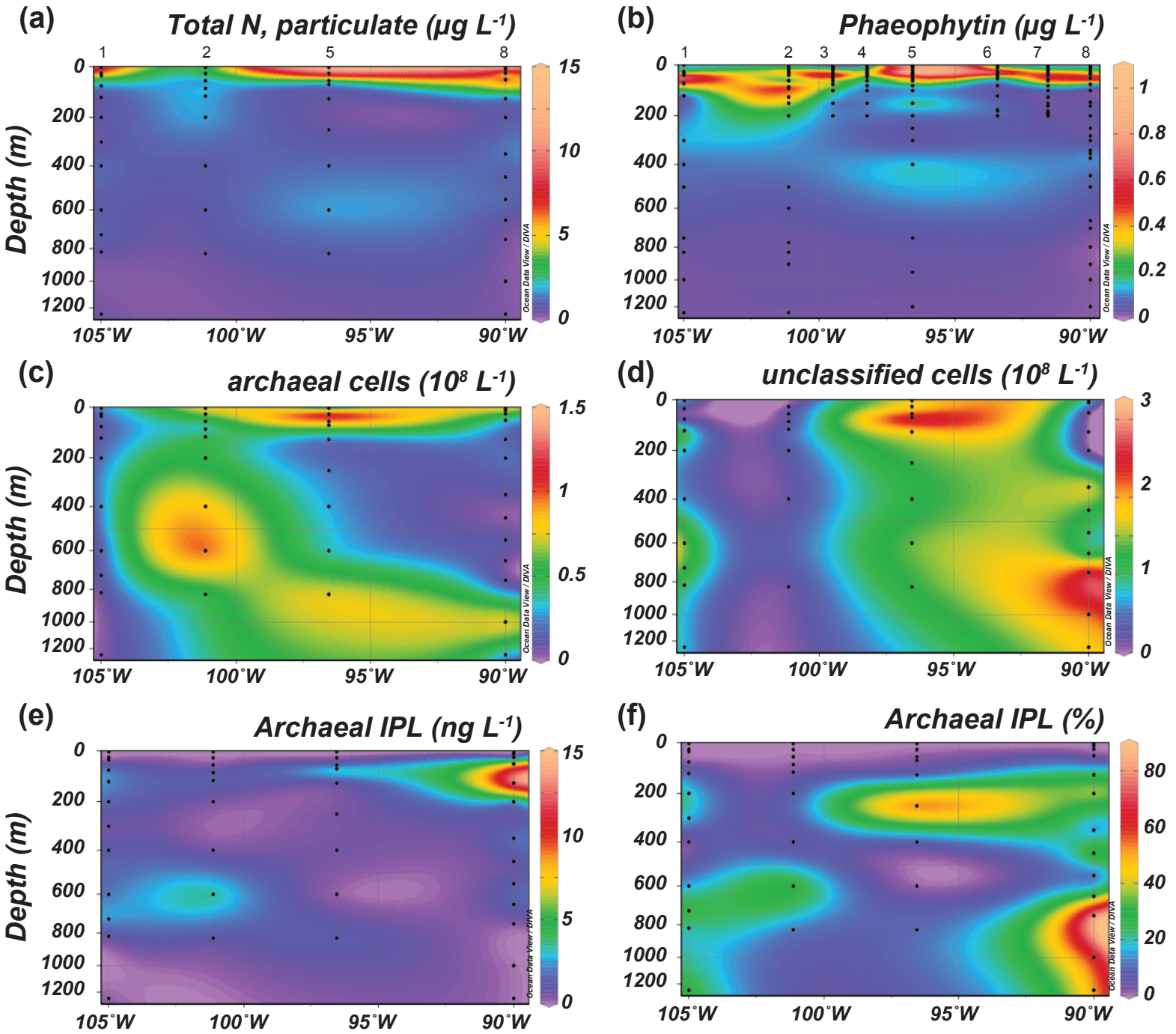
Suppl. Fig 3. Identification of hydroxylated aminolipids and sphingolipids in water column samples of the ETNP. (a) HPLC-MS density map, full scan (MS^1), in the mass range from m/z 600 to 900 and retention time range from 7 to 9 minutes. Representative high-resolution accurate mass MS^2 mass spectrum showing fragmentation patterns of (b) DGTS, (c) 1OH-DGTS, (d) 3OH-DGTS and (e) 1G-2OH-CER in positive ionization mode. Typical fragments for DGTS include monoacylglycerol side chains with the head group still attached. Similar fragmentation patters are observed between DGTS, 1OH-DGTS and 3OH-DGTS with exact masses pointing to additional hydroxyl-groups attached to the fatty acyl side chains. Note, that it's possible that the dihydroxylated fatty acid, could also be an epoxy-hydroxy or keto-hydroxy acid as only one loss of water was observed in the MS2 (from fragment *m/z* 466.281 to *m/z* 448.270). Multiple fatty acid side chain combinations are possible. Fragments of 1G-2OH-CER include the glycosidic head group loss of 180 Da and two hydroxyl-group losses as well as the long chain base (LCB), *m/z* 294.279.

Suppl. Fig 4. Identification of aminolipids AL-I and AL-II and ester/ether-sulfoquinovosyl (SQ-AEG) in water column samples of the ETNP. (a) HPLC-MS density map, full scan (MS^1), in the mass range from *m/z* 600 to 900 and retention time range from 6.5 to 11.5 minutes. Representative high-resolution accurate mass MS^2 mass spectrum showing fragmentation patterns of (b) AL-I and (c) AL-II in positive ionization mode. Fragmentation patterns of AL-I and AL-II are very similar to DGTS (Suppl. Fig. 3) showing monoacylglycerol fragments with the amino-head group still attached. The sum formula of the AL-I headgroup matches the head group of DGCC with an extra methyl group. However, since no head group fragments were observed no further structural inference could be made. The sum formula of AL-II matches exactly the head group of DGCC, however, the DGCC-characteristic head group ion fragment *m/z* 252.144 was not observed and no structural inference from the detected head group fragments *m/z* 132.102 and 104.107 could be made. Representative high-resolution accurate mass MS^2 mass spectrum showing fragmentation patterns of (d) SQ-DAG and (e) SQ-AEG in positive and negative ionization mode. Both compound classes exhibit the sulfoquinovosyl-diagnostic head group loss of 261.05 Da. However, SQ-AEG only has one fatty acyl side chain fragment, whereas SQ-DAG has two fatty acyl fragments in positive and negative ion mode. Furthermore, the exact mass of the parent ion and the fragments indicate that SQ-AEG has one oxygen less than SQ-DAG, indicating the replacement of one of the ester bonds with an ether bond.

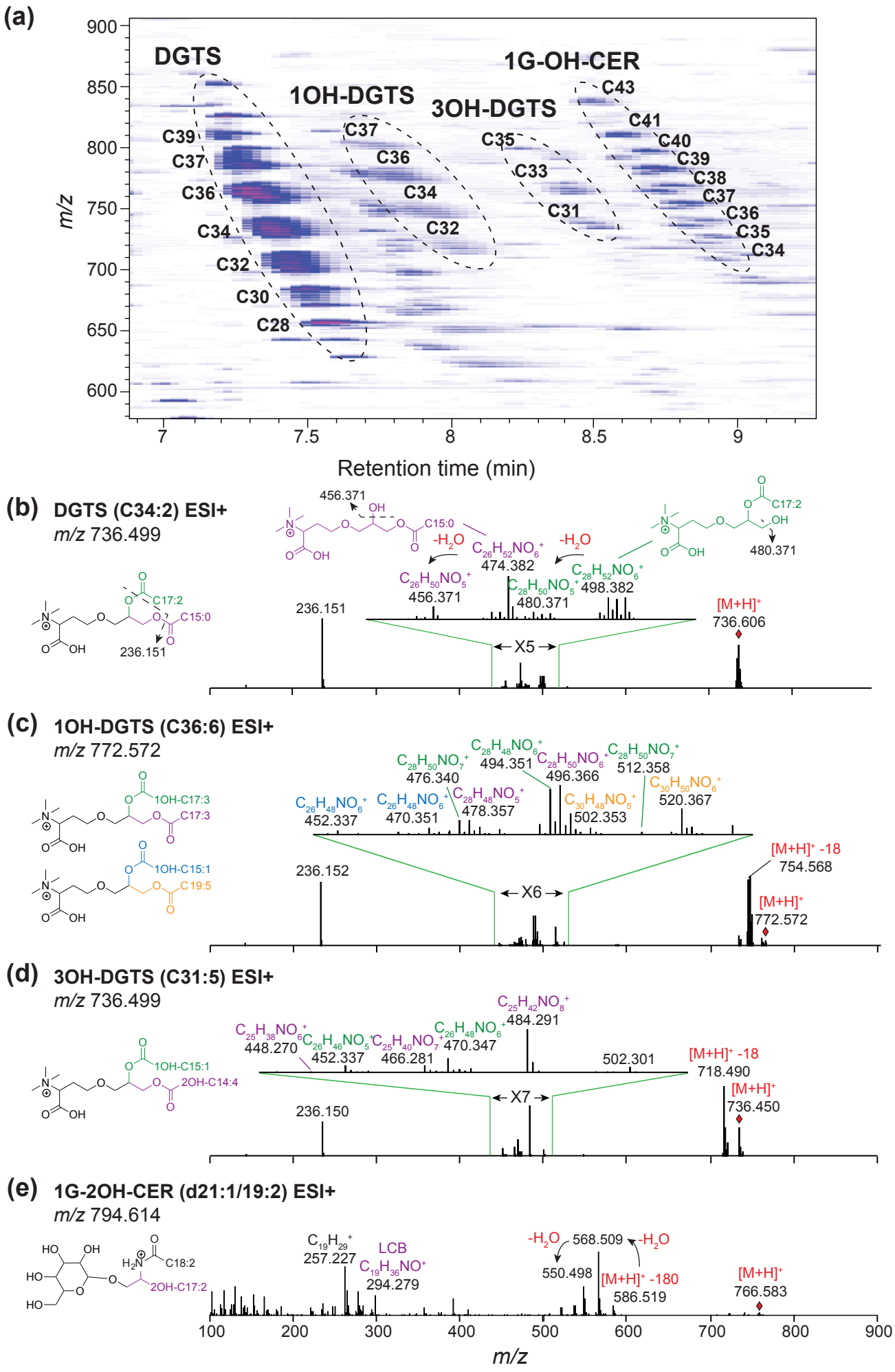
suppl.fig01


(a)
Monoglycosyl (1G), n=1
Diglycosyl (2G), n=2
Triglycosyl (3G), n=3
Sulfoquinovosyl (SQ)
Diphosphatidylglycerol (DPG)
Phosphatidylglycerol (PG)
Phosphatidyl-ethanolamine (PE)
Phosphatidyl-(N) methylethanolamine (PME)
Phosphatidyl-(N,N)-dimethylethanolamine (PDME)
Phosphatidylcholine (PC)
Betaine lipid
Diacylglyceryl trimethylhomoserine (DGTS)
Ornithine lipid (OL)
Phosphatidylinositol (PI)
Diacylglycerol (DAG)
Diether-glycerol (DEG)
Acyl/ether-glycerol (AEG)
Ceramide (CER)
R',R'' - variations:
saturated
Mono-hydroxy
Epoxy-hydroxy
polyunsaturated
Di-hydroxy
Keto-hydroxy
(b)
1G-GDGT, n=1
2G-GDGT, n=2
HPH-GDGT
X,Y - variations:

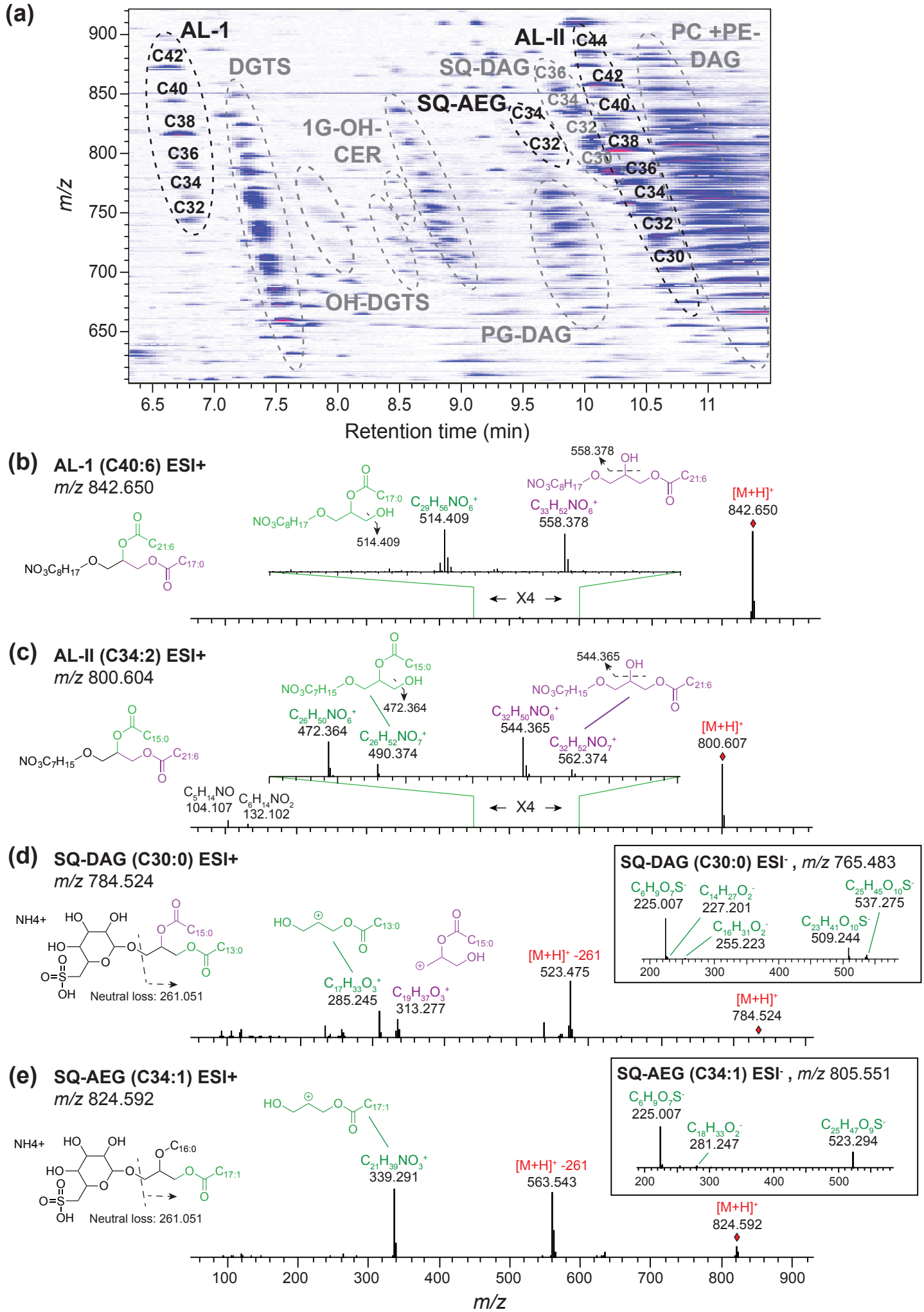
suppl.fig02


(a)
Total N, particulate (µg L-1)
(b)
Phaeophytin (µg L-1)
(c)
archaeal cells (10⁸ L-1)
(d)
unclassified cells (10⁸ L-1)
(e)
Archaeal IPL (ng L-1)
(f)
Archaeal IPL (%)
Depth (m)
105˚W
100˚W
95˚W
90˚W
Ocean Data View / DIVA

suppl.fig03


(a)
DGTS
1OH-DGTS
3OH-DGTS
1G-OH-CER
C39
C37
C36
C34
C32
C30
C28
C37
C36
C34
C32
C35
C33
C31
C43
C41
C40
C39
C38
C37
C36
C35
C34
m/z
Retention time (min)
(b) DGTS (C34:2) ESI+
m/z 736.499
C17:2
C15:0
236.151
456.371
-H2O
C26H52NO6+ 474.382
-H2O
C28H52NO6+ 498.382
C26H50NO5+ 456.371
C28H50NO5+ 480.371
480.371
236.151
[M+H]+ 736.606
X5
(c) 1OH-DGTS (C36:6) ESI+
m/z 772.572
1OH-C17:3
C17:3
1OH-C15:1
C19:5
C28H50NO7+ 476.340
C28H48NO6+ 494.351
C28H50NO6+ 496.366
C28H50NO7+ 512.358
C30H50NO6+ 520.367
C26H48NO6+ 452.337
C26H48NO6+ 470.351
C28H48NO5+ 478.357
C30H48NO5+ 502.353
236.152
X6
[M+H]+ -18 754.568
[M+H]+ 772.572
(d) 3OH-DGTS (C31:5) ESI+
m/z 736.499
1OH-C15:1
2OH-C14:4
C25H42NO8+ 484.291
C25H38NO6+ 448.270
C26H46NO5+ 452.337
C25H40NO7+ 466.281
C26H48NO6+ 470.347
502.301
[M+H]+ -18 718.490
[M+H]+ 736.450
236.150
X7
(e) 1G-2OH-CER (d21:1/19:2) ESI+
m/z 794.614
C18:2
2OH-C17:2
C19H29+ 257.227
LCB
C19H36NO+ 294.279
-H2O
568.509
-H2O
550.498
[M+H]+ -180 586.519
[M+H]+ 766.583
m/z

suppl.fig04


(a)
AL-1
C42
C40
C38
C36
C34
C32
DGTS
1G-OH-CER
OH-DGTS
SQ-AEG
SQ-DAG
AL-II
C44
C42
C40
C38
C36
C34
C32
C30
PC +PE-DAG
PG-DAG
m/z
Retention time (min)
(b) AL-1 (C40:6) ESI+
m/z 842.650
514.409
558.378
842.650
X4
(c) AL-II (C34:2) ESI+
m/z 800.604
472.364
490.374
544.365
562.374
800.607
104.107
132.102
X4
(d) SQ-DAG (C30:0) ESI+
m/z 784.524
Neutral loss: 261.051
285.245
313.277
523.475
784.524
SQ-DAG (C30:0) ESI- , m/z 765.483
225.007
227.201
255.223
509.244
537.275
(e) SQ-AEG (C34:1) ESI+
m/z 824.592
Neutral loss: 261.051
339.291
563.543
824.592
SQ-AEG (C34:1) ESI- , m/z 805.551
225.007
281.247
523.294
m/z