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Supplementary information for Chaves Torres et al.

I. Concentrations and proportions of prokaryotic membrane lipids in OM fractions

Table S1. Concentration (µg/g TOC) of FAs and archaeal ether lipids in soluble and IOM fractions of CP1, CP2 and OP.

		FAs*						Archaeal ether lipids*						
	Sample ID	*i*-C15	*ai*-C15	*n*-C15	*i*-C17	*ai*-C17	*n*-C17	archaeol	GDGT—	GDGT-1	GDGT-2	GDGT-3	GDGT-4	Cren-archaeol
BD	CP1	–	–	12	12	48	37	420	1300	250	280	130	180	51
	CP2	–	–	22	4.4	9.0	47	170	22	12	160	75	310	36
	OP	90	23	19	320	150	40	420	580	390	670	1000	1100	140
Sox	CP1	10	–	10	–	7.8	7.0	91	230	65	63	39	41	16
	CP2	–	–	31	1.5	7.8	70	13	5.2	2.3	36	18	69	8.1
	OP	13	5.1	11	56	27	48	100	180	110	190	360	370	40
BHy	CP1	–	–	40	17	30	28	84	490	100	130	76	74	26
	CP2	–	1.7	6.9	–	1.9	8.7	17	6.2	3.1	39	14	62	9.0
	OP	5.1	1.7	0.87	19	8.4	3.0	7.3	31	21	34	59	75	7.1
AMe	CP1	–	–	–	7.3	9.8	17	58	780	72	97	52	76	29
	CP2	–	–	–	–	–	–	–	2.6	1.7	19	8.0	36	4.5
	OP	31	13	5.3	100	45	5.9	–	30	19	28	54	69	5.9

* See the manuscript Appendix for structures.

Note: Values presented in the current table are the result of quantification by comparison of peak areas with an internal standard (Chaves Torres and Pancost, 2016). There has been no calibration curve developed based on authentic standards. Although that is commonly used in GC or GC-MS approaches, it is understood to be only semi-quantitative for GDGT quantification (due to different ionisation efficiency of GDGTs compared to the internal standard). Reproducabiltiy allows a comparison among samples and fractions used in this study, but abundances shown in the Table above are not quantitative.

Table S2. Concentration (μg/g TOC) of bacterial DAGEs and hopanoids in soluble and IOM fractions of CP1, CP2 and OP.

		Bacterial DAGEs*									Hopanoids**						
	Sample ID	16/16	16/17 (a)	16/17 (b)	16/18	17/17 (a)	17/17 (b)	17/18	18/18	18/19	C31 αβ	C32 αβ	C31 ββ	C32 βα	C32 ββ	C33 ββ	anhydro-BHT
BD	CP1	130	70	790	260	290	1400	84	750	86	–	–	–	–	–	–	–
	CP2	–	–	–	–	–	–	–	–	–	36	35	150	29	370	59	180
	OP	–	–	44	37	49	120	80	220	–	10	19	20	17	47	–	–
Sox	CP1	49	–	190	63	48	370	–	140	–	–	–	–	–	–	–	–
	CP2	–	–	–	–	–	–	–	–	–	–	–	130	30	190	12	360
	OP	–	–	–	11	17	36	20	67	–	–	–	–	–	–	–	–
BHy	CP1	15	–	130	33	–	280	–	97	–	–	–	–	–	–	–	–
	CP2	–	–	–	–	–	–	–	–	–	9.8	11	31	6.4	77	15	–
	OP	–	–	–	0.50	–	1.5	0.77	2.3	–	1.0	1.4	0.32	0.97	3.8	–	–
AMe	CP1	–	–	100	23	20	160	–	100	–	–	–	–	–	–	–	–
	CP2	–	–	–	–	–	–	–	–	–	–	–	21	7.3	49	4.5	410
	OP	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–

*Numbers refer to the number of carbon atoms of each alkyl chain. See exemplary structure in Appendix.
**See exemplary structure in Appendix.
(a) and (b) represent different isomers of the corresponding DAGE.
Note: See comment on Supplementary Table 1 with respect to quantification methodology.

Table S3. Total concentration (mg/g TOC) of target compounds and distribution (%) of compounds within soluble and IOM fractions. Note that Figs. 2–6 and Fig. 7 (a–d) in the manuscript are based on the data below.

		Total concentration (mg/g TOC)				Percentage (%) of total compounds recovered			
	Target comound classes	BD	Sox	BHy	AMe	BD	Sox	BHy	AMe
CP1	Branched FAs	0.060	0.018	0.047	0.017	42	13	33	12
	Hopanoids	–	–	–	–	–	–	–	–
	Bacterial DAGEs	3.8	0.86	0.56	0.41	68	15	9.9	7.3
	Archaeol	0.42	0.091	0.084	0.058	64	14	13	8.8
	i-GDGTs	2.2	0.45	0.90	1.1	47	9.6	19	24
CP2	Branched FAs	0.013	0.0093	0.0036	–	51	35	14	–
	Hopanoids	0.85	0.72	0.15	0.49	38	33	6.8	22
	Bacterial DAGEs	–	–	–	–	–	–	–	–
	Archaeol	0.17	0.013	0.017	–	85	6.4	8.4	–
	i-GDGTs	0.61	0.14	0.13	0.071	64	14	14	7.5
OP	Branched FAs	0.59	0.10	0.034	0.19	64	11	3.7	21
	Hopanoids	0.11	–	0.0075	–	94	–	6.2	–
	Bacterial DAGEs	0.55	0.15	0.0050	–	78	21	0.71	–
	Archaeol	0.42	0.10	0.0073	–	79	19	1.4	–
	i-GDGTs	4.0	1.2	0.23	0.20	70	22	4.0	3.6

II. Chromatograms showing the distribution of major compounds associated with soluble and IOM fractions

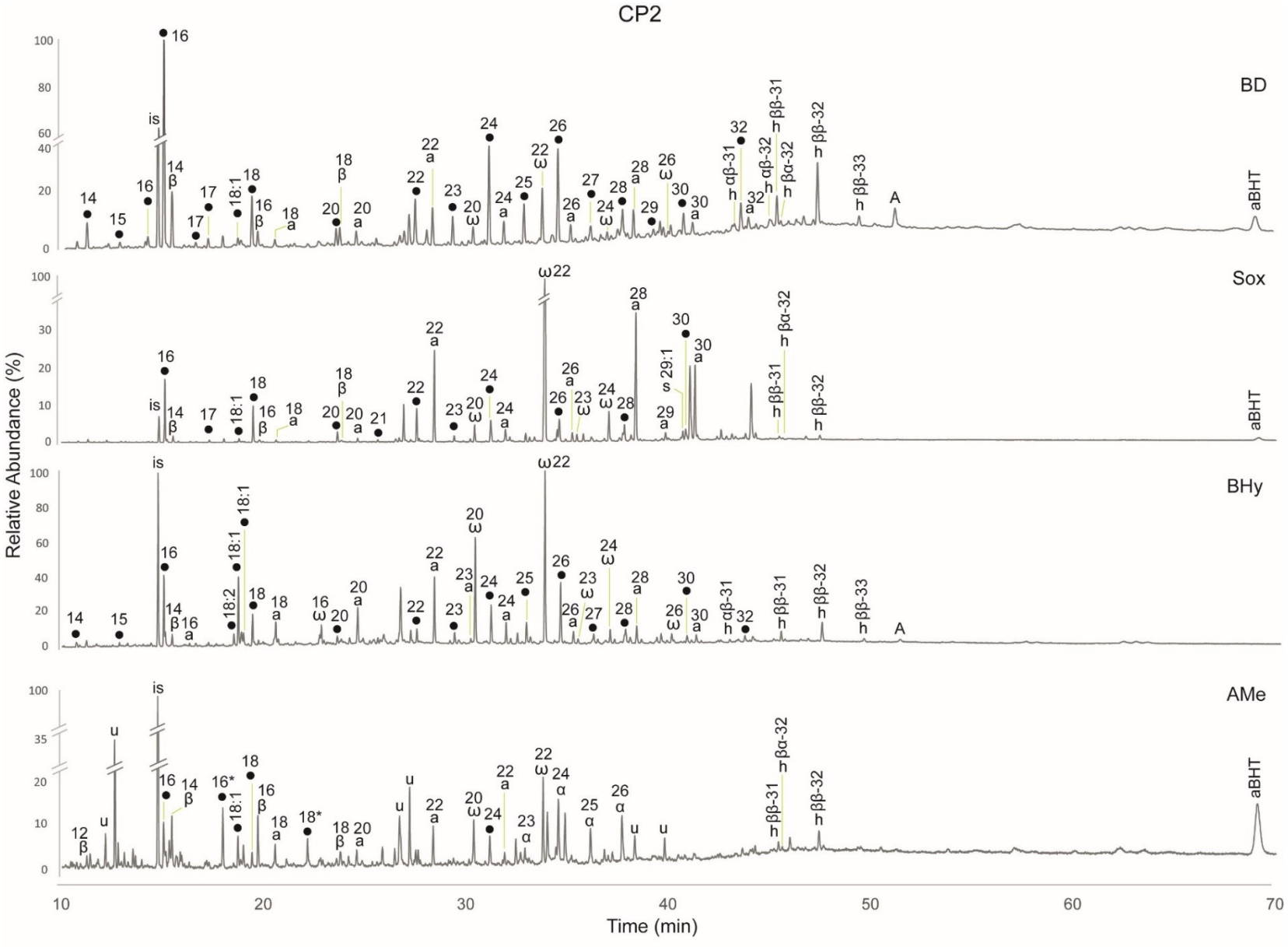

Figure S1. Partial chromatograms of BD (AMe of TLE), Sox (AMe of TLE), BHy and AMe OM fractions from CP2 TVZ silica sinter after GC-MS. Symbols: black circle: alkanoic acids; β: β-hydroxy alkanoic acids; ω: ω-hydroxy alkanoic acids; a: alcohols; P: polycyclic aromatic hydrocarbons (PAHs); d: dialkyl glycerol diethers (DAGEs); s: sterols; α: α-hydroxy alkanoic acids; h: hopanoids; A: archaeol; aBHT: anhydrobacteriohopanetetrol; u: unidentified compound; *: TMS-derivative; is: internal standard (2-hexadecanol).

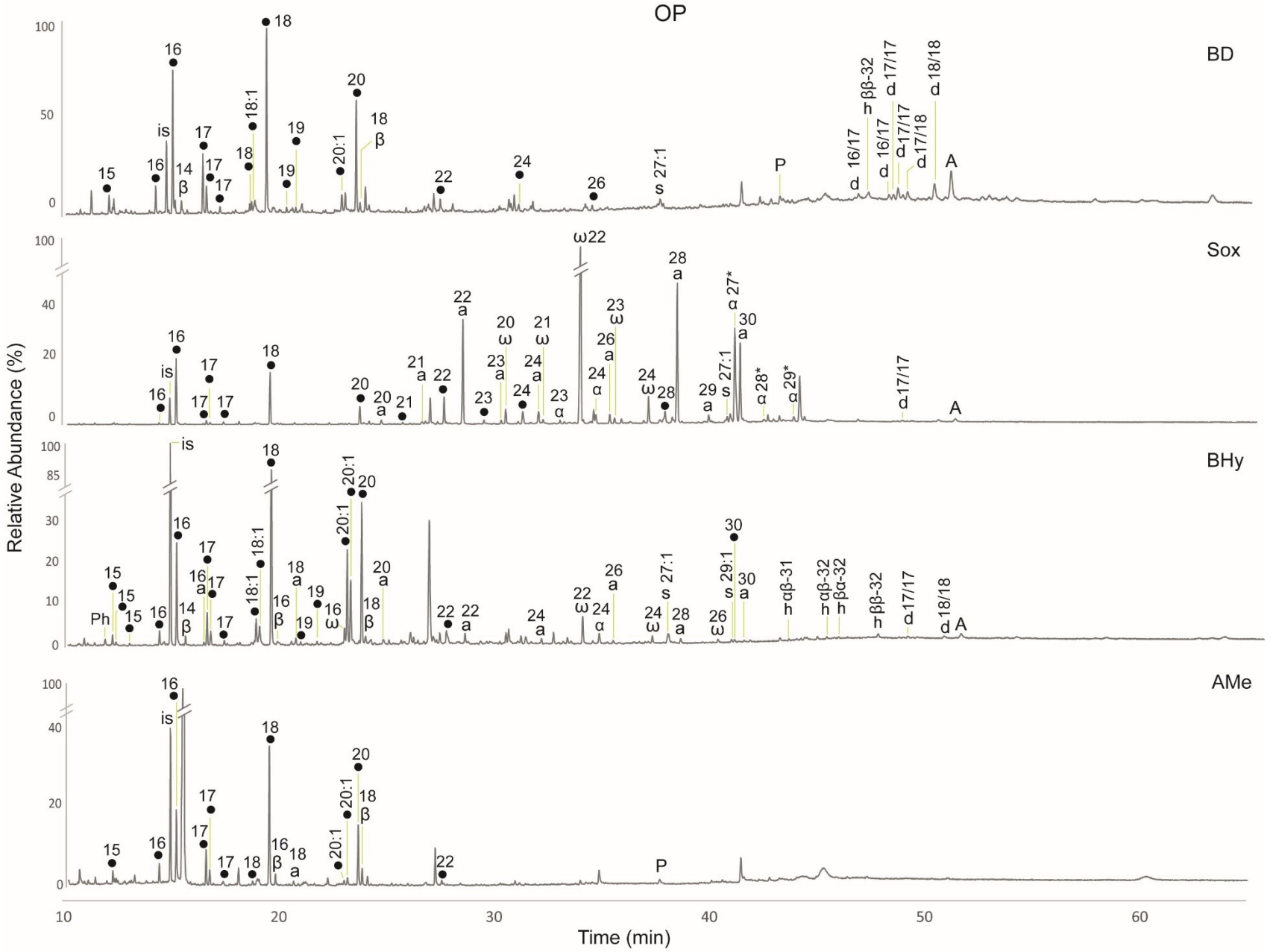
OP
BD
Sox
BHy
AMe
Relative Abundance (%)
Time (min)
10
20
30
40
50
60

Figure S2. Partial chromatograms of BD (AMe of TLE), Sox (AMe of TLE), BHy and AMe OM fractions from CP2 TVZ silica sinter after GC-MS. Symbols: black circle: alkanoic acids; β: β-hydroxy alkanoic acids; ω: ω-hydroxy alkanoic acids; a: alcohols; P: polycyclic aromatic hydrocarbons (PAHs); d: dialkyl glycerol diethers (DAGEs); s: sterols; α: α-hydroxy alkanoic acids; h: hopanoids; A: archaeol; Ph: phenols; u: unidentified compound; *: TMS-derivative; is: internal standard (2-hexadecanol).

III. Overall TLEs content in OM fractions

Table S4. Total concentrations (mg/g TOC) of major compound classes within our analytical window.

		Silica sinters		
OM fraction	**Compound Class**	**CP1**	**CP2**	**OP**
BD	odd-numbered FAs	0.11	0.083	0.65
	even-numbered FAs	3.3	3.5	3.6
	hydroxy FAs	0.93	0.97	0.084
	n-alcohols	0.45	0.85	0.18
	n-alkanes	0.12	0.13	0.012
	PAHs	1.1	–	0.039
	DAGEs	3.8	–	0.55
	Hopanoids	–	0.85	0.11
	sterols	0.049	–	0.013
	phenols	–	–	–
	archaeol	0.42	0.17	0.42
	i-GDGTs	2.2	0.61	4.0
	TOTAL	**12**	**7.2**	**9.6**
Sox	odd-numbered FAs	0.035	0.11	0.16
	even-numbered FAs	0.64	6.4	3.4
	hydroxy FAs	0.63	15	6.2
	n-alcohols	5.4	11	6.4
	n-alkanes	0.059	0.15	0.026
	PAHs	0.083	–	–
	DAGEs	0.86	–	0.15
	Hopanoids	–	0.72	–
	sterols	–	–	0.037
	phenols	–	–	–
	archaeol	0.091	0.013	0.10
	i-GDGTs	0.45	0.14	1.2
	TOTAL	**8.3**	**33**	**18**
BHy	odd-numbered FAs	0.11	0.019	0.038
	even-numbered FAs	2.5	1.1	0.48
	hydroxy FAs	1.1	0.18	0.20
	n-alcohols	0.079	0.49	0.022
	n-alkanes	0.054	0.015	–
	PAHs	0.43	–	–
	DAGEs	0.56	–	0.0050
	Hopanoids	–	0.15	0.0075
	sterols	–	–	0.018
	phenols	0.053	0.026	0.020
	archaeol	0.084	0.017	0.0073
	i-GDGTs	0.90	0.13	0.23
	TOTAL	**5.9**	**2.1**	**1.0**
AMe	odd-numbered FAs	0.034	–	0.20
	even-numbered FAs	1.4	0.26	0.93
	hydroxy FAs	2.4	1.0	0.49
	n-alcohols	0.073	0.15	0.033
	n-alkanes	0.0029	0.0082	0.0083
	PAHs	0.10	–	0.022
	DAGEs	0.41	–	–
	Hopanoids	–	0.49	–
	sterols	–	–	–
	phenols	0.096	0.012	–
	archaeol	0.058	–	–
	i-GDGTs	1.1	0.071	0.20
	TOTAL	**5.6**	**2.0**	**1.9**

Note: See comment on Supplementary Table 1 with respect to quantification methodology.

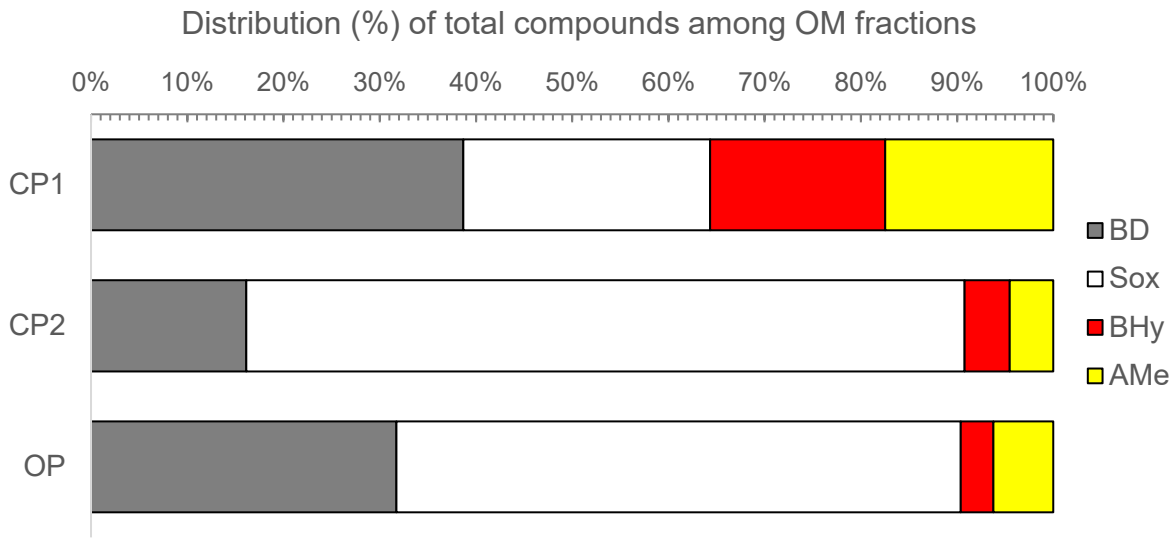

Figure S3. Distribution of major compound classes within our analytical window among soluble and IOM fractions. Note that 10–36% of compunds only occur in IOM fractions.

Table S5. Estimation of the % of TOC recovery based on the carbon content of compounds quantified in TLEs (Table S4).

	% of TOC recovered		
OM fraction	CP1	CP2	OP
BD	0.97	0.53	0.72
Sox	0.65	2.5	1.3
BHy	0.44	0.15	0.075
AMe	0.41	0.15	0.13
TOTAL	**2.5**	**3.3**	**2.3**

*Note that not included in this quantification are unidentified compounds within our analytical window and compounds out of our analytical window, but likely also recovered with our methodology.