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Environmental Chemistry

Supplementary Material

A critical assessment of physicochemical indices used to characterise natural dissolved organic carbon (DOC), their inter- relationships, and the effects of pH

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Table S1. Characterisation of grab samples from Lake Ontario (LO), Preston Flats (PF), Ancient Woods Pond (AP) and Ancient Woods Swamp (AS)

Sample	pH	[DOC]	Na	Ca	K	Mg	Al
LO	6.83	1.52	28.10	80.46	0.36	11.73	0.12
PF	7.35	4.15	106.76	147.33	2.27	22.57	0.08
AP	7.07	22.18	1.31	57.51	0.82	11.12	0.10
AS	6.89	37.96	10.98	171.17	0.75	37.83	0.14

Ions are expressed as milligrams per litre and DOC as milligrams of carbon per litre. Pb, Cu and Ni were below the detection limit of 0.02 (Pb), 0.01 (Cu and Ni)

Table S2. Characterisation of experimental solutions from Lake Ontario (LO), Luther Marsh (LM), Preston Flats (PF), Ancient Woods Pond (AP) and Ancient Woods Swamp (AS).

Source	Na	Ca	K	Mg	Al	[DOC] pH 7	[DOC] pH 4	pH ~7	pH ~4
LO	25.76	18.67	0.38	12.24	0.100	10.20 ± 0.18	10.50 ± 0.16	6.76 ± 0.08	3.94 ± 0.07
PF	24.05	14.93	0.33	7.92	0.09	9.17 ± 0.06	10.66 ± 0.17	6.73 ± 0.03	3.95 ± 0.04
LM	0.13	2.48	ND	0.29	0.08	10.06 ± 0.12	10.03 ± 0.13	6.77 ± 0.27	4.02 ± 0.05
AP	0.18	0.40	0.10	0.22	0.08	9.42 ± 0.005	9.19 ± 0.04	7.01 ± 0.16	3.98 ± 0.01
AS	0.91	0.74	0.17	0.49	0.085	8.82 ± 0.01	8.62 ± 0.09	6.88 ± 0.06	3.99 ± 0.03

DOC and pH values are mean ± range, $n = 2$. Ions are expressed as milligrams per litre and DOC as milligrams of carbon per litre. ND indicates not detectable due to the detection limit of 0.01 for K. Pb, Cu and Ni were below the detection limit of 0.02 (Pb), 0.01 (Cu and Ni)

Table S3. Size fractionation of DOCs from Lake Ontario, Luther Marsh, Preston Flats, Ancient Woods Pond, and Ancient Woods Swamp at neutral pH, achieved by by ultra-filtration using 0.45-μm, 100-kDa, 10-kDa and 3-kDa filters.

	0.45 μm	100 kDa	10 kDa	3 kDa
Lake Ontario				
[DOC] (mg C L^{-1})	9.30	8.44	8.22	7.01
Absorbance at 340 nm	0.0488	0.029	0.027	0.0128
Molecular weight index	9	13.95	13.48	35.55
SAC_{340}	12.07	7.9	7.57	4.21
Relative percentage of fluorophore (PARAFAC Components)	22.50% Pro 46.90% FA 30.60% HA	18.26% Pro 41.45% FA 40.29% HA	19.47% Pro 42.09% FA 38.44% HA	22.88% Pro 58.37% FA 18.75% HA
Fluorescence Index	1.25	1.22	1.23	1.35
Preston Flats				
[DOC] (mg C L^{-1})	9.24	7.98	7.01	8.12
Absorbance at 340 nm	0.0721	0.0417	0.0328	0.0186
Molecular weight index	6.89	9.69	11.31	9.3
SAC_{340}	17.98	12.02	10.78	6.24
Relative percentage fluorophore (PARAFAC Components)	19.42% Pro 40.72% FA 39.86% HA	15.28% Pro 34.47% FA 50.25% HA	15.14% Pro 33.20% FA 51.66% HA	18.56% Pro 53.64% FA 27.79% HA
Fluorescence Index	1.22	1.18	1.19	1.23
Luther Marsh				
[DOC] (mg C L^{-1})	9.86	8.49	6.74	7.64
Absorbance at 340nm	0.112	0.075	0.0609	0.0103
Molecular weight index	5.16	6.14	6.46	18.74
SAC_{340}	26.16	20.33	20.79	3.11
Relative percentage fluorophore	13.44% Pro	13.21% Pro	12.39% Pro	16.18% Pro

	0.45 μm	100 kDa	10 kDa	3 kDa
(PARAFAC Components)				
	66.55% FA	66.69% FA	67.79% FA	73.23% FA
	20.01% HA	20.10% HA	19.81% HA	10.59% HA
Fluorescence Index	1.18	1.2	1.23	1.4
Ancient Woods Pond				
[DOC] (mg C L^{-1})	9.24	8.65	7.84	5.73
Absorbance at 340nm	0.0982	0.0684	0.0582	0.0135
Molecular weight index	6	7.35	7.62	25.09
SAC_{340}	24.48	18.21	17.09	5.42
Relative percentage fluorophore (	21.57% Pro	19.24% Pro	18.07% Pro	18.48% Pro
PARAFAC Components)	30.64% FA	26.68% FA	26.28% FA	56.08% FA
	47.80% HA	54.08% HA	55.65% HA	25.44% HA
Fluorescence Index	1.2	1.17	1.17	1.3
Ancient Woods Swamp				
[DOC] (mg C L^{-1})	8.68	7.54	6.98	5.40
Absorbance at 340nm	0.0765	0.0505	0.0466	0.0147
Molecular weight index	5.91	7.41	7.32	14.7
SAC_{340}	20.34	15.42	15.37	6.25
Relative percentage fluorophore	20.07% Pro	16.85% Pro	17.04% Pro	18.86% Pro
(PARAFAC Components)	38.56% FA	33.53% FA	32.45% FA	60.20% FA
	41.38% HA	49.62% HA	50.51% HA	20.94% HA
Fluorescence Index	1.2	1.18	1.19	1.32

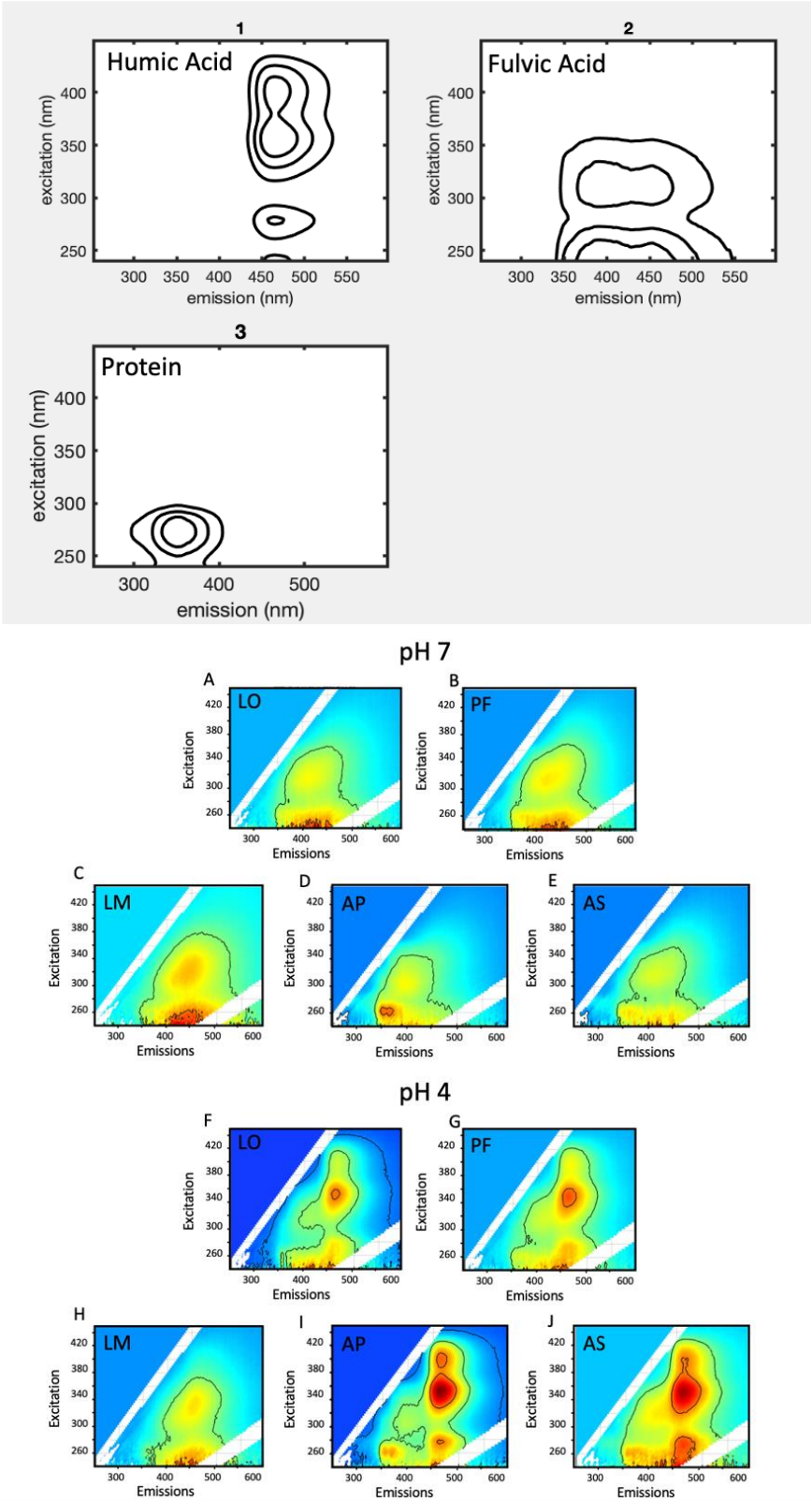

Figure S1. (top) Preselected parallel factor analysis (PARAFAC) excitation and emission fluorophore components and (bottom) parallel factor analysis (PARAFAC) fluorescence excitation-emission matrices for natural DOCs at pH 7 for (A) Lake Ontario, (B) Preston Flats, (C) Luther Marsh, (D) Ancient Woods Pond, and (E) Ancient Woods Swamp, and pH 4 for (F) Lake Ontario, (G) Luther Marsh, (H) Preston Flats, (I) Ancient Pond, and (J) Ancient Swamp.