

Supplementary Materials of
Comparing the spectroscopic and molecular characteristics for different
dissolved organic matter fractions isolated by hydrophobic and anionic
exchange resins using fluorescence spectroscopy and FT-ICR-MS

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Table S1. Samples description including site name, type of area, depth, date of sampling, geographical coordinates and samples names.

Site Name	Characteristics sample			
	Depth (m)	Sampling date	Coordinates	Samples name
DaeCheong Dam	0	2016.11.03	36°28'34.8"N 127°29'6.91"E	D1
	20			D2
	40			D3
DaeCheong River 1	0.4	2016.11.03	36°13'47.31"N 127°43'34.73"E	R1
DaeCheong River 2	0.9		36°17'2.86"N 127°38'43.09"E	R2
DaeCheong River 3	1.1		36°17'56.28"N 127°39'55.18"E	R3

Table S2. Characteristics of compound classes used for categorizing FT-ICR MS molecular formulas.

Compound class	Abbreviation/Name	Criterion
Aromatic formula	AF	$AI_{mod} = 0.5-0.67$
Condensed aromatic structure	CAS	$0.2 \leq H/C \leq 0.7$ $0 \leq O/C \leq 0.67$
Lignin/CRAM	Lignin	$0.7 \leq H/C \leq 1.5$ $0.1 \leq O/C \leq 0.67$
Protein	Protein	$1.5 \leq H/C \leq 2.2$ $0.3 \leq O/C \leq 0.67$
Carbohydrate	Carbohydrate	$1.5 \leq H/C \leq 2.4$ $0.67 \leq O/C \leq 1.2$
Lipid	Lipid	$1.5 \leq H/C \leq 2.0$ $0 \leq O/C \leq 0.3$
Unsaturated hydrocarbon	UnsatHydroC	$0.7 \leq H/C \leq 1.5$ $0 \leq O/C \leq 0.1$
Tannin	Tannin	$0.5 \leq H/C \leq 1.5$ $0.65 \leq O/C \leq 1$

Table S3. Values of chemical, spectroscopic and molecular characteristics of the three chemical fractions for the 6 water samples from Deacheong Reservoir.

	HPOA						TPIA						HPIN/B					
Sample	D1	D2	D3	R1	R2	R3	D1	D2	D3	R1	R2	R3	D1	D2	D3	R1	R2	R3
SUVA ₂₅₄	3.0	/	5.9	4.9	3.2	1.9	0.2	0.4	0.4	0.5	0.6	0.2	0.3	0.1	0.1	0.1	0.6	0.1
%C1	35.3	34.0	27.2	31.0	24.1	29.1	14.4	31.5	32.5	35.3	35.3	33.5	23.9	23.3	19.6	20.2	21.7	/
%C2	21.5	17.7	12.2	20.4	14.2	15.0	3.6	15.3	14.6	14.2	14.2	14.1	7.6	4.7	5.9	6.5	6.7	/
%C3	43.2	48.2	60.6	48.6	61.7	55.9	82.0	53.3	53.0	50.6	50.6	52.4	68.5	72.0	74.6	73.4	71.6	/
FI	1.1	1.2	1.2	1.2	1.2	1.2	1.2	1.3	1.2	1.3	1.3	1.3	1.7	1.6	1.6	1.5	1.6	1.5
HIX	3.4	2.9	1.8	2.9	1.7	2.1	0.5	2.1	1.7	2.0	2.0	1.8	1.0	0.7	0.8	0.8	0.8	0.4
BIX	0.7	0.8	0.9	0.8	0.9	0.9	1.5	0.9	0.9	1.0	1.0	0.9	1.7	1.4	1.9	1.4	1.5	3.5
C1/C2	1.6	1.9	2.2	1.5	1.7	1.9	4.0	2.1	2.2	2.5	2.5	2.4	3.2	5.0	3.3	3.1	3.2	/
C1/C3	0.8	0.7	0.4	0.6	0.4	0.5	0.2	0.6	0.6	0.7	0.7	0.6	0.3	0.3	0.3	0.3	0.3	/
C2/C3	0.5	0.4	0.2	0.4	0.2	0.3	0.0	0.3	0.3	0.3	0.3	0.3	0.1	0.1	0.1	0.1	0.1	/
Number of formul	403	57	1	20	1	7	172	42	332	939	550	230	137	254	267	134	197	231
m/Z _{wa}	395.52	378.91	441.29	351.45	441.29	346.37	387.44	354.68	383.36	395.07	398.22	380.48	346.42	363.22	352.55	376.65	350.68	346.90
C _{wa}	23.62	23.19	27.00	21.00	24.00	19.02	24.07	21.92	23.43	24.14	24.47	23.63	19.66	21.89	21.44	21.42	20.17	19.99
H _{wa}	29.66	29.50	39.00	30.01	42.00	32.60	25.95	23.19	25.92	25.19	25.62	25.48	33.43	27.12	30.44	26.93	30.98	31.31
O _{wa}	3.97	2.66	4.00	3.48	7.00	5.25	2.59	2.47	3.02	3.53	3.31	2.64	4.10	4.34	3.34	5.18	3.94	4.15
N _{wa}	0.42	0.45	1.00	0.31	0.00	0.05	0.68	0.62	0.61	0.54	0.56	0.64	0.13	0.09	0.14	0.12	0.21	0.21
S _{wa}	0.42	0.70	0.00	0.31	0.00	0.05	0.69	0.64	0.61	0.52	0.58	0.64	0.32	0.11	0.31	0.28	0.38	0.22
H/C _{wa}	1.31	1.32	1.44	1.50	1.75	1.73	1.13	1.11	1.16	1.12	1.12	1.13	1.73	1.35	1.51	1.36	1.59	1.62
O/C _{wa}	0.20	0.14	0.15	0.19	0.29	0.28	0.14	0.15	0.16	0.18	0.17	0.14	0.23	0.24	0.18	0.28	0.22	0.23
N/C _{wa}	0.01	0.02	0.04	0.01	0.00	0.00	0.03	0.03	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01	0.01
S/C _{wa}	0.01	0.03	0.00	0.01	0.00	0.00	0.03	0.03	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.02	0.01
DBE _{wa}	10.0	9.7	9.0	7.1	4.0	3.7	12.43	11.63	11.77	12.82	12.94	12.21	4.01	9.37	7.29	9.01	5.78	5.44
DBE _{wa} /C _{wa}	0.4	0.4	0.3	0.3	0.2	0.2	0.5	0.5	0.5	0.5	0.5	0.5	0.2	0.4	0.3	0.4	0.3	0.3
A _{Imod,wa}	0.3	0.3	0.3	0.2	0.0	0.1	0.43	0.43	0.40	0.42	0.42	0.42	0.06	0.26	0.20	0.23	0.14	0.13
CHO (%)	43.2	29.8	0.0	10.0	100.0	42.9	14.0	26.2	27.4	38.6	34.2	36.5	72.3	86.2	73.4	78.4	66.0	71.9
CHON (%)	0.0	0.0	100.0	0.0	0.0	0.0	0.0	0.0	0.0	11.2	0.0	0.0	0.0	2.4	0.0	0.0	2.0	0.0
CHOS (%)	0.0	17.5	0.0	0.0	0.0	0.0	1.2	4.8	0.3	1.0	2.9	0.0	3.6	3.5	2.2	6.7	2.5	0.0
CHONS (%)	36.2	0.0	0.0	20.0	0.0	0.0	55.2	14.3	51.5	38.2	49.5	40.4	0.0	0.4	0.4	4.5	17.8	0.0
Others (%)	20.6	52.6	0.0	70.0	0.0	57.1	29.7	54.8	20.8	11.1	13.5	23.0	24.1	7.5	24.0	10.4	11.7	28.1
AF (%)	34.7	47.4	0.0	70.0	0.0	42.9	61.6	50.0	49.1	28.3	41.8	47.8	16.1	8.3	16.9	6.0	21.8	17.7
CAS (%)	3.2	0.0	0.0	0.0	0.0	0.0	1.2	19.0	2.7	20.8	18.5	0.9	0.0	28.0	10.5	21.6	1.5	0.9
Lignin/CRAM (%)	22.3	12.3	100.0	0.0	0.0	0.0	12.8	7.1	23.2	35.6	26.5	20.0	9.5	16.1	16.5	24.6	20.3	18.6
Protein (%)	12.7	14.0	0.0	0.0	0.0	14.3	7.6	9.5	11.1	11.4	10.0	14.8	32.1	20.1	19.1	39.6	22.3	21.2
Carbohydrate (%)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.0	0.0	1.0	0.0
Lipid (%)	11.2	21.1	0.0	10.0	100.0	28.6	2.3	4.8	2.7	3.4	1.6	5.2	39.4	26.8	31.8	9.7	32.0	36.8
UnsatHydroC (%)	53.8	57.9	0.0	90.0	0.0	57.1	79.1	64.3	63.9	32.3	46.4	62.6	24.1	10.6	25.8	11.2	27.9	27.3
Tannin (%)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.6	0.0	0.0	0.0	0.0

Note: wa-intensity-weighted average, DBE-Double Bond Equivalent, AImod-modified Aromatic Index, AF-Aromatic Formulas, CAS-Condensed Aromatic Structures, UnsatHydroC-Unsaturated HydroCarbons, CHO-only elements C, H and, O in the formulas, CHON-only elements C, H, O and, N in the formulas, CHOS-only elements C, H, O and, S in the formulas, CHONS-only elements C, H, O, N and, S in the formulas and others-the remaining formulas excluding the previous four groups.

Table S4. *p*-values of all the chemical, fluorescence and molecular parameters for each chemical fraction between the dam and river samples. *p*-values < 0.05 are in bold font.

	<i>p</i> -value Dam vs River		
	HPOA	TPIA	HPIN/B
SUVA ₂₅₄	0.5340	0.4781	0.3904
%C1	0.2781	0.2192	0.5161
%C2	0.8600	0.4751	0.6331
%C3	0.5030	0.2972	0.7646
FI	0.3549	0.0482	0.2557
HIX	0.5237	0.3533	0.2886
BIX	0.4564	0.4996	0.5502
C1/C2	0.3713	0.6546	0.4412
C1/C3	0.3432	0.2028	0.5559
C2/C3	0.6560	0.4021	0.7320
Number of formula	0.3153	0.1523	0.5582
m/z _{wa}	0.5176	0.2399	0.7231
C _{wa}	0.1581	0.2392	0.5950
H _{wa}	0.6781	0.6810	0.8099
O _{wa}	0.2006	0.2150	0.3634
N _{wa}	0.0762	0.2123	0.1496
S _{wa}	0.3240	0.1751	0.6280
H/C _{wa}	0.0296	0.4777	0.9650
O/C _{wa}	0.0684	0.2878	0.3583
N/C _{wa}	0.0852	0.1070	0.0476
S/C _{wa}	0.3361	0.1071	0.7952
DBE _{wa}	0.0154	0.1011	0.9440
DBE _{wa} /C _{wa}	0.0621	0.3909	0.9765
AI _{mod,wa}	0.0280	0.9021	0.9323
CHO (%)	0.4140	0.0361	0.4129
CHON (%)	0.3739	0.3739	0.9203
CHOS (%)	0.3739	0.6513	0.9769
CHONS (%)	0.7149	0.8696	0.2509
Others (%)	0.5335	0.1503	0.8354
AF (%)	0.7007	0.1128	0.8039
CAS (%)	0.3739	0.5359	0.6747
Lignin/CRAM (%)	0.1808	0.1169	0.0691
Protein (%)	0.5609	0.2062	0.6168

Carbohydrate (%)	/	/	0.8679
Lipid (%)	0.2756	0.9098	0.5144
UnsatHydroC (%)	0.7329	0.0949	0.8029
Tannin (%)	/	/	0.3739

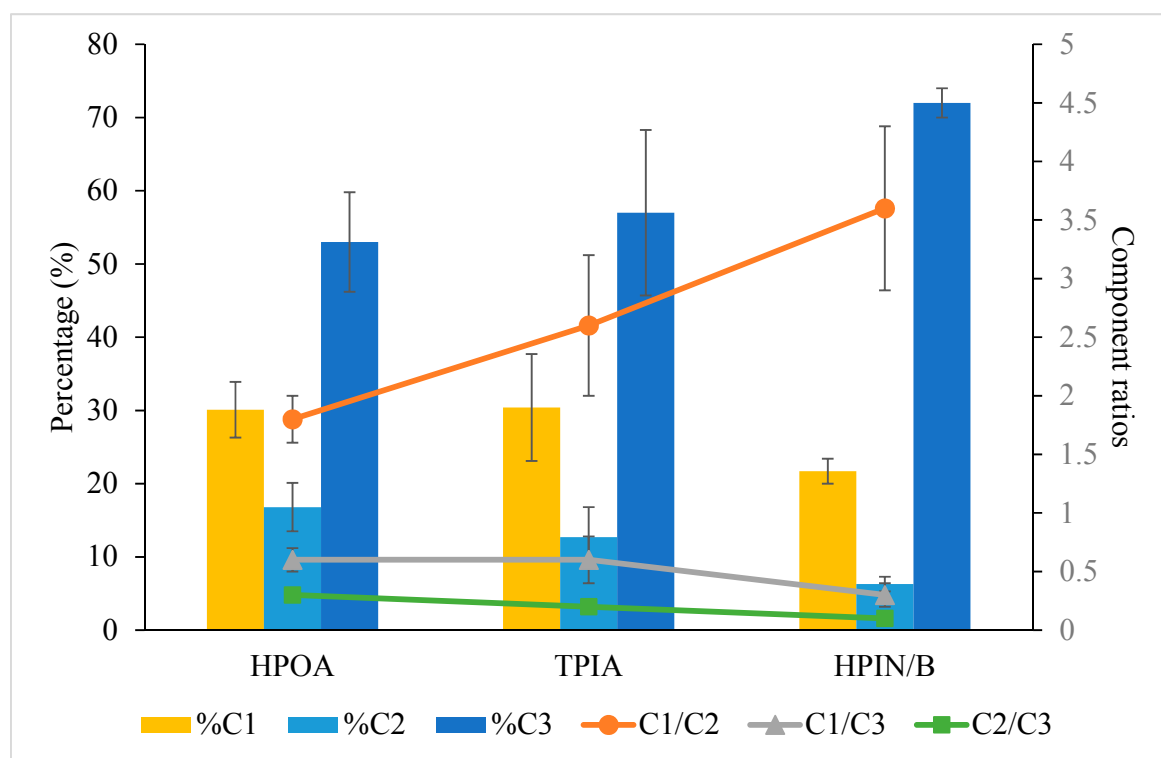
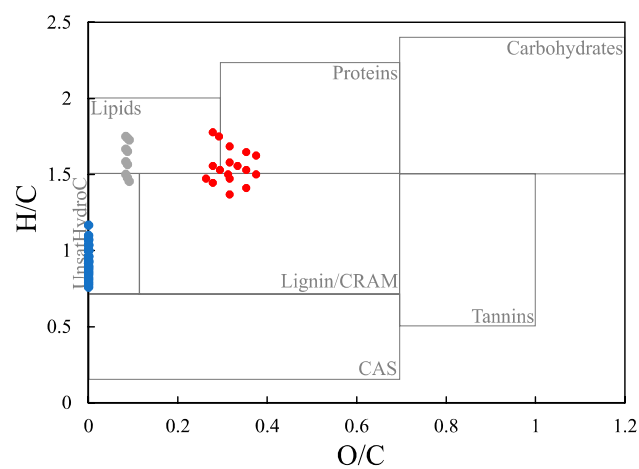
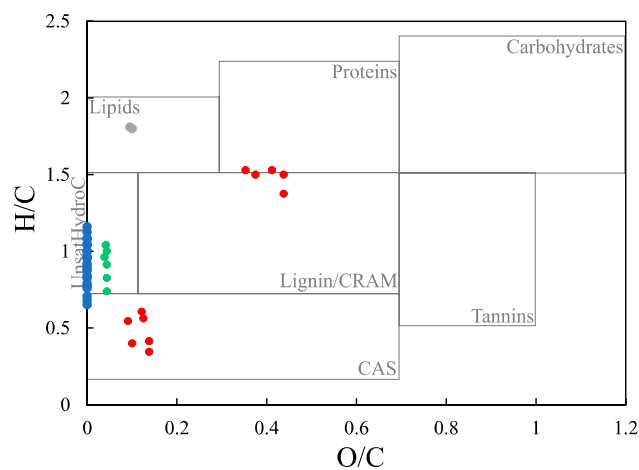


Figure S1. Average percentage of the component and ratios of these components for each fractions.

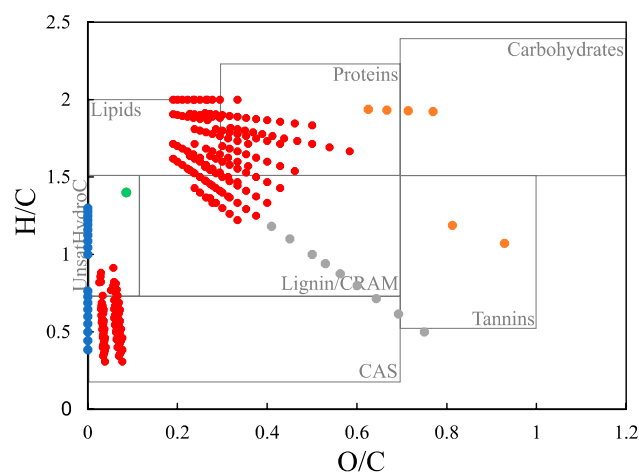
D2-HPOA



D2-TPIA

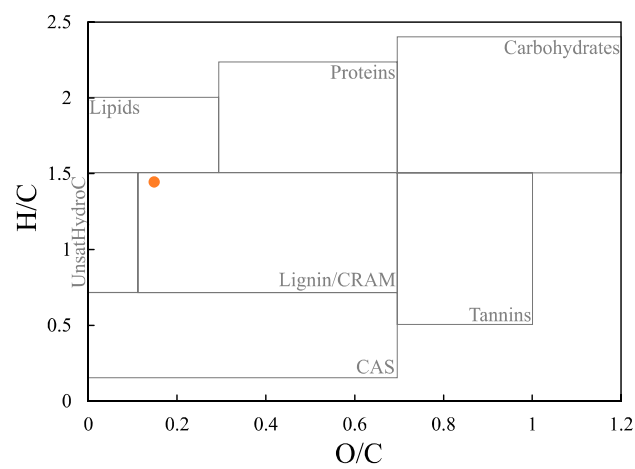


D2-HPIN/B

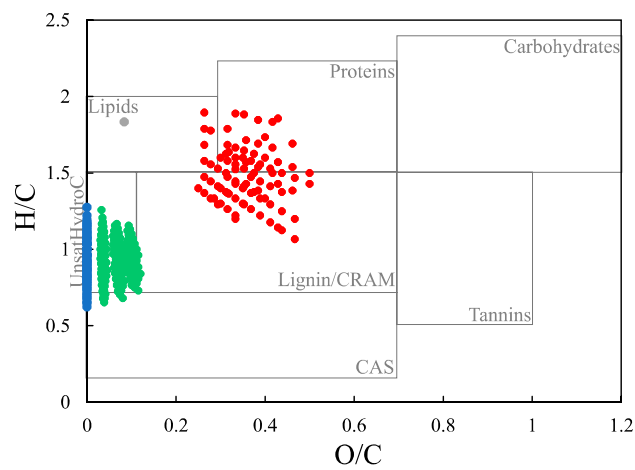


● CHO ● CHON ● CHOS ● CHONS ● Others

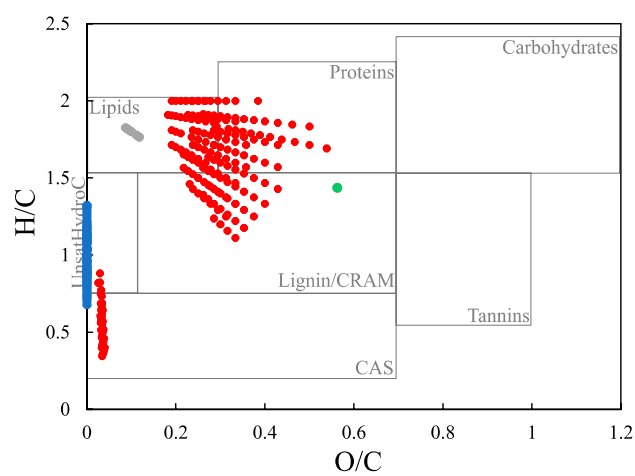
D3-HPOA



D3-TPIA

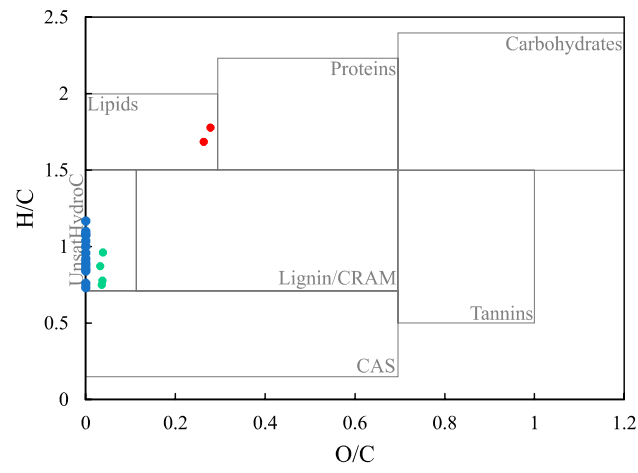


D3-HPIN/B

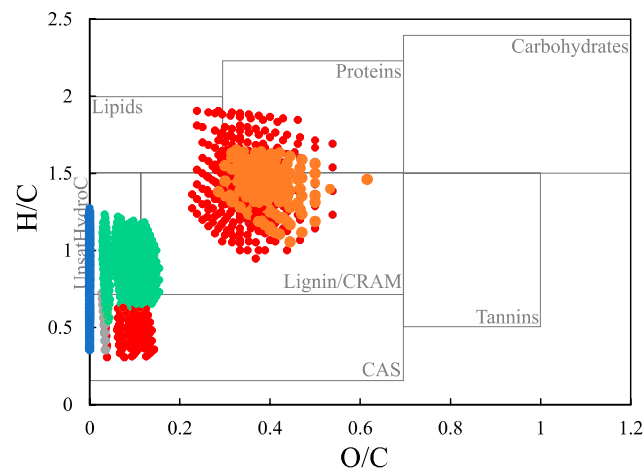


● CHO ● CHON ● CHOS ● CHONS ● Others

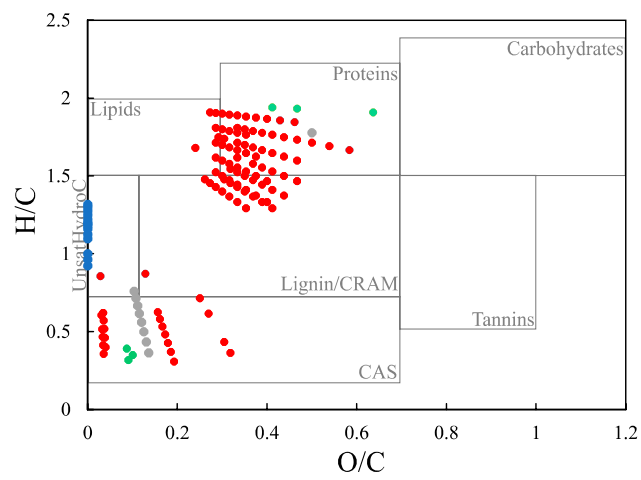
R1-HPOA



R1-TPIA

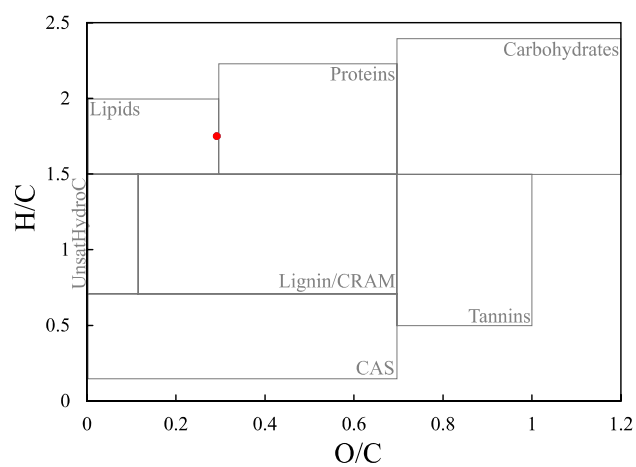


R1-HPIN/B

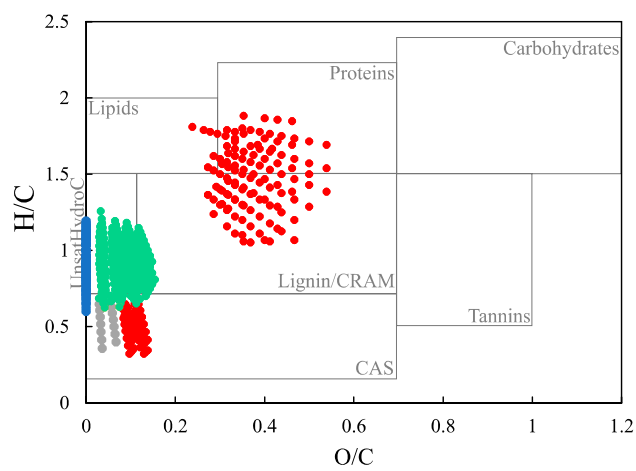


● CHO ● CHON ● CHOS ● CHONS ● Others

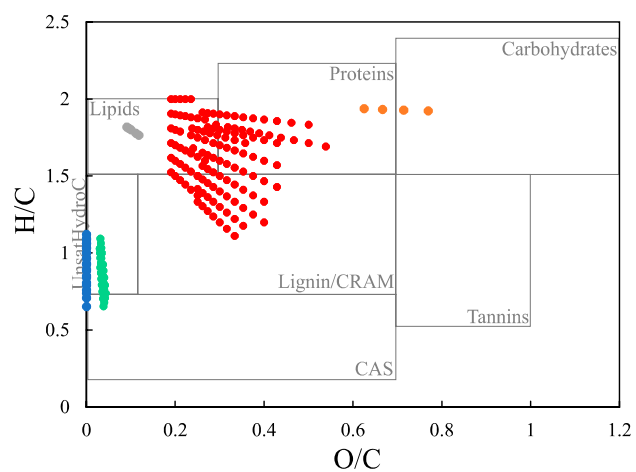
R2-HPOA



R2-TPIA



R2-HPIN/B



● CHO ● CHON ● CHOS ● CHONS ● Others

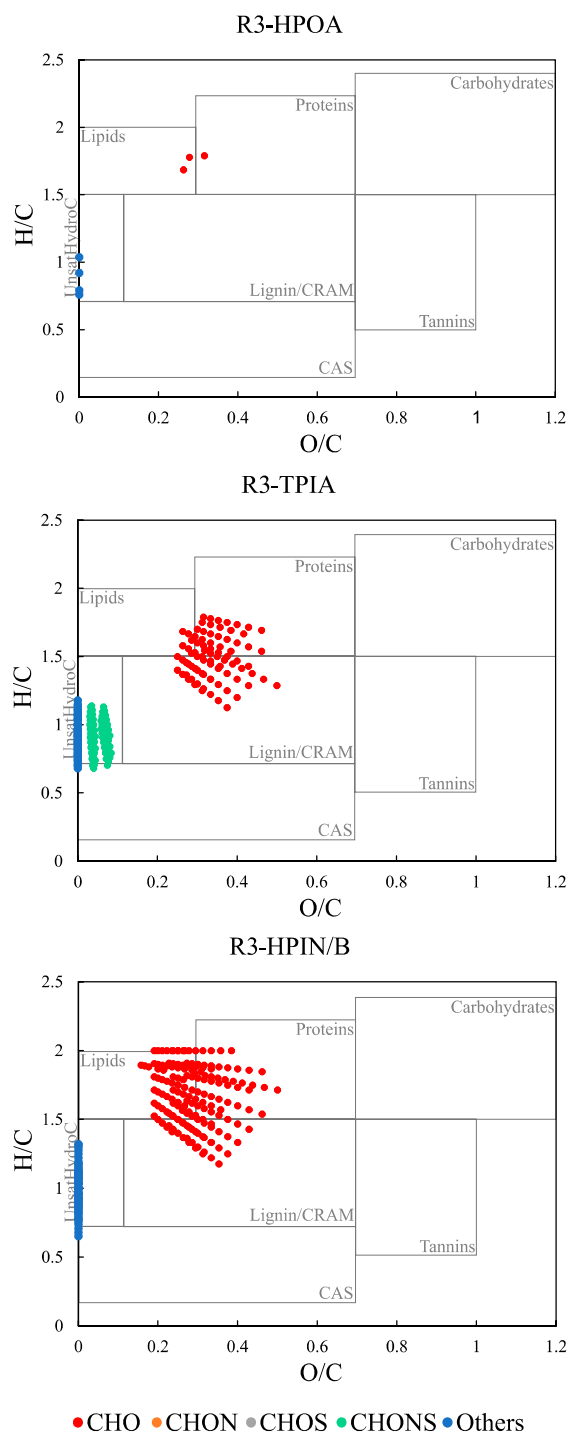


Figure S2. Van Krevelen diagram of the identified formulas group of the three chemical fraction for the D2, D3, R1, R2, and R3 samples assigned by the FT-ICR MS. Overlain rectangular are used as broad indicators of the compound classes defined in Table S2.