

Supplement of Biogeosciences, 17, 317–330, 2020  
<https://doi.org/10.5194/bg-17-317-2020-supplement>  
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*Supplement of*

## **Structural elucidation and environmental distributions of butanetriol and pentanetriol dialkyl glycerol tetraethers (BDGTs and PDGTs)**

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**Supplementary Table S1:** Sample general properties, organic matter and geochemical parameters.

# in dataset	core ID	latitude (decimal)	longitude (decimal)	water depth (m)	sample depth (cmbsf)	estimated age (ka BP)	CH <sub>4</sub> (μmol/L)	SO <sub>4</sub> <sup>2-</sup> (μmol/L)	HS <sup>-</sup> (μmol/L)	Fe <sup>2+</sup> (μmol/L)	TOC (%)	C/N (molar ratio)	δ <sup>13</sup> C <sub>TOC</sub> (‰)	DOC (μmol/L)	DIC (μmol/L)
1	GeoB15103-1	33.03	32.63	1424	3.0	0.68	0.002	30600	5.0	0.00	0.27	15.8	-18.3	382	2710
2	GeoB15103-1	33.03	32.63	1424	26.5	9.30	0.30	30800	5.0	14.0	1.58	15.4	-20.9	755	3140
3	GeoB15103-1	33.03	32.63	1424	297	73.15	0.16	28600	5.0	54.3	0.16	9.30	-17.8	768	4030
4	GeoB15103-1	33.03	32.63	1424	314	77.21	0.28	28500	5.0	46.5	2.33	18.1	-19.6	1243	4060
5	GeoB15103-1	33.03	32.63	1424	460	121.05	0.82	27600	5.0	18.5	4.34	20.3	-20.1	1047	4660
6	GeoB15103-2	33.03	32.63	1367	27.5	9.30	0.08	29800	5.3	0.00	1.89	17.0	-21.2	428	2770
7	GeoB15103-2	33.03	32.63	1367	230	60.24	0.28	28500	5.9	31.4	0.50	19.4	-19.9	373	3640
8	GeoB15103-2	33.03	32.63	1367	293	77.21	0.26	28200	5.6	48.8	2.02	18.1	-19.5	797	3760
9	GeoB15103-2	33.03	32.63	1367	445	121.05	0.10	27800	5.4	25.7	3.77	20.9	-20.7	1388	4000
10	GeoB15103-2	33.03	32.63	1367	473	131.90	0.54	27500	5.4	25.6	0.10	11.7	-20.2	5332	4060
11	GeoB15103-2	33.03	32.63	1367	559	173.30	0.64	26500	5.4	18.9	1.31	17.0	-21.2	1663	4000
12	GeoB15104-1	40.80	27.72	606	3.0	0.05	0.17	30400	5.3	0.20	0.86	10.0	-22.9	438	2890
13	GeoB15104-1	40.80	27.72	606	35	0.63	0.30	30800	5.7	14.4	0.69	10.1	-22.9	166	3070
14	GeoB15104-2	40.80	27.72	600	188	4.76	0.70	29500	9.1	1.00	1.03	13.4	-24.1	286	3620
15	GeoB15104-2	40.80	27.72	600	288	10.10	0.80	29900	5.9	0.00	0.87	14.5	-25.4	322	3420
16	GeoB15104-2	40.80	27.72	600	368	14.99	0.20	29200	5.7	0.30	0.45	13.1	-25.8	251	4170
17	GeoB15104-2	40.80	27.72	600	628	19.87	2.2	26700	5.6	27.6	0.58	11.3	-26.1	543	5490
18	GeoB15105-4	41.53	30.88	1266	9.0	0.23	9.6	12800	1700	0.30	1.26	10.5	-24.5	1053	9080
19	GeoB15105-4	41.53	30.88	1266	39	0.92	26.5	10200	3430	0.20	1.20	10.8	-24.8	522	12000
20	GeoB15105-2	41.53	30.88	1266	113	2.60	1230	2810	5600	0.20	1.32	11.8	-24.8	2070	22000
21	GeoB15105-2	41.53	30.88	1266	155	3.57	920	2690	4580	0.20	1.43	11.9	-24.7	3340	21800
22	GeoB15105-2	41.53	30.88	1266	273	5.31	1120	2040	2005	0.40	1.88	12.9	-24.3	2120	22000
23	GeoB15105-2	41.53	30.88	1266	398	7.16	850	1330	680	2.50	4.37	15.4	-24.5	4180	20800
24	GeoB15105-2	41.53	30.88	1266	428	7.84	920	965	265	2.00	1.23	11.0	-26.1	2990	21600
25	GeoB15105-2	41.53	30.88	1266	605	15.13	814	660	120	54.0	1.12	11.9	-26.1	2300	18050
26	GeoB17302-5	42.33	3.48	741	3.5	0.04	0.17	30400	0.0	60.1	0.58	9.70	-22.8	265	1950
27	GeoB17302-5	42.33	3.48	741	60	0.60	0.26	28200	0.0	71.6	0.30	11.7	-23.9	274	1240
28	GeoB17302-5	42.33	3.48	741	180	1.80	0.27	27000	0.0	65.4	0.30	11.7	-24.0	289	1260

29	GeoB17304-3	41.99	4.84	2291	8.0	1.87	0.00	30200	0.0	0.00	0.15	5.80	-22.3	225	838
30	GeoB17304-3	41.99	4.84	2291	19.5	3.36	0.00	29700	0.0	9.44	0.08	4.70	-22.2	181	1684
31	GeoB17304-3	41.99	4.84	2291	57.5	7.25	0.00	29400	0.0	28.3	0.15	17.5	-22.8	294	2320
32	GeoB17304-3	41.99	4.84	2291	180	17.09	0.00	21100	0.0	83.9	0.26	15.2	-24.5	486	1065
33	GeoB17306-1	43.32	4.87	30	4.5	0.00	7.56	36600	0.0	45.0	1.31	13.9	-26.7	351	1190
34	GeoB17306-1	43.32	4.87	30	32.5	0.00	28.5	25200	0.0	31.9	1.42	15.1	-26.9	715	8240
35	GeoB17306-2	43.32	4.87	29	70	0.00	295	3260	0.0	281	1.16	13.5	-26.3	2252	31500
36	GeoB17306-2	43.32	4.87	29	255	0.01	3500	880	0.0	224	1.40	14.8	-26.9	3571	22600
37	GeoB17306-2	43.32	4.87	29	382	0.01	4440	810	0.0	426	0.58	33.8	-24.2	3936	25100
38	GeoB17306-2	43.32	4.87	29	430	0.01	2030	396	0.0	207	1.21	14.1	-25.9	3413	29100
39	GeoB17307-5	43.30	4.86	52	4.5	0.00	6.14	30500	0.0	206	1.21	14.1	-26.6	241	1200
40	GeoB17307-5	43.30	4.86	52	22.5	0.00	26.0	15000	0.0	78.1	1.08	14.0	-26.4	659	14200
41	GeoB17307-8	43.30	4.86	52	62.5	0.00	8.18	13700	0.0	7.69	1.00	14.6	-26.3	1529	16700
42	GeoB17307-8	43.30	4.86	52	108	0.01	2150	4920	0.0	39.8	0.73	12.2	-26.2	3220	20600
43	GeoB17307-8	43.30	4.86	52	339	0.02	3500	0.0	0.0	269	1.05	15.3	-25.9	3298	27700
44	GeoB17307-8	43.30	4.86	52	446	0.03	1520	0.0	0.0	103	1.39	16.2	-26.0	3119	20100
45	GeoB17308-1	43.27	4.73	62	1.5	0.01	1.86	30800	0.0	53.4	0.91	11.8	-24.9	133	1780
46	GeoB17308-4	43.27	4.73	61	25.0	0.04	1.33	27300	0.0	168	0.63	12.3	-24.7	422	2790
47	GeoB17308-4	43.27	4.73	61	225	0.36	60.7	3880	0.0	55.4	0.50	9.70	-24.7	1078	6760
48	GeoB17308-4	43.27	4.73	61	275	0.44	72.4	1050	0.0	74.2	0.51	9.90	-25.0	1334	4760

**Supplementary Table S2:** Absolute concentration, relative abundance and distribution indices of GDGTs, BDGTs and PDGTs. (n.d.: not detected; n.a.: not applicable).

# in dataset	IGSN	core ID	sample depth (cmbfsf)	[2G-BDGTs] (µg/g OC)	[1G-BDGTs] (µg/g OC)	[CL-BDGT-0] (µg/g OC)	[CL-BDGT-1] (µg/g OC)	[CL-BDGT-2] (µg/g OC)	sum [CL-BDGTs] (µg/g OC)	sum [IPL-BDGTs] (µg/g OC)	sum [BDGTs] (µg/g OC)	f(2G-BDGTs) (%)	f(1G-BDGTs) (%)	f(IPL-BDGTs) (%)	f(CL-BDGTs) (%)
1	IGSN: GEOB0151EXIH101	GeoB15103-3	3	n.d.	n.d.	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
2	IGSN: GEOB0151EXCG101	GeoB15103-1	26.5	1.55	1.15	0.99	0.35	0.10	1.45	2.71	4.15	37	28	65	35
3	IGSN: GEOB0151EXIG101	GeoB15103-1	297	n.d.	0.20	0.73	n.d.	n.d.	0.73	0.20	0.93	n.a.	22	22	78
4	IGSN: GEOB0151EXKG101	GeoB15103-1	314	3.26	2.08	0.48	0.22	0.05	0.76	5.35	6.11	53	34	88	12
5	IGSN: GEOB0151EXQG101	GeoB15103-1	460	2.02	2.40	1.59	0.48	0.16	2.23	4.42	6.65	30	36	66	34
6	IGSN: GEOB0151EXOH101	GeoB15103-2	27.5	0.97	1.18	0.16	0.07	n.d.	0.23	2.15	2.37	41	50	90	10
7	IGSN: GEOB0151EXSH101	GeoB15103-2	230	n.d.	0.02	0.005	n.d.	0.03	0.03	0.02	0.05	n.a.	39	39	61
8	IGSN: GEOB0151EX7H101	GeoB15103-2	293	2.15	3.20	0.28	0.09	0.03	0.39	5.35	5.74	37	56	93	7
9	IGSN: GEOB0151EXBH101	GeoB15103-2	445	0.98	2.02	0.33	0.16	0.04	0.52	3.00	3.53	28	57	85	15
10	IGSN: GEOB0151EXCH101	GeoB15103-2	473	0.13	0.24	0.05	n.d.	0.05	0.10	0.36	0.46	27	51	78	22
11	IGSN: GEOB0151EXEH101	GeoB15103-2	559	n.d.	0.81	0.27	0.02	0.02	0.31	0.81	1.12	n.a.	72	72	28
12	IGSN: GEOB0151EX5J101	GeoB15104-1	3.0	0.09	0.45	0.25	0.06	0.02	0.32	0.53	0.86	10	52	62	38
13	IGSN: GEOB0151EXLJ101	GeoB15104-1	35	0.28	0.53	0.24	0.03	n.d.	0.26	0.81	1.08	26	49	76	24
14	IGSN: GEOB0151EXVJ101	GeoB15104-2	188	0.27	0.41	0.30	0.12	0.01	0.43	0.68	1.11	24	37	61	39
15	IGSN: GEOB0151EXXJ101	GeoB15104-2	288	1.34	1.59	0.33	0.17	n.d.	0.50	2.93	3.43	39	46	85	15
16	IGSN: GEOB0151EX0K101	GeoB15104-2	368	0.24	0.20	0.80	0.10	n.d.	0.90	0.44	1.34	18	15	33	67
17	IGSN: GEOB0151EX5K101	GeoB15104-2	628	n.d.	n.d.	0.35	0.01	n.d.	0.36	n.a.	0.36	n.a.	n.a.	n.a.	100
18	IGSN: GEOB0151EXAM101	GeoB15105-4	9.0	0.77	5.69	1.92	0.51	0.25	2.69	6.46	9.15	8	62	71	29
19	IGSN: GEOB0151EXPM101	GeoB15105-4	39	0.32	1.75	2.03	0.60	0.39	3.02	2.07	5.09	6	34	41	59
20	IGSN: GEOB0151EX0L101	GeoB15105-2	113	0.81	2.18	1.70	0.46	0.15	2.32	2.99	5.31	15	41	56	44
21	IGSN: GEOB0151EX1L101	GeoB15105-2	155	0.54	1.72	1.50	0.49	0.18	2.17	2.26	4.43	12	39	51	49
22	IGSN: GEOB0151EX4L101	GeoB15105-2	273	0.25	1.44	1.20	0.44	0.12	1.76	1.69	3.45	7	42	49	51
23	IGSN: GEOB0151EX6L101	GeoB15105-2	398	n.d.	1.17	0.46	0.15	0.04	0.65	1.17	1.82	n.a.	64	64	36
24	IGSN: GEOB0151EX8L101	GeoB15105-2	428	n.d.	1.31	0.36	0.22	0.08	0.65	1.31	1.95	n.a.	67	67	33
25	IGSN: GEOB0151EXCL101	GeoB15105-2	605	n.d.	0.16	0.10	0.04	0.03	0.17	0.16	0.33	n.a.	48	48	52
26	IGSN: GEOB0173EXYS001	GeoB17302-5	3.5	1.17	0.98	0.11	0.03	0.01	0.15	2.15	2.30	51	42	93	7
27	IGSN: GEOB0173EX0T001	GeoB17302-5	60	0.38	0.63	0.71	0.08	0.04	0.83	1.01	1.84	21	34	55	45

28	IGSN: GEOB0173EX4T001	GeoB17302-5	180	0.86	0.86	0.86	0.17	0.13	1.15	1.72	2.87	30	30	60	40
29	IGSN: GEOB0173EX2V001	GeoB17304-3	8.0	n.d.	n.d.	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
30	IGSN: GEOB0173EX3V001	GeoB17304-3	19.5	n.d.	n.d.	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
31	IGSN: GEOB0173EX7V001	GeoB17304-3	57.5	0.14	0.32	0.12	0.08	n.d.	0.24	0.46	0.70	20	45	65	35
32	IGSN: GEOB0173EXMV001	GeoB17304-3	180	0.32	0.67	0.22	0.13	0.09	0.44	0.99	1.44	22	47	69	31
33	IGSN: GEOB0173EXDL001	GeoB17306-1	4.5	0.66	0.38	0.10	0.04	0.03	0.18	1.04	1.22	54	31	86	14
34	IGSN: GEOB0173EXKL001	GeoB17306-1	32.5	2.50	0.79	0.12	0.04	0.03	0.19	3.28	3.47	72	23	95	5
35	IGSN: GEOB0173EX8E001	GeoB17306-2	70	2.89	0.77	0.13	0.04	0.02	0.19	3.66	3.85	75	20	95	5
36	IGSN: GEOB0173EXCE001	GeoB17306-2	255	3.33	1.53	0.54	0.10	0.03	0.67	4.86	5.53	60	28	88	12
37	IGSN: GEOB0173EXHE001	GeoB17306-2	382	1.21	0.32	0.14	0.07	0.05	0.25	1.54	1.79	68	18	86	14
38	IGSN: GEOB0173EXIE001	GeoB17306-2	430	3.29	0.82	0.12	0.03	0.01	0.16	4.12	4.28	77	19	96	4
39	IGSN: GEOB0173EX5M001	GeoB17307-5	4.5	1.77	0.95	0.61	0.16	0.07	0.83	2.72	3.55	50	27	77	23
40	IGSN: GEOB0173EXAM001	GeoB17307-5	22.5	3.30	1.00	0.16	0.07	0.04	0.27	4.29	4.56	72	22	94	6
41	IGSN: GEOB0173EX8Y001	GeoB17307-8	62.5	2.27	0.99	0.22	0.16	0.11	0.48	3.25	3.74	61	26	87	13
42	IGSN: GEOB0173EXBY001	GeoB17307-8	108	2.97	1.06	0.21	0.06	0.03	0.30	4.04	4.33	69	25	93	7
43	IGSN: GEOB0173EXMY001	GeoB17307-8	339	3.00	0.96	0.34	0.12	0.05	0.51	3.96	4.47	67	21	89	11
44	IGSN: GEOB0173EXPY001	GeoB17307-8	446	2.72	0.79	0.19	0.11	0.06	0.36	3.51	3.88	70	20	91	9
45	IGSN: GEOB0173EXCM001	GeoB17308-1	1.5	5.01	2.21	0.70	0.15	0.08	0.93	7.22	8.15	61	27	89	11
46	IGSN: GEOB0173EXLZ001	GeoB17308-4	25.0	3.22	1.48	0.26	0.06	0.03	0.34	4.70	5.04	64	29	93	7
47	IGSN: GEOB0173EXUZ001	GeoB17308-4	225	2.01	0.95	0.38	0.05	0.03	0.46	2.96	3.42	59	28	86	14
48	IGSN: GEOB0173EXWZ001	GeoB17308-4	275	1.13	0.60	0.10	0.03	0.01	0.15	1.73	1.88	60	32	92	8

**Supplementary Table S2 (continued):** Absolute concentration, relative abundance and distribution indices of GDGTs, BDGTs and PDGTs. (n.d.: not detected; n.a.: not applicable).

# in dataset	IGSN	core ID	sample depth (cmbsf)	[2G-PDGTs] ( $\mu\text{g/g OC}$ )	[1G-PDGTs] ( $\mu\text{g/g OC}$ )	[CL-PDGTs] ( $\mu\text{g/g OC}$ )	sum [IPL-PDGTs] ( $\mu\text{g/g OC}$ )	sum [PDGTs] ( $\mu\text{g/g OC}$ )	f(2G-PDGT) (%)	f(1G-PDGT) (%)	f(CL-PDGT) (%)	f(IPL-PDGTs) (%)
1	IGSN: GEOB0151EXIH101	GeoB15103-3	3	n.d.	0.87	n.d.	0.87	0.87	n.a.	100	n.a.	100
2	IGSN: GEOB0151EXCG101	GeoB15103-1	26.5	0.20	0.55	0.19	0.76	0.95	22	58	20	80
3	IGSN: GEOB0151EXJG101	GeoB15103-1	297	n.d.	0.20	n.d.	0.20	0.20	n.a.	100	n.a.	100
4	IGSN: GEOB0151EXKG101	GeoB15103-1	314	1.54	0.40	0.13	1.94	2.07	74	19	6	94
5	IGSN: GEOB0151EXQG101	GeoB15103-1	460	1.09	0.96	1.05	2.05	3.10	35	31	34	66
6	IGSN: GEOB0151EXOH101	GeoB15103-2	27.5	0.09	0.72	0.01	0.81	0.82	10	88	2	98

7	IGSN: GEOB0151EX5H101	GeoB15103-2	230	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
8	IGSN: GEOB0151EX7H101	GeoB15103-2	293	0.90	0.68	n.d.	1.58	1.58	57	43	n.a.	100
9	IGSN: GEOB0151EXBH101	GeoB15103-2	445	0.43	0.65	0.17	1.08	1.25	34	52	14	86
10	IGSN: GEOB0151EXCH101	GeoB15103-2	473	0.22	0.24	n.d.	0.46	0.46	49	51	n.a.	100
11	IGSN: GEOB0151EXEH101	GeoB15103-2	559	0.43	0.22	0.10	0.65	0.75	57	29	13	87
12	IGSN: GEOB0151EX5J101	GeoB15104-1	3.0	n.d.	0.89	n.d.	0.89	0.89	n.a.	100	n.a.	100
13	IGSN: GEOB0151EXLJ101	GeoB15104-1	35	n.d.	0.91	0.02	0.91	0.93	n.a.	98	2	98
14	IGSN: GEOB0151EXVJ101	GeoB15104-2	188	n.d.	0.73	0.07	0.73	0.79	n.a.	92	8	92
15	IGSN: GEOB0151EXXJ101	GeoB15104-2	288	n.d.	0.90	0.06	0.90	0.96	n.a.	94	6	94
16	IGSN: GEOB0151EXOK101	GeoB15104-2	368	n.d.	0.10	0.13	0.10	0.23	n.a.	44	56	44
17	IGSN: GEOB0151EX5K101	GeoB15104-2	628	n.d.	n.d.	0.04	n.a.	0.04	n.a.	n.a.	100	n.a.
18	IGSN: GEOB0151EXAM101	GeoB15105-4	9.0	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
19	IGSN: GEOB0151EXPM101	GeoB15105-4	39	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
20	IGSN: GEOB0151EXOL101	GeoB15105-2	113	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
21	IGSN: GEOB0151EX1L101	GeoB15105-2	155	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
22	IGSN: GEOB0151EX4L101	GeoB15105-2	273	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
23	IGSN: GEOB0151EX6L101	GeoB15105-2	398	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
24	IGSN: GEOB0151EX8L101	GeoB15105-2	428	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
25	IGSN: GEOB0151EXCL101	GeoB15105-2	605	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
26	IGSN: GEOB0173EXYS001	GeoB17302-5	3.5	n.d.	0.49	n.d.	0.49	0.49	n.a.	100	n.a.	100
27	IGSN: GEOB0173EXOT001	GeoB17302-5	60	n.d.	n.d.	0.20	n.a.	0.20	n.a.	n.a.	100	n.a.
28	IGSN: GEOB0173EX4T001	GeoB17302-5	180	n.d.	n.d.	0.40	n.a.	0.40	n.a.	n.a.	100	n.a.
29	IGSN: GEOB0173EX2V001	GeoB17304-3	8.0	n.d.	0.35	n.d.	0.35	0.35	n.a.	100	n.a.	100
30	IGSN: GEOB0173EX3V001	GeoB17304-3	19.5	n.d.	0.46	n.d.	0.46	0.46	n.a.	100	n.a.	100
31	IGSN: GEOB0173EX7V001	GeoB17304-3	57.5	n.d.	0.08	0.12	0.08	0.20	n.a.	39	61	39
32	IGSN: GEOB0173EXMV001	GeoB17304-3	180	n.d.	n.d.	0.10	n.a.	0.10	n.a.	n.a.	100	n.a.
33	IGSN: GEOB0173EXDL001	GeoB17306-1	4.5	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
34	IGSN: GEOB0173EXKL001	GeoB17306-1	32.5	0.85	n.d.	n.d.	0.85	0.85	100	n.a.	n.a.	100
35	IGSN: GEOB0173EX8E001	GeoB17306-2	70	0.84	n.d.	n.d.	0.84	0.84	100	n.a.	n.a.	100
36	IGSN: GEOB0173EXCE001	GeoB17306-2	255	n.d.	n.d.	n.d.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
37	IGSN: GEOB0173EXHE001	GeoB17306-2	382	0.28	n.d.	n.d.	0.28	0.28	100	n.a.	n.a.	100
38	IGSN: GEOB0173EXIE001	GeoB17306-2	430	0.60	n.d.	n.d.	0.60	0.60	100	n.a.	n.a.	100

39	IGSN: GEOB0173EX5M001	GeoB17307-5	4.5	0.55	n.d.	n.d.	0.55	0.55	100	n.a.	n.a.	100
40	IGSN: GEOB0173EXAM001	GeoB17307-5	22.5	0.62	n.d.	n.d.	0.62	0.62	100	n.a.	n.a.	100
41	IGSN: GEOB0173EX8Y001	GeoB17307-8	62.5	1.02	n.d.	n.d.	1.02	1.02	100	n.a.	n.a.	100
42	IGSN: GEOB0173EXBY001	GeoB17307-8	108	1.55	n.d.	n.d.	1.55	1.55	100	n.a.	n.a.	100
43	IGSN: GEOB0173EXMY001	GeoB17307-8	339	1.09	n.d.	n.d.	1.09	1.09	100	n.a.	n.a.	100
44	IGSN: GEOB0173EXPY001	GeoB17307-8	446	0.92	n.d.	n.d.	0.92	0.92	100	n.a.	n.a.	100
45	IGSN: GEOB0173EXCM001	GeoB17308-1	1.5	1.23	n.d.	n.d.	1.23	1.23	100	n.a.	n.a.	100
46	IGSN: GEOB0173EXLZ001	GeoB17308-4	25.0	1.23	n.d.	n.d.	1.23	1.23	100	n.a.	n.a.	100
47	IGSN: GEOB0173EXUZ001	GeoB17308-4	225	0.72	n.d.	n.d.	0.72	0.72	100	n.a.	n.a.	100
48	IGSN: GEOB0173EXWZ001	GeoB17308-4	275	0.57	n.d.	n.d.	0.57	0.57	100	n.a.	n.a.	100

**Supplementary Table S2 (continued):** Absolute concentration, relative abundance and distribution indices of GDGTs, BDGTs and PDGTs. (n.d.: not detected; n.a.: not applicable).

# in dataset	IGSN	core ID	sample depth (cmbfsf)	[2G-GDGT-0] ( $\mu\text{g/g OC}$ )	[1G-GDGT-0] ( $\mu\text{g g}^{-1}\text{ OC}$ )	[CL-GDGT-0] ( $\mu\text{g g}^{-1}\text{ OC}$ )	sum [IPL-GDGT-0] ( $\mu\text{g/g OC}$ )	sum [GDGT-0] ( $\mu\text{g/g OC}$ )	f(GDGT-0) (%)	f(IPL-GDGT-0) (%)	(sum-BDGTs)/(sum-GDGT-0) (%)	(sum-PDGTs)/(sum-GDGT-0) (%)
1	IGSN: GEOB0151EXIH101	GeoB15103-3	3	n.d.	0.48	4.42	0.48	4.91	90.14	9.86	n.a.	17.7
2	IGSN: GEOB0151EXCG101	GeoB15103-1	26.5	2.63	6.14	358.44	8.77	367.21	97.61	2.39	1.1	0.3
3	IGSN: GEOB0151EXJG101	GeoB15103-1	297	n.d.	1.35	5.94	1.35	7.29	81.43	18.57	12.8	2.7
4	IGSN: GEOB0151EXKG101	GeoB15103-1	314	5.96	7.57	341.97	13.52	355.49	96.20	3.80	1.7	0.6
5	IGSN: GEOB0151EXQG101	GeoB15103-1	460	5.76	9.29	315.86	15.04	330.91	95.45	4.55	2.0	0.9
6	IGSN: GEOB0151EXOH101	GeoB15103-2	27.5	1.38	8.09	65.05	9.47	74.52	87.29	12.71	3.2	1.1
7	IGSN: GEOB0151EX5H101	GeoB15103-2	230	n.d.	0.53	1.83	0.53	2.36	77.68	22.32	1.6	n.a.
8	IGSN: GEOB0151EX7H101	GeoB15103-2	293	2.58	8.81	150.82	11.40	162.22	92.98	7.02	3.5	1.0
9	IGSN: GEOB0151EXBH101	GeoB15103-2	445	1.96	8.94	163.56	10.91	174.47	93.75	6.25	2.0	0.7
10	IGSN: GEOB0151EXCH101	GeoB15103-2	473	n.d.	4.27	11.01	4.27	15.28	72.06	27.94	3.0	3.0
11	IGSN: GEOB0151EXEH101	GeoB15103-2	559	0.52	7.26	95.22	7.79	103.00	92.44	7.56	1.1	0.7
12	IGSN: GEOB0151EX5J101	GeoB15104-1	3.0	0.12	1.12	48.38	1.25	49.62	97.49	2.51	1.7	1.8
13	IGSN: GEOB0151EXLJ101	GeoB15104-1	35	0.51	3.87	74.68	4.38	79.06	94.46	5.54	1.4	1.2
14	IGSN: GEOB0151EXVJ101	GeoB15104-2	188	0.28	3.75	52.87	4.02	56.89	92.93	7.07	1.9	1.4
15	IGSN: GEOB0151EXXJ101	GeoB15104-2	288	4.08	13.75	147.76	17.83	165.59	89.23	10.77	2.1	0.6
16	IGSN: GEOB0151EXOK101	GeoB15104-2	368	0.08	1.14	47.59	1.22	48.81	97.51	2.49	2.7	0.5
17	IGSN: GEOB0151EX5K101	GeoB15104-2	628	n.d.	3.13	18.80	3.13	21.93	85.73	14.27	1.7	0.2

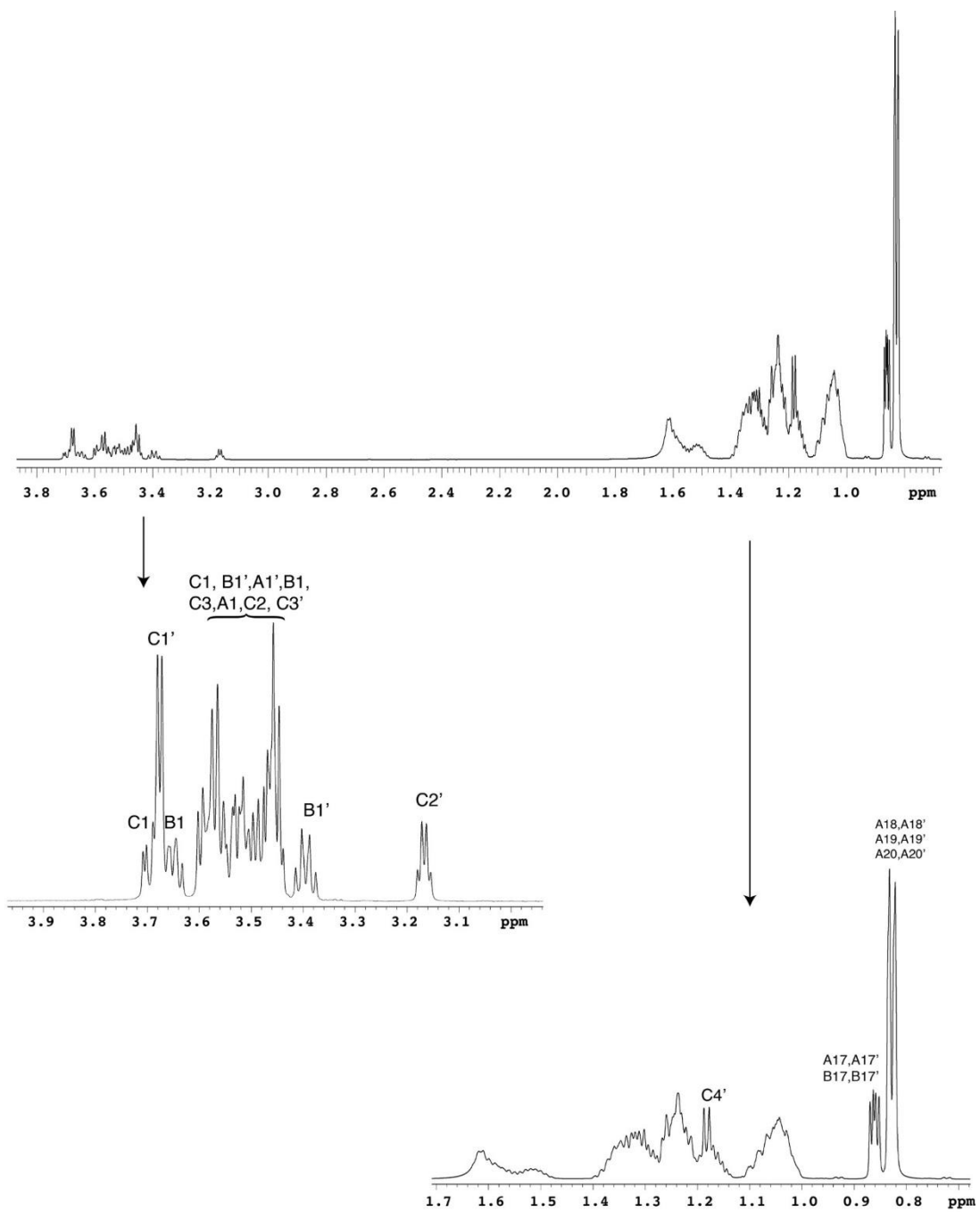
18	IGSN: GEOB0151EXAM101	GeoB15105-4	9.0	5.40	25.24	364.58	30.65	395.23	92.25	7.75	2.3	n.a.
19	IGSN: GEOB0151EXPM101	GeoB15105-4	39	7.98	23.26	262.00	31.24	293.24	89.35	10.65	1.7	n.a.
20	IGSN: GEOB0151EXOL101	GeoB15105-2	113	6.36	29.87	360.43	36.24	396.67	90.86	9.14	1.3	n.a.
21	IGSN: GEOB0151EX1L101	GeoB15105-2	155	6.23	22.59	287.18	28.82	316.00	90.88	9.12	1.4	n.a.
22	IGSN: GEOB0151EX4L101	GeoB15105-2	273	2.93	23.27	264.75	26.21	290.96	90.99	9.01	1.2	n.a.
23	IGSN: GEOB0151EX6L101	GeoB15105-2	398	1.68	15.47	372.46	17.16	389.62	95.60	4.40	0.5	n.a.
24	IGSN: GEOB0151EX8L101	GeoB15105-2	428	0.21	3.65	173.44	3.86	177.30	97.82	2.18	1.1	n.a.
25	IGSN: GEOB0151EXCL101	GeoB15105-2	605	0.36	4.02	121.51	4.38	125.89	96.52	3.48	0.3	n.a.
26	IGSN: GEOB0173EXYS001	GeoB17302-5	3.5	1.45	4.29	20.27	5.74	26.01	77.94	22.06	8.9	1.9
27	IGSN: GEOB0173EXOT001	GeoB17302-5	60	0.42	2.18	122.19	2.60	124.79	97.92	2.08	1.5	0.2
28	IGSN: GEOB0173EX4T001	GeoB17302-5	180	0.72	2.93	157.17	3.65	160.81	97.73	2.27	1.8	0.2
29	IGSN: GEOB0173EX2V001	GeoB17304-3	8.0	n.d.	0.22	3.37	0.22	3.59	93.93	6.07	n.a.	9.8
30	IGSN: GEOB0173EX3V001	GeoB17304-3	19.5	n.d.	0.24	4.24	0.24	4.48	94.71	5.29	n.a.	10.4
31	IGSN: GEOB0173EX7V001	GeoB17304-3	57.5	0.06	0.99	28.64	1.05	29.69	96.47	3.53	2.4	0.7
32	IGSN: GEOB0173EXMV001	GeoB17304-3	180	0.26	1.21	17.27	1.47	18.74	92.16	7.84	7.7	0.5
33	IGSN: GEOB0173EXDL001	GeoB17306-1	4.5	2.89	4.53	16.61	7.42	24.03	69.12	30.88	5.1	n.a.
34	IGSN: GEOB0173EXKL001	GeoB17306-1	32.5	3.11	4.82	10.10	7.93	18.03	56.02	43.98	19.2	4.7
35	IGSN: GEOB0173EX8E001	GeoB17306-2	70	2.61	4.09	8.74	6.70	15.44	56.61	43.39	24.9	5.4
36	IGSN: GEOB0173EXCE001	GeoB17306-2	255	5.65	9.41	14.15	15.06	29.22	48.44	51.56	18.9	n.a.
37	IGSN: GEOB0173EXHE001	GeoB17306-2	382	0.85	1.01	26.66	1.85	28.52	93.50	6.50	6.3	1.0
38	IGSN: GEOB0173EXIE001	GeoB17306-2	430	6.76	7.69	0.92	14.46	15.37	5.96	94.04	27.9	3.9
39	IGSN: GEOB0173EX5M001	GeoB17307-5	4.5	5.50	10.02	20.92	15.52	36.44	57.41	42.59	9.7	1.5
40	IGSN: GEOB0173EXAM001	GeoB17307-5	22.5	2.38	5.49	22.42	7.87	30.29	74.02	25.98	15.1	2.0
41	IGSN: GEOB0173EX8Y001	GeoB17307-8	62.5	2.64	3.71	9.42	6.35	15.77	59.74	40.26	23.7	6.5
42	IGSN: GEOB0173EXBY001	GeoB17307-8	108	3.26	4.45	8.13	7.71	15.84	51.33	48.67	27.3	9.8
43	IGSN: GEOB0173EXMY001	GeoB17307-8	339	4.41	5.56	7.66	9.97	17.63	43.45	56.55	25.4	6.2
44	IGSN: GEOB0173EXPY001	GeoB17307-8	446	2.74	3.50	9.03	6.24	15.26	59.13	40.87	25.4	6.0
45	IGSN: GEOB0173EXCM001	GeoB17308-1	1.5	2.39	14.36	120.32	16.75	137.07	87.78	12.22	5.9	0.9
46	IGSN: GEOB0173EXLZ001	GeoB17308-4	25.0	1.34	7.11	29.09	8.45	37.54	77.50	22.50	13.4	3.3
47	IGSN: GEOB0173EXUZ001	GeoB17308-4	225	0.50	2.37	20.72	2.87	23.59	87.84	12.16	14.5	3.1
48	IGSN: GEOB0173EXWZ001	GeoB17308-4	275	0.49	2.38	10.23	2.87	13.11	78.09	21.91	14.3	4.3



**Supplementary Table S3:** Carbon isotopic composition ( $\delta^{13}\text{C}$ ) of the biphytanes derived from IPL-GDGT-0 and IPL-BDGT-0 together with the carbon isotopic composition ( $\delta^{13}\text{C}$ ) of the total organic carbon (TOC), dissolved inorganic carbon (DIC) and methane.

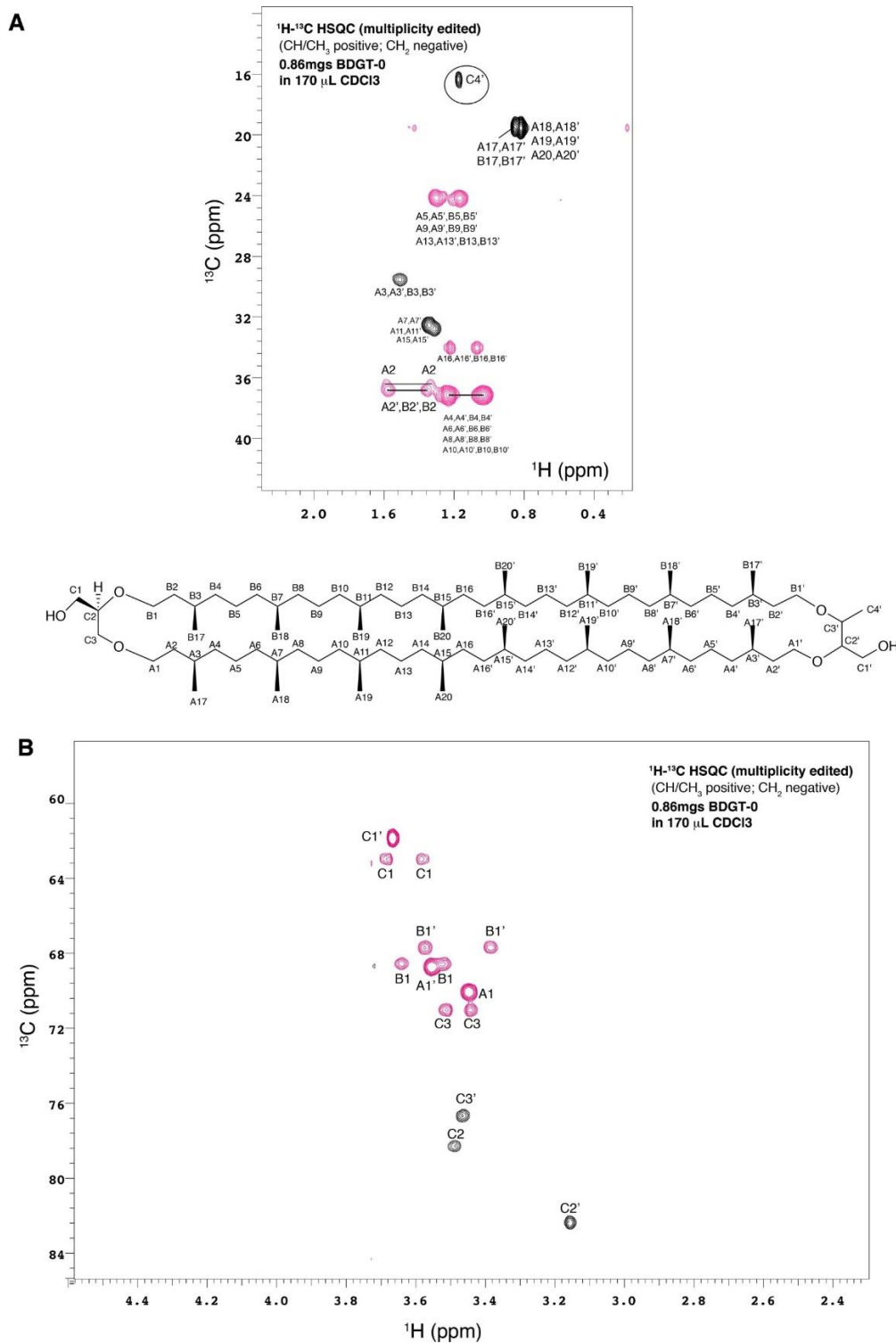
# in dataset	core ID	sample depth (cmbfsf)	$\delta^{13}\text{C}(\text{bp-0 IPL-GDGT}) (\text{‰})$	$\delta^{13}\text{C}(\text{bp-0 IPL-BDGT}) (\text{‰})$	$\delta^{13}\text{C}(\text{TOC}) (\text{‰})$	$\delta^{13}\text{C}(\text{DIC}) (\text{‰})$	$\delta^{13}\text{C}(\text{CH}_4) (\text{‰})$
5	GeoB15103-1	459.5	$-23 \pm 0.3$	$-28.0 \pm 0.1$	-20.1	-7.9	-67.8
8	GeoB15103-2	292.5	$-22.5 \pm 0.03$	$-28.7 \pm 0.1$	-19.5	-6.2	-69.1
20	GeoB15105-2	112.5	$-30.4 \pm 0.3$	$-51.8 \pm 0.2$	-24.8	-19.9	-88.5
22	GeoB15105-2	272.5	$-24.3 \pm 0.2$	$-41.0 \pm 0.8$	-24.3	-20.3	-87.0
34	GeoB17306-1	32.5	$-30.2 \pm 0.2$	$-56.3 \pm 0.9$	-26.9	-4.1	-63.6
38	GeoB17306-2	429.5	$-24.7 \pm 0.3$	$-53.0 \pm 0.2$	-25.9	2.9	-73.7

**Supplementary Figure S1.** 1-D  $^1\text{H}$  spectrum and expansions of BDGT-0 in  $\text{CDCl}_3$ .



## Supplementary Figure S2. $^1\text{H}$ - $^{13}\text{C}$ HSQC 2-D spectra of BDGT-0.

Methine and Methyl signals are positive (black) and methylene signals are negative (red). A) Carbon atoms (A, A', B, B') 2 to (A, A', B, B') 20 and C4' (circled). C4' is well resolved in 2D from the remaining methyl signals. A3, A3', B3 and B3' although overlapped with each other are well resolved from the remaining branched alkyl chain methine groups (7, 11 and 15). B) Ether linked  $^1\text{H}$ - $^{13}\text{C}$  correlations and glycerol and butanetriol correlations. The butanetriol moiety gives a distinctive set of two well resolved methine signals (C2' and C3') that correlate with C4' in the  $^1\text{H}$ - $^{13}\text{C}$  HMBC experiment.



**Supplementary Figure S3.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC 2-D spectra of BDGT-0.

A) Methyl and alkyl side-chain correlations. 17-methyls are resolved from 18, 19 and 20. A1 and A1' correlations allow discrimination of A2/A2' and A3/A3' chemical shifts. Weaker (due to multiplicity and non-degenerate protons) B1 and B1' correlations are visible but are just above the noise and not plotted at this level here. B) Carbon bonded to oxygen chemical shift region. Several key correlations are highlighted including key correlations from C4' to methine C3' and C2' (black box). Each of the correlation across the four ether linkages is highlighted.

