

Supplementary information for: Assessment of sample freezing as a preservation technique for analysing the molecular composition of dissolved organic matter in aquatic systems


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Supplementary figure 1&2: Error analysis for formula assignments in both cases

Supplementary table 1: sample processing information and mass spectrometry metrics

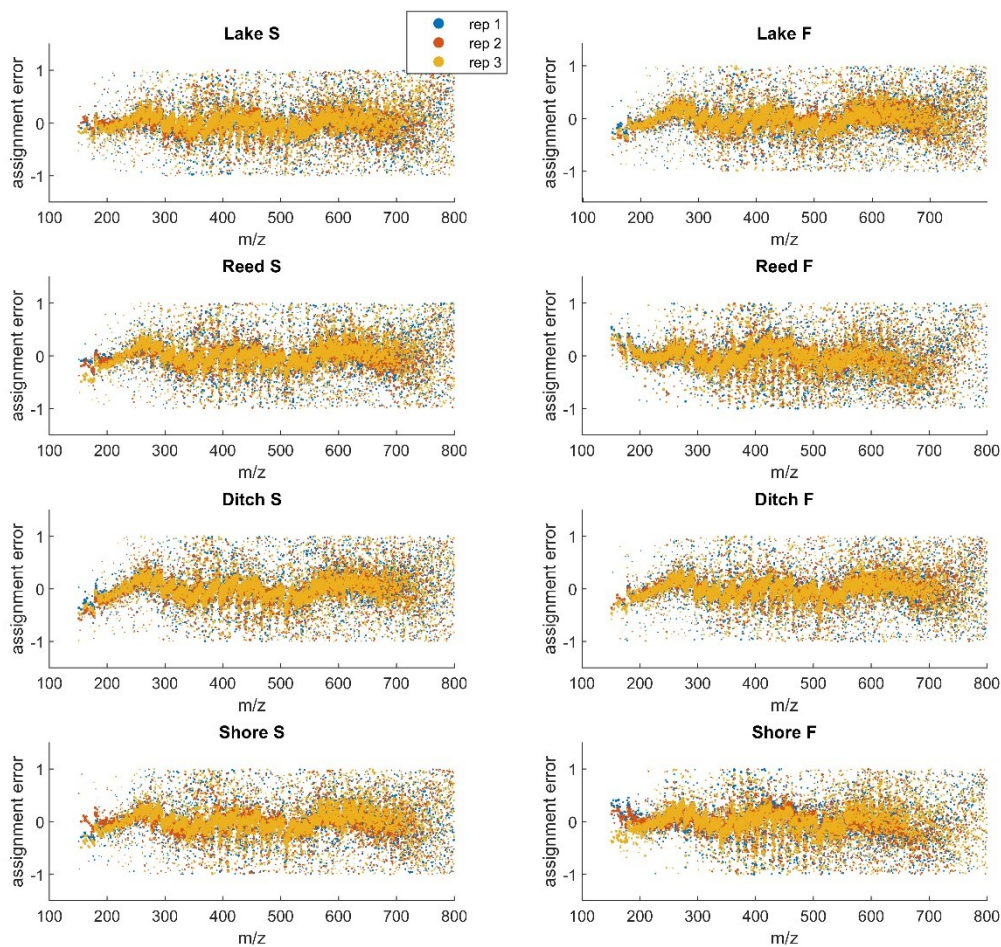


Figure S11: Error analysis for the Swedish systems. Assignment error in ppm plotted vs mass to charge ratio, with each of three replicates overlaid. Point size is shown as logarithm of intensity to emphasise the most intense peaks. See methods for further information on molecular assignment errors.

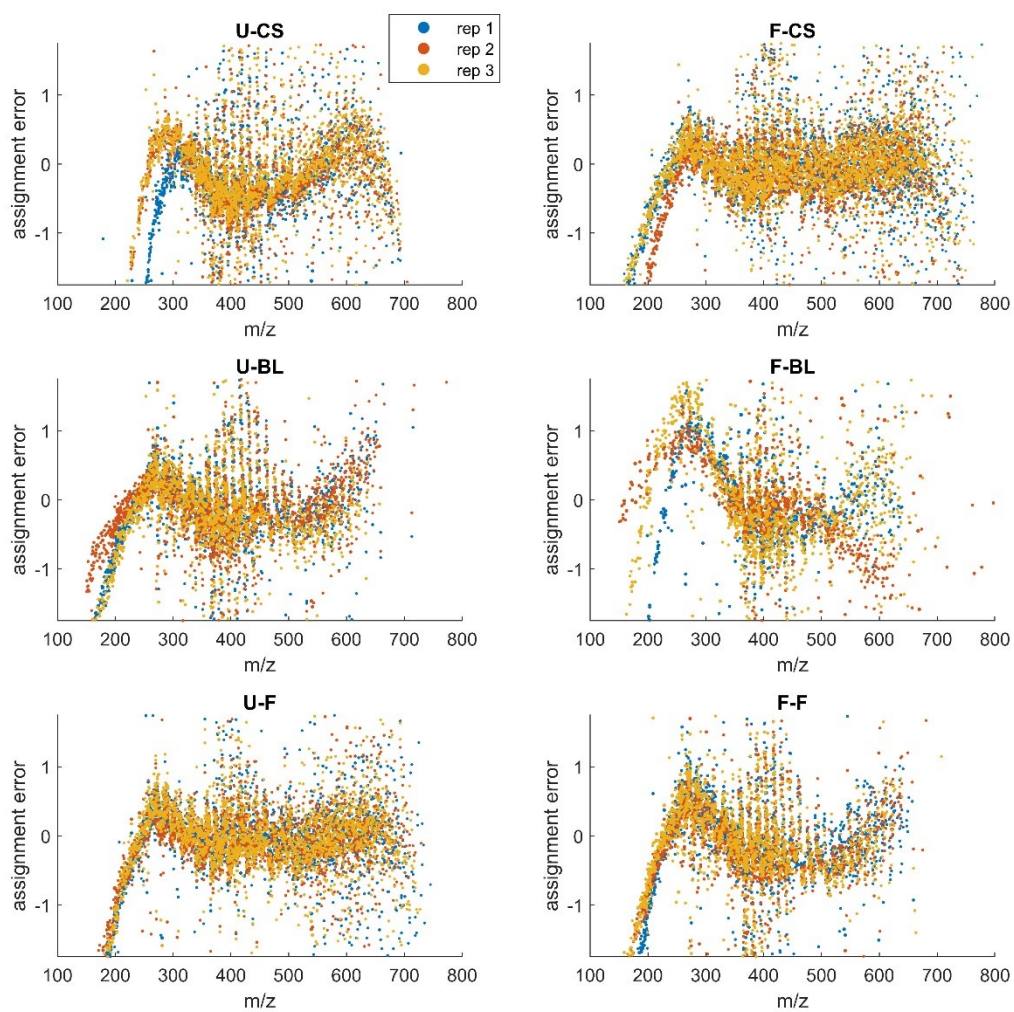


Figure S12: Error analysis for the UK systems. Assignment error in ppm plotted vs mass to charge ratio, with each of three replicates overlaid. Point size is shown as logarithm of intensity to emphasise the most intense peaks. See methods for further information on molecular assignment errors.

Table S1: Sample processing information (carbon injected and Volume of sample extracted) alongside high-resolution mass spectrometry peak metrics showing number of peaks (Peaks) and the intensity weighted average of oxygen to carbon (O/C_{wa}), hydrogen to carbon (H/C_{wa}) and mass to charge (m/z_{wa}) for each sample.

Sample	Country	Frozen	Sample code	Peaks	Total current	O/C_{wa}	H/C_{wa}	m/z_{wa}	millilitres Extracted
Marine	SW	N	U-M-1	2074	1.64E+06	0.5	1.25	361.91	54
Marine	SW	N	U-M-2	2018	1.85E+06	0.5	1.26	362.52	54
Marine	SW	N	U-M-3	2154	1.67E+06	0.48	1.28	364.33	54
Marine	SW	Y	F-M-1	2142	2.61E+06	0.5	1.25	362.17	53
Marine	SW	Y	F-M-2	2527	2.41E+06	0.51	1.26	359.78	53
Marine	SW	Y	F-M-3	2292	2.66E+06	0.5	1.25	361.62	56
Swedish Lake	SW	N	U-SL-1	3804	3.25E+06	0.52	1.12	404.35	54
Swedish Lake	SW	N	U-SL-2	3466	3.10E+06	0.52	1.12	397.62	54
Swedish Lake	SW	N	U-SL-3	3442	2.91E+06	0.51	1.13	401.71	54
Swedish Lake	SW	Y	F-SL-1	3576	3.01E+06	0.51	1.12	402.6	53
Swedish Lake	SW	Y	F-SL-2	3455	3.15E+06	0.52	1.12	402.65	55
Swedish Lake	SW	Y	F-SL-3	3328	3.00E+06	0.52	1.12	397.15	53
Reed Bed	SW	N	U-RB-1	3836	3.62E+06	0.52	1.13	403.75	54
Reed Bed	SW	N	U-RB-2	3813	3.63E+06	0.51	1.13	404.14	54
Reed Bed	SW	N	U-RB-3	4043	3.62E+06	0.51	1.13	403.47	54
Reed Bed	SW	Y	F-RB-1	3532	3.28E+06	0.51	1.14	402.37	52
Reed Bed	SW	Y	F-RB-2	3826	3.20E+06	0.51	1.13	403.57	53
Reed Bed	SW	Y	F-RB-3	3904	3.45E+06	0.52	1.13	403.46	52
Drainage Ditch	SW	N	U-DD-1	3561	3.05E+06	0.5	1.12	413.8	54
Drainage Ditch	SW	N	U-DD-2	3680	3.22E+06	0.51	1.11	413.5	54
Drainage Ditch	SW	N	U-DD-3	3682	3.05E+06	0.5	1.13	413.28	54
Drainage Ditch	SW	Y	F-DD-1	3811	3.18E+06	0.52	1.09	417.21	53
Drainage Ditch	SW	Y	F-DD-2	3851	3.21E+06	0.5	1.13	409.63	52
Drainage Ditch	SW	Y	F-DD-3	3808	3.22E+06	0.51	1.11	413.43	52
Chalk Stream	UK	N	U-CS-1	1699	2.15E+10	0.49	1.26	415.93	30
Chalk Stream	UK	N	U-CS-2	1717	2.24E+10	0.51	1.22	416.89	30
Chalk Stream	UK	N	U-CS-3	1689	2.25E+10	0.51	1.2	419.1	30
Chalk Stream	UK	Y	F-CS-1	888	1.49E+10	0.5	1.28	396.79	19
Chalk Stream	UK	Y	F-CS-2	863	1.33E+10	0.51	1.2	399.34	26
Chalk Stream	UK	Y	F-CS-3	1073	2.38E+10	0.48	1.39	379.83	18
British Lake	UK	N	U-BL-1	2592	2.84E+10	0.55	1.05	425.14	30
British Lake	UK	N	U-BL-2	2142	2.63E+10	0.55	1.05	425.92	30
British Lake	UK	N	U-BL-3	2564	3.29E+10	0.55	1.04	423.84	30
British Lake	UK	Y	F-BL-1	2196	1.96E+10	0.55	1.1	410.64	23
British Lake	UK	Y	F-BL-2	1974	2.16E+10	0.53	1.13	403.87	23
British Lake	UK	Y	F-BL-3	2134	2.19E+10	0.54	1.11	409.67	26
Fen	UK	N	U-F-1	1720	1.51E+10	0.49	1.25	352.96	30
Fen	UK	N	U-F-2	1836	1.61E+10	0.49	1.25	354.99	30
Fen	UK	N	U-F-3	1415	1.61E+10	0.49	1.25	351.64	30
Fen	UK	Y	F-F-1	1671	2.02E+10	0.49	1.28	357.92	22
Fen	UK	Y	F-F-2	1577	1.86E+10	0.5	1.24	353.56	22
Fen	UK	Y	F-F-3	1489	2.09E+10	0.49	1.31	344.8	12

