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Supplementary Material

Molecular composition and spatial distribution of dissolved organic matter (DOM) in the Pearl River Estuary, China

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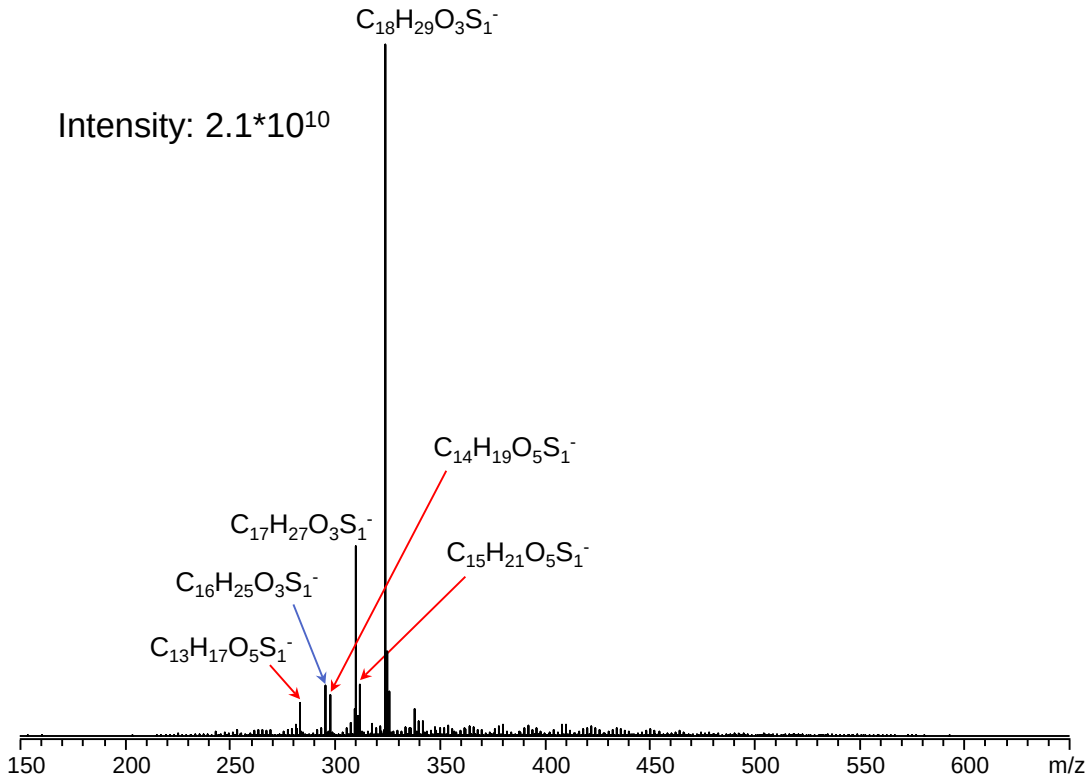

Fig. S1. Negative-ion ESI FT-ICR mass spectrum of the SPE-DOM from site A in Pearl River Estuary.

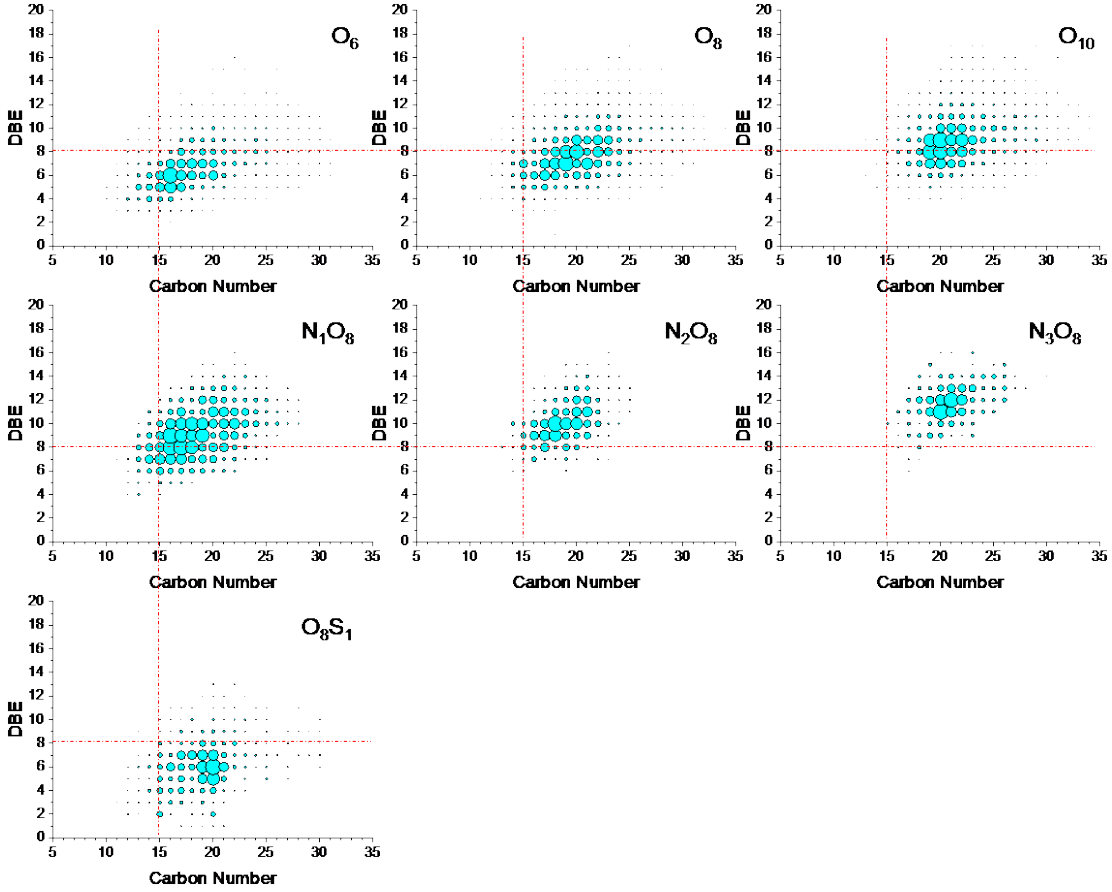

Fig. S2. Ion relative abundance plots of DBE versus carbon numbers for O_6, O_8, O_{10}, N_1O_8, N_2O_8, N_3O_8 and O_8S_1 class species assigned from the negative ion mass spectrum of the SPE-DOM form site A.

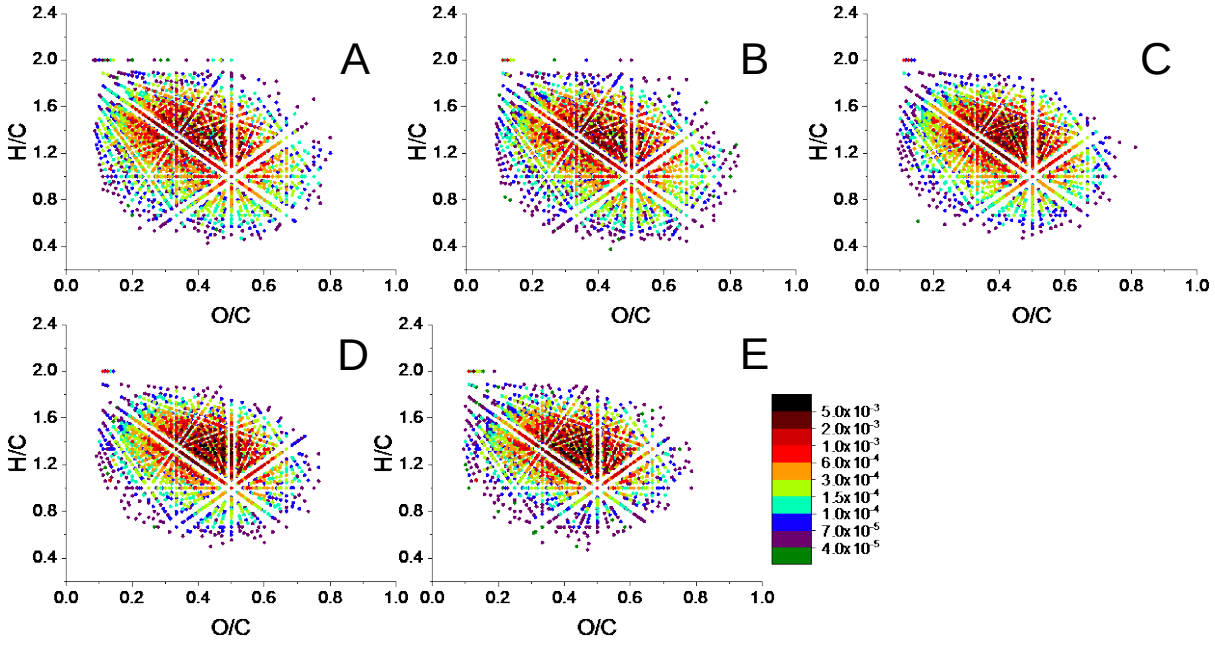

Fig. S3. van Krevelen diagram of CHO classes for DOM in A, B, C, D and E sites detected by negative-ion ESI FT-ICR MS.

Table S1

FT-ICR MS intensity-weighted average (wa) molecular parameters of the DOM in all samples.

Sample	A	B	C	D	E	K1	K2	K3	K4	K5
m/z_{wa}	386.9	390.1	401.5	409.2	405.3	396.0	407.2	397.8	399.1	396.2
Num	5518	5156	4710	4344	4233	5376	4984	4612	5439	5422
C_{wa}	19.49	19.45	19.97	20.19	19.95	19.89	20.07	19.83	19.90	19.94
H_{wa}	25.09	24.62	25.93	26.34	26.23	25.23	24.85	25.05	25.02	25.37
O_{wa}	7.57	7.90	8.13	8.45	8.42	7.91	8.52	8.06	8.07	7.86
N_{wa}	0.31	0.30	0.32	0.30	0.30	0.32	0.32	0.29	0.32	0.30
S_{wa}	0.10	0.07	0.07	0.06	0.05	0.06	0.05	0.08	0.08	0.07
CHO	70.2% (2211)	73.5% (2219)	70.6% (1954)	73.7% (1878)	75.2% (1871)	73.2% (2448)	73.6% (2207)	72.0% (2077)	71.7% (2312)	72.9% (2357)
CHON	11.3% (1087)	11.3% (1081)	15.4% (1237)	13.0% (1080)	11.8% (985)	12.2% (1157)	12.7% (1164)	12.6% (1057)	12.6% (1208)	11.5% (1148)
CHON2	5.4% (645)	5.4% (606)	4.1% (369)	4.5% (381)	5.5% (456)	6.0% (671)	6.0% (612)	5.0% (478)	5.4% (612)	5.3% (634)
CHON3	3.1% (439)	2.8% (426)	2.7% (368)	2.8% (376)	2.7% (379)	3.1% (453)	2.8% (405)	2.5% (312)	2.7% (436)	2.8% (430)
CHOS	8.9% (904)	6.4% (755)	6.6% (724)	5.6% (612)	4.4% (529)	5.0% (601)	4.5% (563)	7.4% (665)	6.8% (771)	6.7% (757)
CHONS	1.1% (232)	0.6% (135)	0.6% (124)	0.4% (83)	0.3% (79)	0.5% (112)	0.4% (99)	0.5% (89)	0.8% (166)	0.7% (162)
O/C_{wa}	0.39	0.41	0.41	0.42	0.43	0.40	0.43	0.41	0.41	0.40
H/C_{wa}	1.29	1.26	1.30	1.30	1.31	1.27	1.23	1.26	1.25	1.27
DBE_{wa}	8.10	8.29	8.16	8.16	7.99	8.43	8.80	8.45	8.55	8.41
$AI_{mod, wa}$	0.27	0.28	0.25	0.24	0.23	0.28	0.29	0.28	0.28	0.28

Sample	A	B	C	D	E	K1	K2	K3	K4	K5
Polycyclic aromatics (%)	1.4	1.6	0.7	0.5	0.3	1.4	1.5	1.2	1.4	1.3
Highly aromatics (%)	8.2	8.5	5.9	4.3	3.1	8.2	8.6	8.2	8.4	8.3
Highly unsaturated (%)	71.1	73.7	76.3	80.2	81.9	75.0	78.2	75.4	75.7	73.7
Unsaturated aliphatics (%)	19.2	16.2	17.0	14.9	14.6	15.2	11.6	15.2	14.4	16.4
CRAM(%)	64.3	66.9	67.7	68.9	68.8	68.1	71.2	68.5	69.1	67.3

Num: number of assigned formulae; AI_{mod}: modified aromaticity index; DBE: double bond equivalents; O/C: oxygen to carbon ratio; H/C: hydrogen to carbon ratio; CRAM: carboxylic-rich alicyclic compounds.