

Supporting information for:

Validation and evaluation of High-resolution Orbitrap mass spectrometry on molecular characterization of dissolved organic matter (DOM)

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Table S1. Instrumental parameter of ESI-Orbitrap MS

Group	Sequence	Neg ion spray voltage	sheath gas	aux gas	ion transfer tube temp	rf lens	AGC target
A	1	2600	10	2	300	60	500000
A	2	2700	10	2	300	60	500000
A	3	2800	10	2	300	60	500000
A	4	2900	10	2	300	60	500000
A	5	3000	10	2	300	60	500000
A	6	3100	10	2	300	60	500000
B	1	2600	5	2	300	60	500000
B	2	2600	7	2	300	60	500000
B	3	2600	9	2	300	60	500000
B	4	2600	11	2	300	60	500000
B	5	2600	13	2	300	60	500000
B	6	2600	15	2	300	60	500000
C	1	2600	10	1	300	60	500000
C	2	2600	10	2	300	60	500000
C	3	2600	10	4	300	60	500000
C	4	2600	10	6	300	60	500000
D	1	2600	10	2	200	60	500000
D	2	2600	10	2	225	60	500000
D	3	2600	10	2	250	60	500000
D	4	2600	10	2	275	60	500000
D	5	2600	10	2	300	60	500000
E	1	2600	10	2	300	20	500000
E	2	2600	10	2	300	40	500000
E	3	2600	10	2	300	60	500000
E	4	2600	10	2	300	80	500000
E	5	2600	10	2	300	100	500000
E	6	2600	10	2	300	120	500000
F	1	2600	10	2	300	60	300000
F	2	2600	10	2	300	60	350000
F	3	2600	10	2	300	60	400000
F	4	2600	10	2	300	60	450000
F	5	2600	10	2	300	60	500000

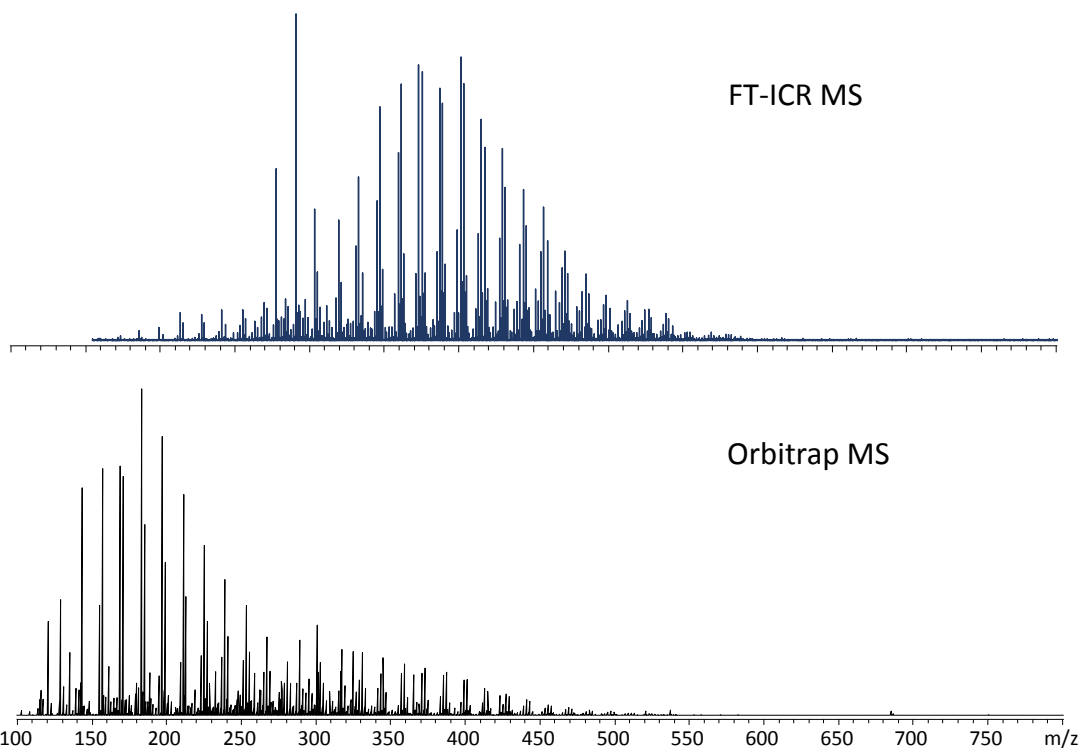


Figure S1. Mass distribution of condensate oil spectra of FT-ICR MS and Orbitrap MS

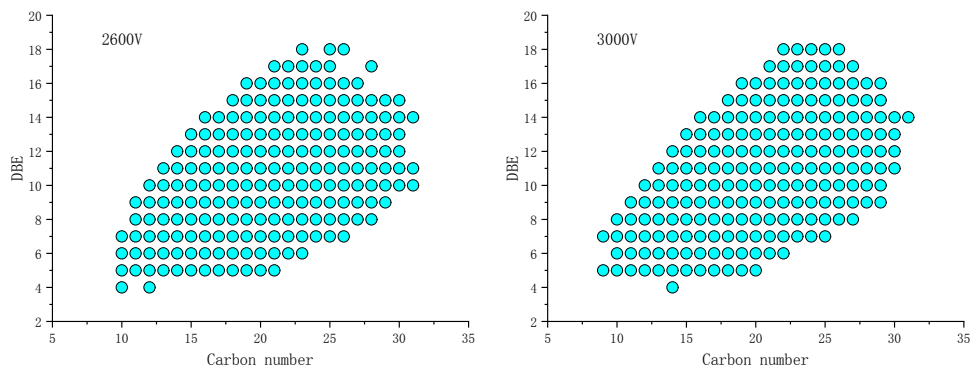


Figure S2. Distribution of O10 compounds under different ion spray voltage

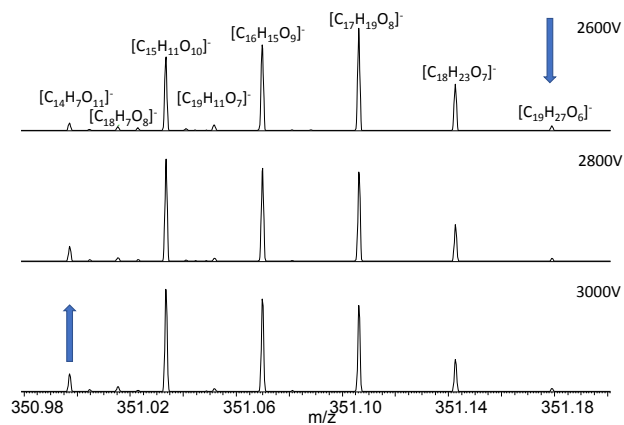


Figure S3. Expanded spectra under evaluated ion spray voltage at m/z 351

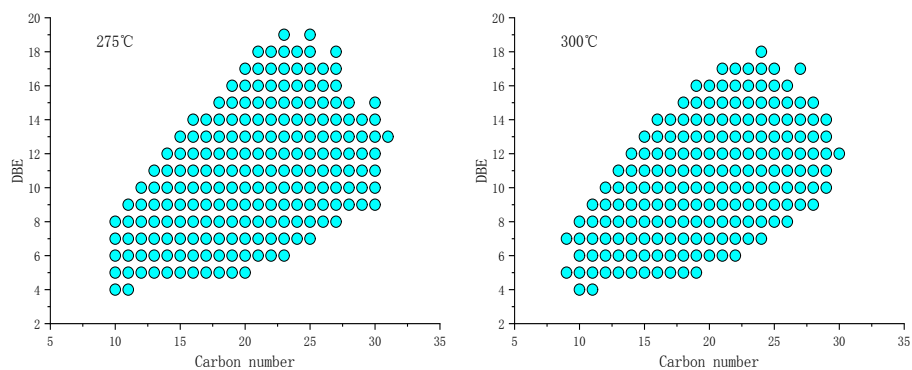


Figure S4. Distribution of O10 compounds under 275°C (left), 300°C (right) ion transfer tube temperature

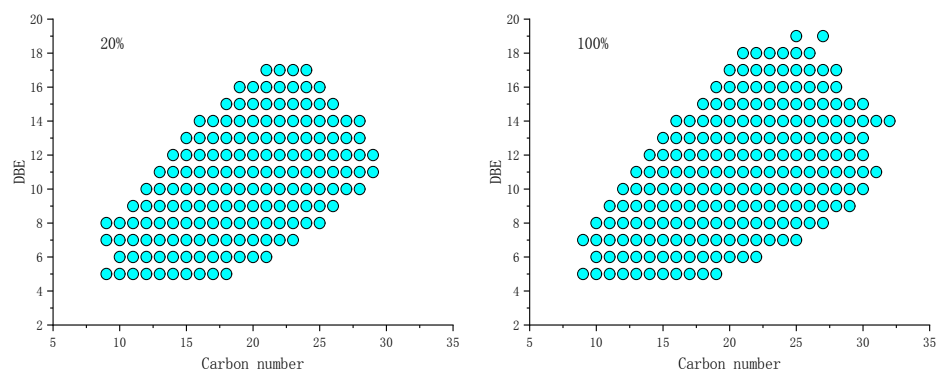


Figure S5. Distribution of O10 compounds under 20% (left), 100% (right) rf lens

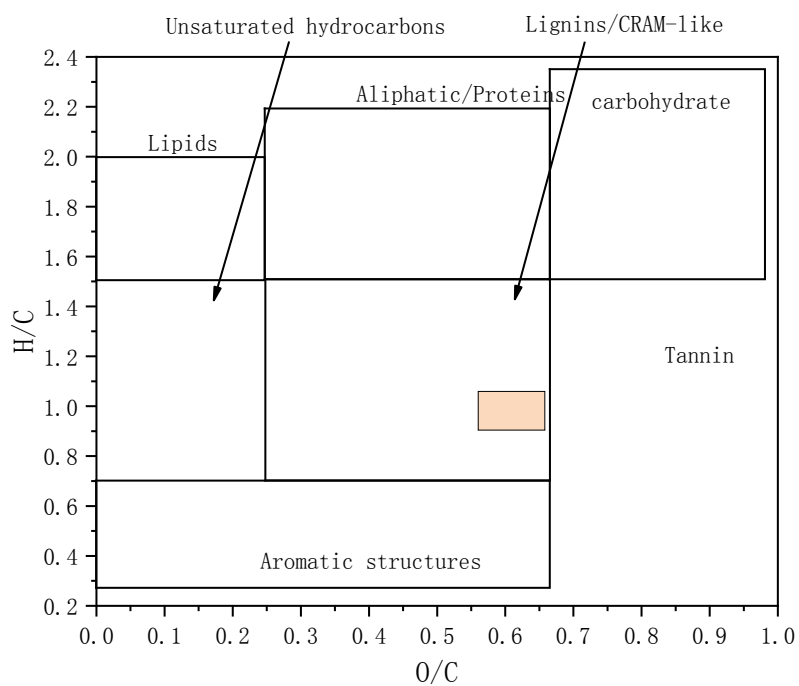


Figure S6. Typical category of compounds in different area of van Krevelen diagram