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Intact polar lipids in the water column of the eastern tropical North Pacific: abundance and structural variety of non-phosphorus lipids

Florence Schubotz et al.

Correspondence to: Florence Schubotz (schubotz@uni-bremen.de)

Table S1. Relative abundance of detected intact polar lipids (IPL) at all four stations (1, 2, 5 and 8) in the Eastern Tropical North Pacific, t.a. - trace amonts, n.d. - not detected. For IPL abbreviations refer to main text.

				Relative Abundance (%)																						
Station	Depth (m)	Water filtered (L)	Total IPL (ng/L)	1G-DAG	2G-DAG	SQ-DAG	DGTS	PE+PC-AEG	PE-DAG	PC-DAG	PG-DAG	DPG	3G-DAG	SQ-DEG	1G-Cer	AL-1	AL-II	OL	PME-DAG	PDME-DAG	PI-DAG	1G-OH-DAG	1G-OH-Cer	OH-DGTS	1G-GDGT	2G-GDGT	HPH-GDGT
1	3	575	882.3	17.4	9.8	51.2	1.3	1.4	2.8	3.5	9.0	0.0	0.2	1.3	0.3	t.a.	0.9	n.d.	n.d.	n.d.	0.5	0.1	0.2	n.d.	n.d.	n.d.	n.d.
1	25	193	1357.8	18.4	9.6	34.3	5.3	4.9	3.2	5.0	13.5	0.0	0.2	1.7	0.6	0.1	1.9	n.d.	n.d.	n.d.	0.3	0.3	0.8	n.d.	n.d.	n.d.	n.d.
1	35	1636	361.6	15.0	13.5	16.7	2.4	29.8	3.0	8.5	4.0	0.1	0.5	0.3	0.8	0.3	2.2	n.d.	n.d.	n.d.	1.8	0.4	0.7	n.d.	n.d.	n.d.	n.d.
1	75	1013	304.0	28.5	8.7	39.8	0.9	4.2	1.5	3.7	7.7	0.2	0.2	n.d.	0.4	0.2	1.9	n.d.	n.d.	n.d.	0.4	0.3	0.5	n.d.	0.2	0.1	0.4
1	120	1347	22.3	22.9	4.5	8.6	5.5	11.8	4.2	10.7	14.4	1.1	0.1	n.d.	1.4	0.2	2.9	n.d.	0.1	0.4	0.3	n.d.	0.5	n.d.	3.3	2.6	4.5
1	200	1578	8.4	23.2	1.0	0.7	14.0	11.9	3.8	10.9	5.7	0.8	n.d.	n.d.	1.1	0.4	2.9	n.d.	1.1	2.3	n.d.	n.d.	0.3	n.d.	16.4	3.2	0.3
1	300	1337	2.9	21.4	2.9	4.0	7.8	4.5	4.1	4.9	18.5	4.8	n.d.	n.d.	1.2	1.2	3.2	n.d.	2.8	n.d.	n.d.	n.d.	1.2	n.d.	14.9	2.6	n.d.
1	400	1300	56.4	3.1	2.9	11.3	2.7	0.0	8.8	8.1	50.6	3.1	n.d.	0.4	0.4	1.5	2.3	n.d.	2.0	0.6	0.1	n.d.	n.d.	n.d.	1.4	0.8	n.d.
1	600	1748	11.4	5.6	0.9	2.8	3.5	3.9	15.1	8.0	33.9	3.1	n.d.	n.d.	n.d.	1.3	0.2	n.d.	4.3	0.1	n.d.	0.1	n.d.	n.d.	13.3	3.8	n.d.
1	725	800	9.7	9.8	1.0	1.9	9.6	8.7	6.1	13.2	16.2	1.5	n.d.	n.d.	0.3	0.3	2.1	n.d.	n.d.	n.d.	0.2	n.d.	0.5	n.d.	14.9	10.4	3.2
1	820	1571	3.3	12.3	2.0	1.1	8.4	11.4	7.3	15.1	16.8	1.8	n.d.	n.d.	0.3	0.2	3.0	n.d.	n.d.	n.d.	0.1	n.d.	0.5	n.d.	9.3	9.4	1.2
1	1250	1374	0.8	32.4	1.3	1.9	14.9	1.9	0.8	1.6	13.0	1.4	n.d.	n.d.	0.6	0.3	1.6	n.d.	n.d.	n.d.	n.d.	0.2	0.5	n.d.	21.0	6.3	0.3
2	3	1071	266.2	9.3	18.9	35.7	6.8	4.8	1.4	8.6	6.2	0.1	0.2	1.4	0.8	0.2	2.5	t.a.	n.d.	0.3	0.4	t.a.	0.5	1.7	0.0	n.d.	n.d.
2	6	1166	349.6	30.1	14.9	20.3	7.2	5.9	0.8	3.5	9.0	0.1	t.a.	5.0	0.1	0.0	1.0	n.d.	0.1	n.d.	0.4	0.1	1.4	t.a.	0.0	n.d.	n.d.
2	55	1647	21.9	18.1	17.5	12.4	3.7	26.5	2.8	8.9	3.6	0.1	0.2	0.4	0.3	0.3	3.4	t.a.	t.a.	n.d.	0.4	0.1	t.a.	n.d.	0.3	n.d.	n.d.
2	85	1435	160.0	24.3	7.5	33.5	3.5	7.3	2.7	7.1	4.7	0.9	t.a.	0.4	0.8	0.1	4.2	t.a.	0.6	0.6	0.3	0.5	0.3	n.d.	0.6	0.2	0.0
2	115	1517	50.0	7.0	6.6	18.2	5.0	7.4	5.8	9.1	21.9	2.0	1.6	0.9	1.8	0.3	6.2	0.1	1.5	0.3	0.3	n.d.	1.1	n.d.	2.1	1.0	n.d.
2	200	193	6.0	80.0	0.0	0.4	10.8	0.2	0.2	0.3	0.7	0.0	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.5	n.d.	n.d.	6.8	0.0	n.d.
2	400	1725	12.6	4.2	2.8	4.8	5.4	4.1	13.0	17.2	31.2	4.7	0.5	n.d.	0.9	n.d.	1.6	0.5	3.9	1.9	0.1	n.d.	n.d.	n.d.	1.7	0.7	1.0
2	600	1476	11.8	2.4	0.0	12.5	2.1	1.9	0.1	1.9	34.1	11.3	n.d.	n.d.	n.d.	n.d.	0.0	0.0	n.d.	6.1	n.d.	n.d.	n.d.	n.d.	6.5	13.8	7.5
2	830	1397	7.2	6.2	3.5	6.8	7.7	12.5	8.7	11.5	15.0	1.6	1.0	0.5	1.2	0.2	5.1	0.0	2.9	1.7	0.6	n.d.	1.1	n.d.	5.1	1.8	5.1
5	3	223	244.4	23.1	16.1	18.4	24.6	3.8	0.8	4.1	4.6	0.1	n.d.	1.2	1.1	t.a.	0.4	n.d.	n.d.	n.d.	0.1	0.8	0.5	0.1	n.d.	n.d.	n.d.

5	25	128	1187.6	66.1	1.0	4.1	22.9	0.0	0.2	0.4	4.5	0.0	n.d.	n.d.	0.0	0.2	0.2	n.d.	n.d.	n.d.	0.1	0.3	n.d.	n.d.	n.d.	n.d.	n.d.
5	35	1683	38.1	67.7	0.7	4.0	14.5	2.8	0.4	1.7	3.3	0.0	n.d.	n.d.	0.6	n.d.	0.2	n.d.	t.a.	n.d.	0.0	0.8	n.d.	1.0	2.2	n.d.	n.d.
5	75	995	174.8	20.5	11.0	49.3	2.9	0.2	0.3	0.9	8.6	1.8	t.a.	0.2	0.2	t.a.	0.3	t.a.	0.1	0.2	0.2	0.4	n.d.	t.a.	1.1	0.8	0.8
5	125	1289	2.3	3.9	6.7	35.3	5.6	9.3	3.6	2.8	3.6	0.8	0.2	0.2	1.8	0.2	5.6	n.d.	11.9	0.4	0.1	0.1	n.d.	t.a.	7.1	n.d.	0.8
5	250	1362	1.1	41.7	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	58.3	n.d.	n.d.
5	400	1365	11.2	5.4	2.8	5.0	7.7	3.4	11.8	11.3	33.0	3.4	0.4	n.d.	0.4	0.1	2.1	0.5	5.1	1.3	0.1	n.d.	0.3	n.d.	4.0	0.8	1.1
5	600	968	21.4	3.9	4.2	6.3	5.8	2.1	17.1	15.1	22.0	5.5	1.3	0.4	2.2	0.3	4.1	0.7	5.4	2.8	0.4	n.d.	0.7	n.d.	0.0	n.d.	0.0
5	830	1595	12.4	5.7	3.6	7.2	7.7	12.8	8.6	11.6	15.4	1.6	1.0	0.5	1.3	0.2	5.3	0.1	3.1	2.0	0.7	n.d.	1.2	n.d.	4.1	1.3	5.1
8	3	387	955.4	11.2	16.2	14.9	9.0	5.8	4.0	13.6	8.6	0.5	t.a.	2.4	1.1	t.a.	3.5	0.3	0.5	0.2	0.7	0.2	0.2	6.9	0.0	n.d.	0.0
8	10	309	1458.8	8.5	18.5	19.2	6.0	12.1	3.2	11.6	8.3	0.2	0.1	2.5	1.4	0.1	3.8	0.1	t.a.	0.1	1.1	n.d.	0.2	3.0	0.0	n.d.	n.d.
8	25	1648	348.7	13.2	22.2	11.6	6.8	12.9	3.9	9.5	8.2	0.0	0.1	1.4	1.0	0.6	3.7	0.1	0.1	n.d.	t.a.	0.1	1.3	3.2	0.0	n.d.	n.d.
8	50	887	474.4	18.0	18.3	18.4	5.7	10.2	5.3	11.3	3.1	0.2	0.1	0.3	1.1	0.6	3.2	n.d.	n.d.	n.d.	0.3	0.5	0.7	0.9	0.8	0.2	0.7
8	125	1231	54.2	9.8	1.9	1.7	4.4	14.1	8.5	15.8	6.5	0.9	t.a.	0.1	1.3	0.4	3.5	t.a.	1.9	0.8	0.2	n.d.	0.4	1.0	9.1	6.7	11.0
8	200	1698	3.8	41.1	0.2	0.3	14.5	n.d.	t.a.	0.3	1.8	1.0	n.d.	n.d.	0.1	0.3	0.7	n.d.	n.d.	n.d.	0.5	n.d.	0.3	1.1	22.3	0.4	15.0
8	350	1633	19.5	6.7	1.3	1.1	10.5	8.5	7.5	12.6	11.3	5.6	0.1	n.d.	2.3	0.5	7.2	0.2	6.0	4.3	0.1	n.d.	1.0	1.8	6.5	1.0	3.6
8	450	1440	1.5	24.2	0.0	n.d.	22.6	2.1	1.2	2.4	1.5	0.5	n.d.	n.d.	0.5	0.8	1.1	n.d.	1.1	3.2	n.d.	n.d.	0.3	2.4	22.8	0.9	12.7
8	550	1251	17.2	9.4	1.4	3.5	8.7	9.4	11.4	15.5	15.1	1.9	0.2	n.d.	n.d.	0.4	5.8	0.1	5.3	2.9	0.2	n.d.	0.7	0.6	4.0	1.4	2.1
8	650	1633	5.1	32.4	n.d.	n.d.	30.4	1.2	0.1	0.6	1.2	0.0	n.d.	n.d.	n.d.	1.3	1.0	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	1.6	19.5	0.1	10.5
8	750	1926	0.1	14.5	n.d.	n.d.	0.4	n.d.	0.1	0.1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	t.a.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	61.2	n.d.	23.8
8	1000	1633	0.1	37.9	n.d.	n.d.	1.6	n.d.	0.1	0.1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	40.7	n.d.	19.8
8	1250	1417	0.1	47.3	n.d.	n.d.	0.6	n.d.	0.1	0.1	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	t.a.	n.d.	n.d.	n.d.	n.d.	0.1	n.d.	0.8	36.3	0.0	14.9

Table S2. List of commercially available standards used to determine response factors of intact polar lipids (IPL) in this study. For absolute quantification by HPLC-ion trap-MS the response factor was evaluated relative to the injection standard C19:0 PC-DAG. For determining relative abundances of IPLs via HPLC-QTOF-MS (see methods in the main text), the absolute responses of the individual standards were used. For IPL abbreviations refer to main text.

Short ID	Full Name	Fatty acid distribution	Company	Used for IPL class (HPLC-ion trap-MS)	Used for IPL class (HPLC-QTOF-MS)
16:0 PE-DAG	1,2-dipalmitoyl-sn-glycero-3-phosphoethanolamine	16:0/16:0	Avanti Polar Lipids, USA	PE-DAG, PME-DAG, PDME-DAG	PE-DAG
16:0 PC-DAG	1,2-dipalmitoyl-sn-glycero-3-phosphocholine	16:0/16:0	Avanti Polar Lipids, USA	PC-DAG	PC-DAG
19:0 PC-DAG	1,2-dinonadecanoyl-sn-glycero-3-phosphocholine	19:0/19:0	Avanti Polar Lipids, USA		internal standard for all IPLs
16:0 PME-DAG	1,2-dipalmitoyl-sn-glycero-3-phosphoethanolamine-N-methyl	16:0/16:0	Avanti Polar Lipids, USA		PME-DAG
16:0 PDME-DAG	1,2-dipalmitoyl-sn-glycero-3-phosphoethanolamine-N,N-dimethyl	16:0/16:0	Avanti Polar Lipids, USA		PDME-DAG
16:0 PG-DAG	1,2-dipalmitoyl-sn-glycero-3-phospho-(1'-rac-glycerol)	16:0/16:0	Avanti Polar Lipids, USA	PG-DAG, SQ-DAG, DPG	PG-DAG, SQ-DAG
16:1 DPG	1',3'-bis(1,2-dipalmitoleoyl-sn-glycero-3-phospho)-glycerol	16:1/16:1/16:1/16:1	Avanti Polar Lipids, USA		DPG
1Glc-DAG	1,2-diacyl-3-O-(a-D-glucopyranosyl)-sn-glycerol (E.coli)	18:1/16:0, 18:1/16:1, 16:1/16:0, 18:1/18:1	Avanti Polar Lipids, USA	1G-DAG	1G-DAG
2G-DAG	Digalactosyldiacylglcyerol (plant, hydrogenated)	18:0/18:0, 18:0/16:0	Avanti Polar Lipids, USA	2G-DAG	2G-DAG
DGTS	1,2-dipalmitoyl-sn-glycero-3-O-4'-[N,N,N-trimethyl)-homoserine	16:0/16:0	Avanti Polar Lipids, USA	DGTS	DGTS
C18 1G-CER	D-galactosyl-b-1,1'-N-stearoyl-D-erythro-sphingosine	d18:1/18:0	Avanti Polar Lipids, USA	1G-CER	1G-CER
1G-GDGT-PG	Main phospholipid of Thermoplasma acidophilum (>95% pure)		Matreya LLC, USA	HPH-GDGT, 1G-GDGT, 2G-GDGT	HPH-GDGT, 1G-GDGT, 2G-GDGT

Table S3. Examples of HPLC-MS fragmentation patterns (MS2) in positive ionization mode for select major ions (MS1) of intact polar lipids (IPLs) detected in this study.

IPL	MS1 (pos ion mode) Select major ions (m/z)	MS2 (pos ion mode) Neutral loss (Da)	MS2 (pos ion mode) Select diagnostic ions (m/z)
Glycolipids			
1G-DAG	766.546, 718.546, 716.531 $[M+NH_4]^+$	Hexose plus NH_3 (179.079)	335.258, 305.211, 313.277, 285.245
1G-OH-DAG	732.526, 730.510 $[M+NH_4]^+$	Hexose plus NH_3 (179.079)	313.277, 285.245
2G-DAG	936.662, 934.646, 882.615, 880.599 $[M+NH_4]^+$	Two hexoses plus NH_3 (341.132)	339.291, 337.274, 313.277, 285.245
SQ-DAG	812.555, 784.524, 782.508, 756.493 $[M+H]^+$	Sulfoquinovosyl (261.052)	313.277, 313.277, 311.258, 285.245
SQ-AEG	824.592, 798.576 $[M+H]^+$	Sulfoquinovosyl (261.052)	339.291
1G-CER	748.572, 734.557 $[M+H]^+$	Hexose plus H_2O (180.063)	294.279 (LCB)
1G-OH-CER	780.598, 766.583, 752.567 $[M+H]^+$	Hexose plus H_2O (180.063)	294.279 (LCB)
1G-GDGT	1481.402, 1471.324 $[M+NH_4]^+$	Hexose plus NH_3 (179.079)	1302.323, 1292.44
2G-GDGT	1639.424 $[M+NH_4]^+$	Two hexoses plus NH_3 (341.132)	1298.291
HPH-GDGT	1723.421, 1713.343 $[M+NH_4]^+$	Hexose plus NH_3 (179.079), hexose (162.053)	1544.342, 1382.289, 1534.264, 1372.211
Phospholipids			
PE-DAG	730.538, 718.538, 704.522, 678.507 $[M+H]^+$	Phosphoethanolamine (141.019)	DAG fragments
PE-AEG	706.575, 702.543 $[M+H]^+$	Phosphoethanolamine (141.019)	
PC-DAG	806.569, 780.554, 746.569, 706.538 $[M+H]^+$	-	184.073, DAG fragments
PC-AEG	746.606 742.575, 716.559 $[M+H]^+$	-	184.073
PG-DAG	766.559, 764.544, 762.528 $[M+NH_4]^+$	Phosphoglycerol plus NH_3 (189.040)	DAG fragments
DPG	1404.990, 1380.990, 1352.959, 1338.943 $[M+NH_4]^+$	-	DAG fragments
PME-DAG	732.554, 718.538, 692.522 $[M+H]^+$	Phosphomethylethanolamine (155.035)	DAG fragments
PDME-DAG	732.554, 730.538, 704.522 $[M+H]^+$	Phosphodimethylethanolamine (169.050)	DAG fragments
PI-DAG	902.575, 900.560 $[M+NH_4]^+$	Phosphoinositol plus NH_3 (277.056)	DAG fragments

Aminolipids			
DGTS	764.640, 760.609, 736.609, 732.577 $[M+H]^+$	-	498.382, 480.371, 474.382, 456.237, 236.149
OH-DGTS	754.619, 746.557 $[M+H]^+$	-	512.358, 494.351, 476.340, 496.366, 478.357, 236.149
OL	693.614, 653.583 $[M+H]^+$	-	115.087
AL-I	842.650, 814.619, 742.619 $[M+H]^+$	-	558.378, 514.409
AL-II	800.603, 728.603, 700.572 $[M+H]^+$	-	562.374, 544.365, 490.374, 472.364

Table S4. Absolute concentrations of pigments detected in surface waters of the Eastern Tropical North Pacific at stations 1, 5 and 8.

Concentration (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

Table S5. Fatty acyl combinations (number of carbon atoms and double bond equivalents, DBE, in the alkyl side chains) 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)	Carbon atoms	DBE	FA combination	Mean	SD	Mean	SD	Mean	SD	Mean	SD
1G-DAG	788.531	36	8	18:4/18:4	1.86	1.03	3.55	4.15	0.74	0.50	1.10	0.24
	786.515	36	9	18:4/18:5	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 ; 16:1/16:0	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 ; 15:0/14:0	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-DAG	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 ; 19:1/16:1	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-DAG	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 ; 17:1/17:1	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-DAG	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	11	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 ; 17:0/15:0	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 ; 20:0/16:4	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

Table S6. Goodness of fit statistics for the NMDS analyses of normalized intact polar lipid (IPL) composition and quantitative microbial data (FISH), number of double bond equivalents (DBE) and carbon atoms in the alkyl side chains of IPLs.

	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 DBE			
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

	Number of 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

Figure S1. Fluctuations in (A) absolute and (B) relative responses of select commercially available IPL standards over time. The values represent the slope of standards measured in different concentrations (usually 100 pg to 10 ng injected on column). Standard Mix A, B and C represents newly prepared standard mixtures. The standard mix used in this study was from November 2015.

Figure S2. Depth profiles of (a) total particulate nitrogen and (b) phaeophytin concentrations, at the investigated four stations in the ETNP.

Figure S3. Structures of (a) bacterial/eukaryotic and (b) archaeal intact polar lipids (IPLs) observed in the ETNP. The position of the double bonds or rings and the OH-, epoxy- and keto-groups of the R' and R'' side chains were not determined.

Figure S4. Extracted ion chromatograms of intact polar and core GDGTs showing the ring distribution within each individual compound class. Analyses were performed by HPLC-QTOF-MS with reversed phase chromatography as described in Zhu et al., (2016). Extracted ions for HPH-GDGTs were: *m/z* 1723.421, 1721.406, 1719.390, 1717.374, 1715.359, 1713.343; for 2G-GDGT: *m/z* 1643.455, 1641.439, 1639.424, 1637.408, 1635.392, 1633.377; for 1G-GDGT: *m/z* 1481.402, 1479.386, 1477.371, 1475.355, 1473.339, 1471.324 and for core GDGTs: *m/z* 1302.323, 1300.307, 1298.291, 1296.276, 1294.2, 1292.244. The numbers denote number of rings: 0 – GDGT-0, 1 – GDGT-1, 2 – GDGT-2, 5 – crenarchaeol.

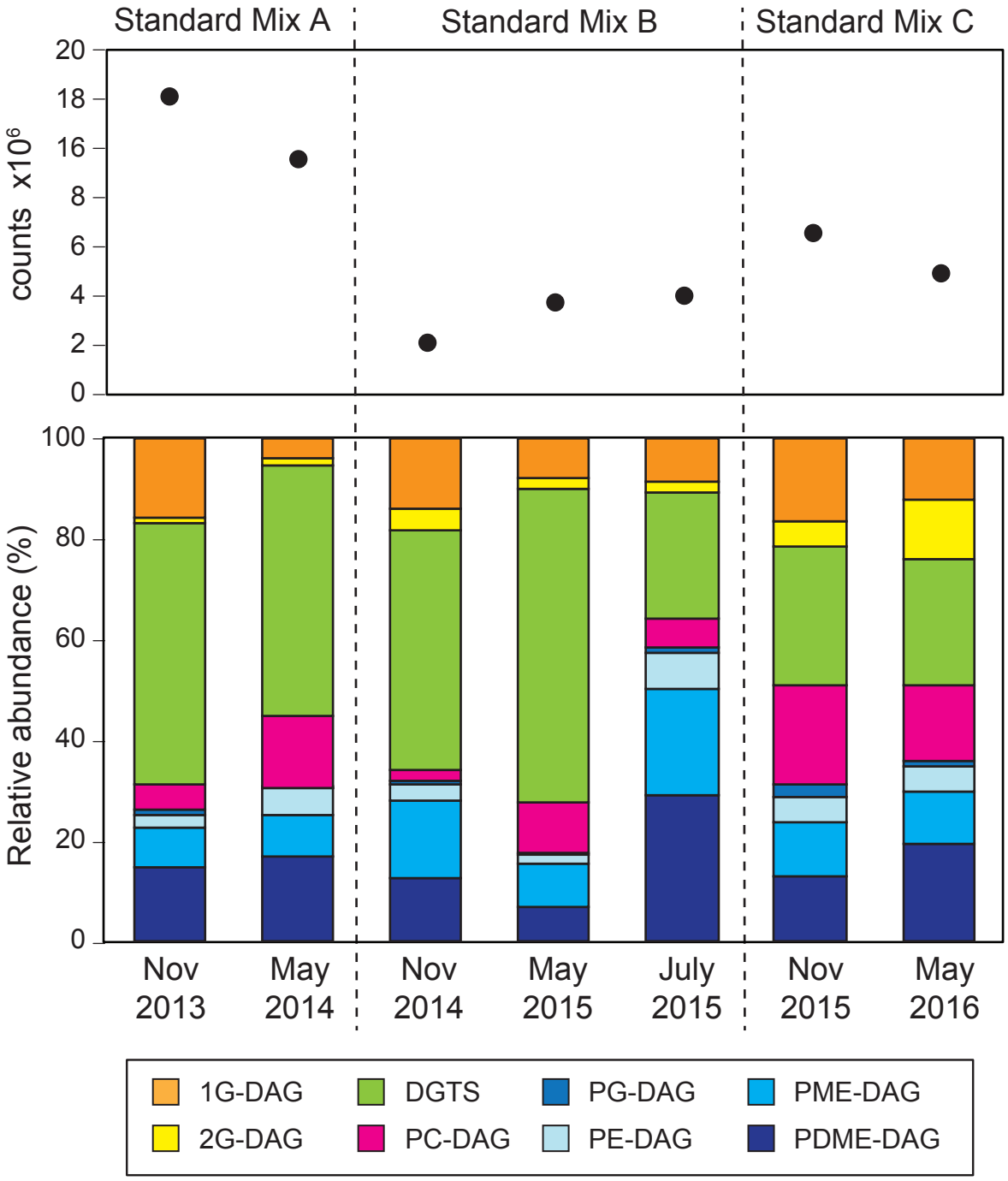
Figure S5. Identification of hydroxylated aminolipids and sphingolipids in water column samples of the

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.

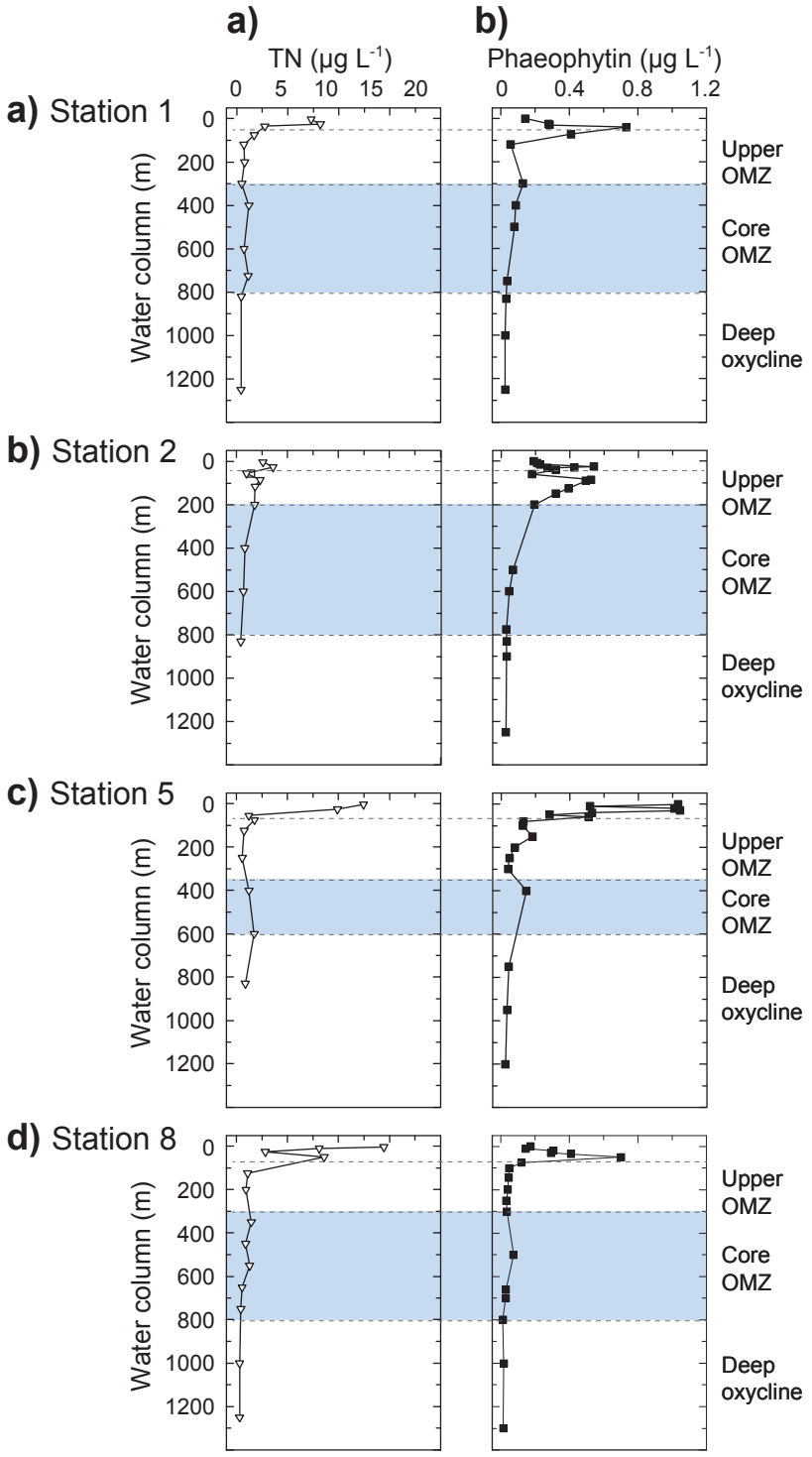
Figure S6. Identification of aminolipids AL-I and AL-II and ester/ether-sulfoquinovosyl (SQ-AEG) in water column samples of the ETNP. (a) HPLC-MS density map, full scan (MS^1), in the mass range from *m/z* 600 to 900 and retention time range from 6.5 to 11.5 minutes. Representative high-resolution accurate 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.

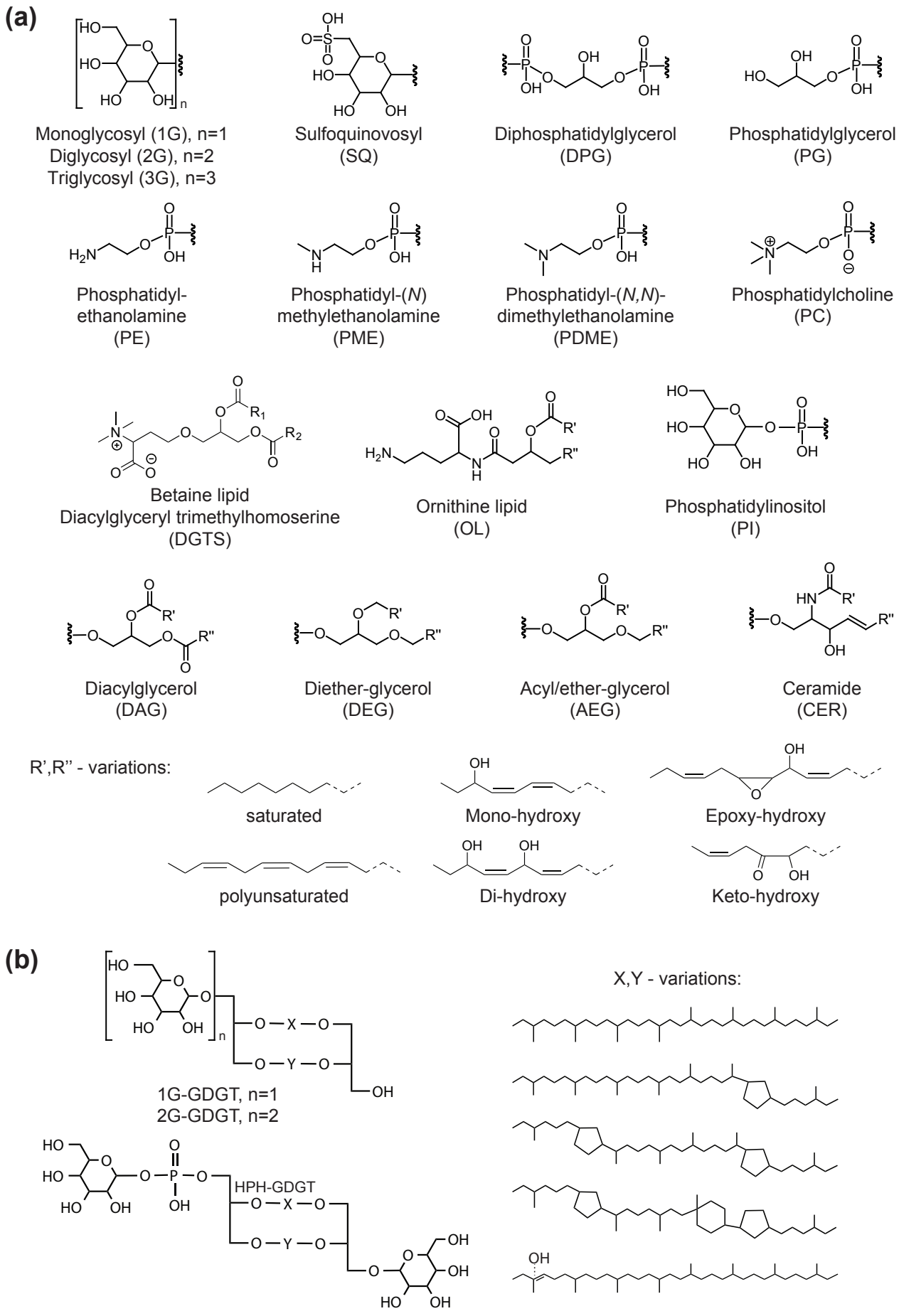
figS01


Standard Mix A
Standard Mix B
Standard Mix C
counts x10^6
20
18
16
8
6
4
2
0
Relative abundance (%)
100
80
60
40
20
0
Nov 2013
May 2014
Nov 2014
May 2015
July 2015
Nov 2015
May 2016
1G-DAG
2G-DAG
DGTS
PC-DAG
PG-DAG
PE-DAG
PME-DAG
PDME-DAG

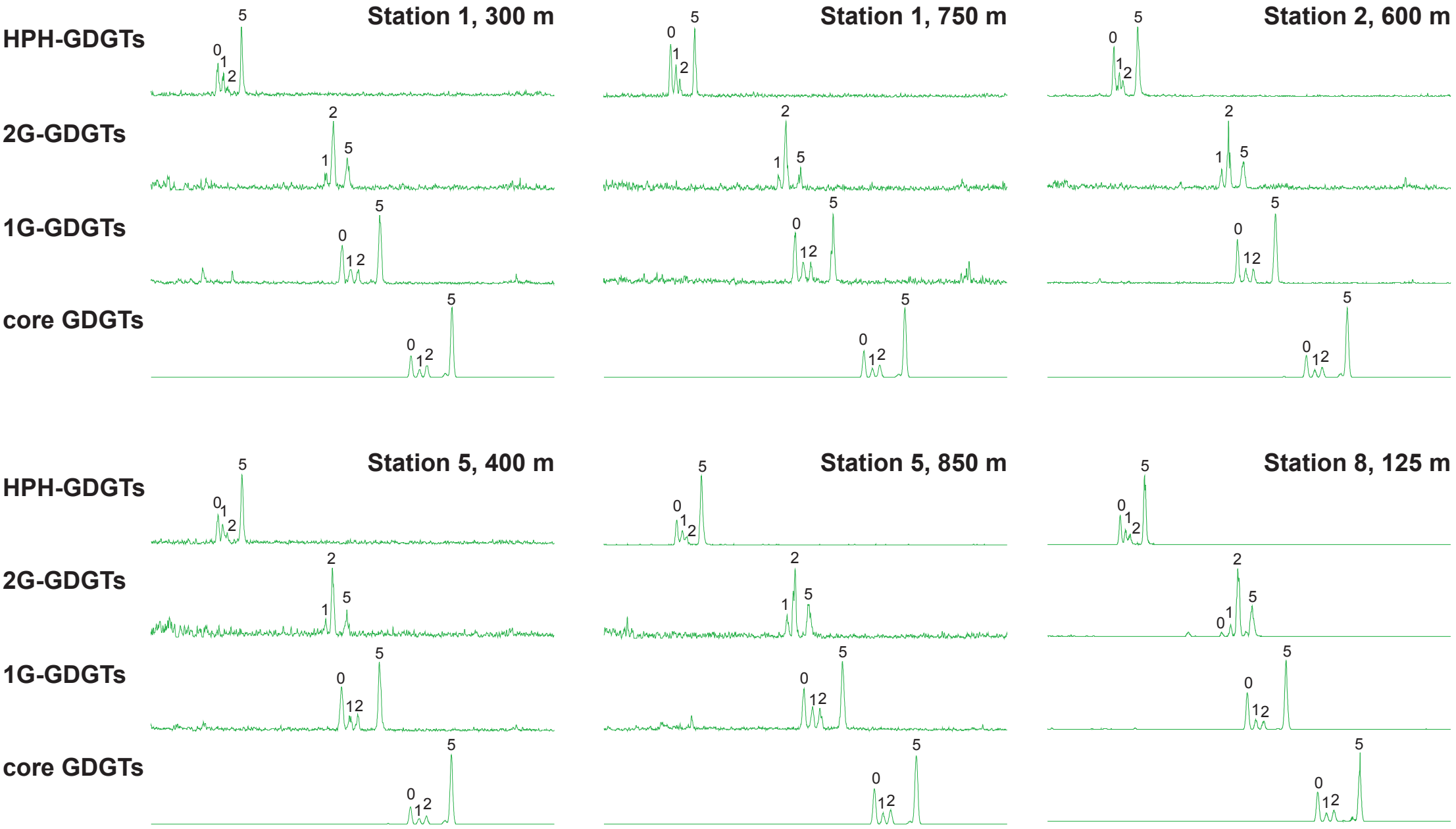
figS02


a)
b)
TN (µg L-1)
Phaeophytin (µg L-1)
0 5 10 15 20
0 0.4 0.8 1.2
a) Station 1
b) Station 2
c) Station 5
d) Station 8
Water column (m)
0
200
400
600
800
1000
1200
Upper OMZ
Core OMZ
Deep oxycline

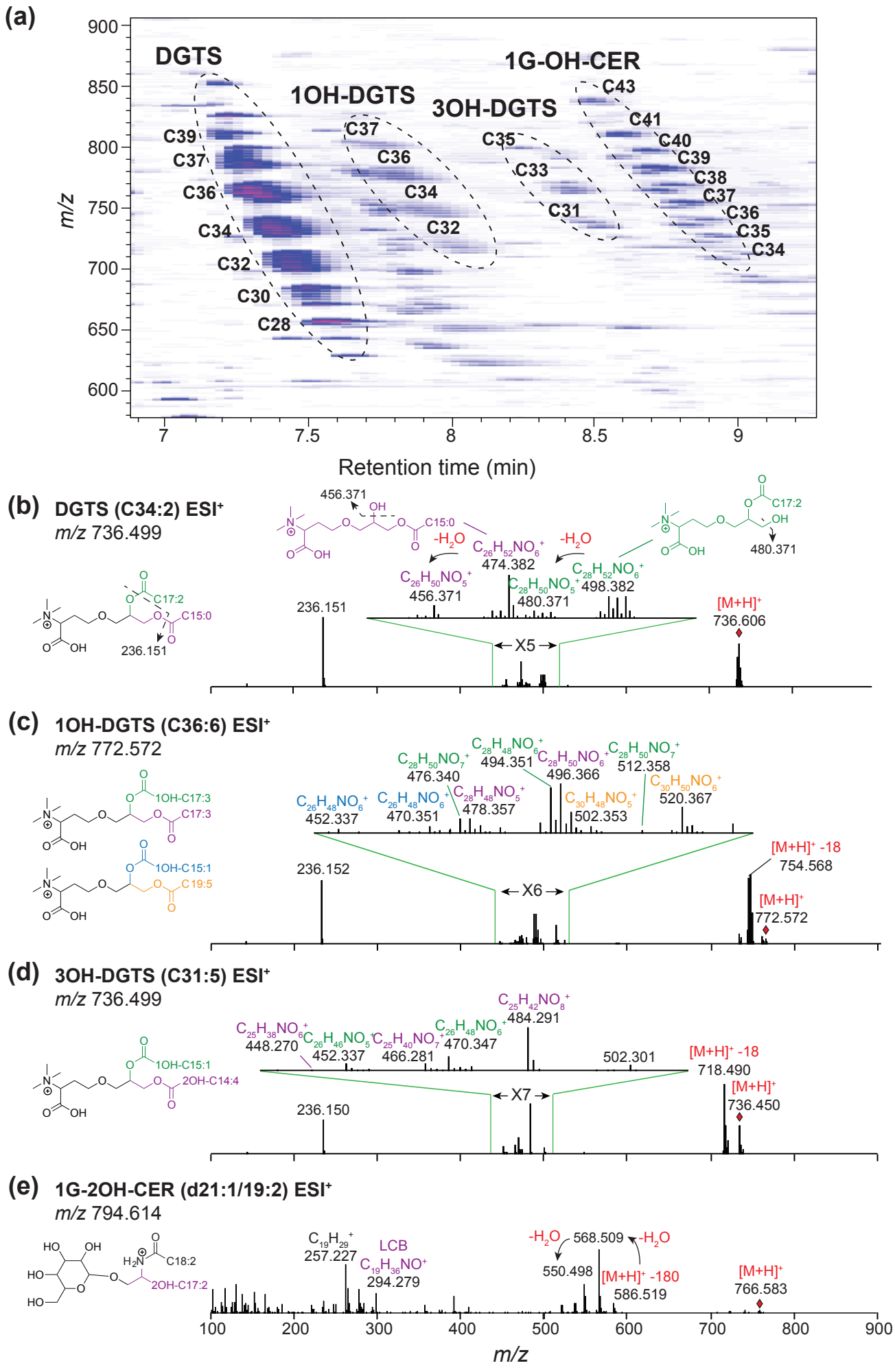
figS03


(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:

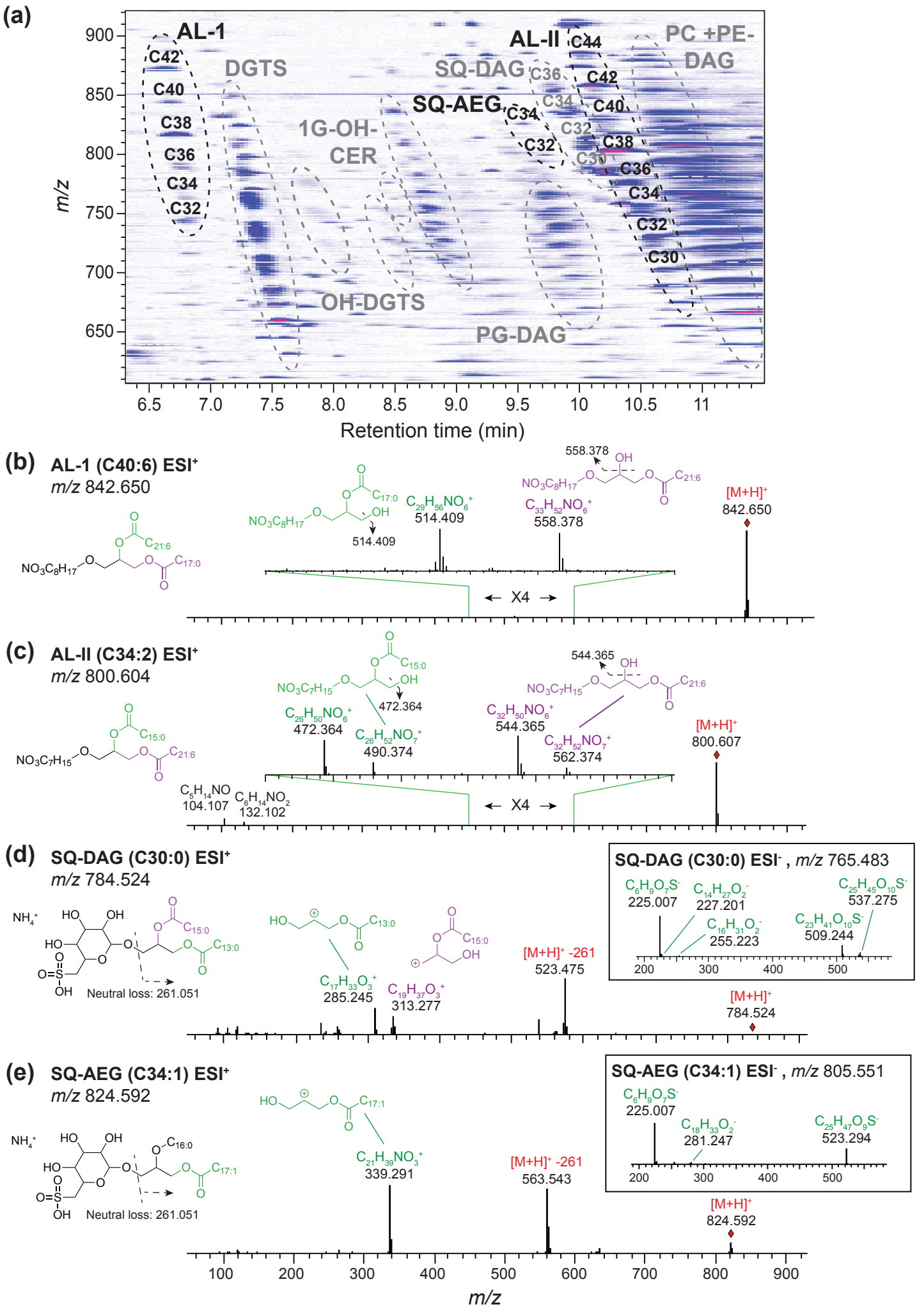
figS04


Station 1, 300 m
Station 1, 750 m
Station 2, 600 m
Station 5, 400 m
Station 5, 850 m
Station 8, 125 m
HPH-GDGTs
2G-GDGTs
1G-GDGTs
core GDGTs

figS05


(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
456.371
C15:0
-H2O
C26H52NO6+ 474.382
-H2O
C28H52NO6+ 498.382
C26H50NO5+ 456.371
C28H50NO5+ 480.371
C17:2
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
C28H48NO6+ 494.351
C28H50NO7+ 476.340
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
100
200
300
400
500
600
700
800
900
m/z

figS06


(a)
AL-1
C42
C40
C38
C36
C34
C32
DGTS
1G-OH-CER
OH-DGTS
SQ-DAG
SQ-AEG
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
[M+H]+ -261
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
[M+H]+ -261
563.543
824.592
SQ-AEG (C34:1) ESI- , m/z 805.551
225.007
281.247
523.294
m/z