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Environmental Chemistry

Supplementary Material

Nickel and copper complexation by natural dissolved organic matter – titration of two contrasting lake waters and comparison of measured and modelled free metal ion concentrations

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Table S1. Excitation and emission maxima for PARAFAC components C_1, C_2, C_3 and C_4 presented in a previous study (Mueller *et al.* 2012a), as determined using the protocol outlined by Stedmon and Bro (2008), including spectral pre-processing, outlier analysis and model validation.

	PARAFAC Components			
	C_1	C_2	C_3	C_4
Emission maximum 1 (nm)	482	412	440	340
Emission maximum 2 (nm)				526
Excitation maximum 1 (nm)	250	240	250	240
Excitation maximum 2 (nm)	340	310		285

Table S2. Root Mean Squared Log Error (RMSLE) values for each metal–lake combination and each WHAM modelling scenario.

	65% fulvic	65% humic	C_1/C_T opt% aFA
Ni Lake Geneva	0.27	0.26	0.44
Ni Lake Opasatica	0.39	0.38	1.77
Cu Lake Geneva	0.93	1.04	0.86
Cu Lake Opasatica	0.49	0.57	0.30

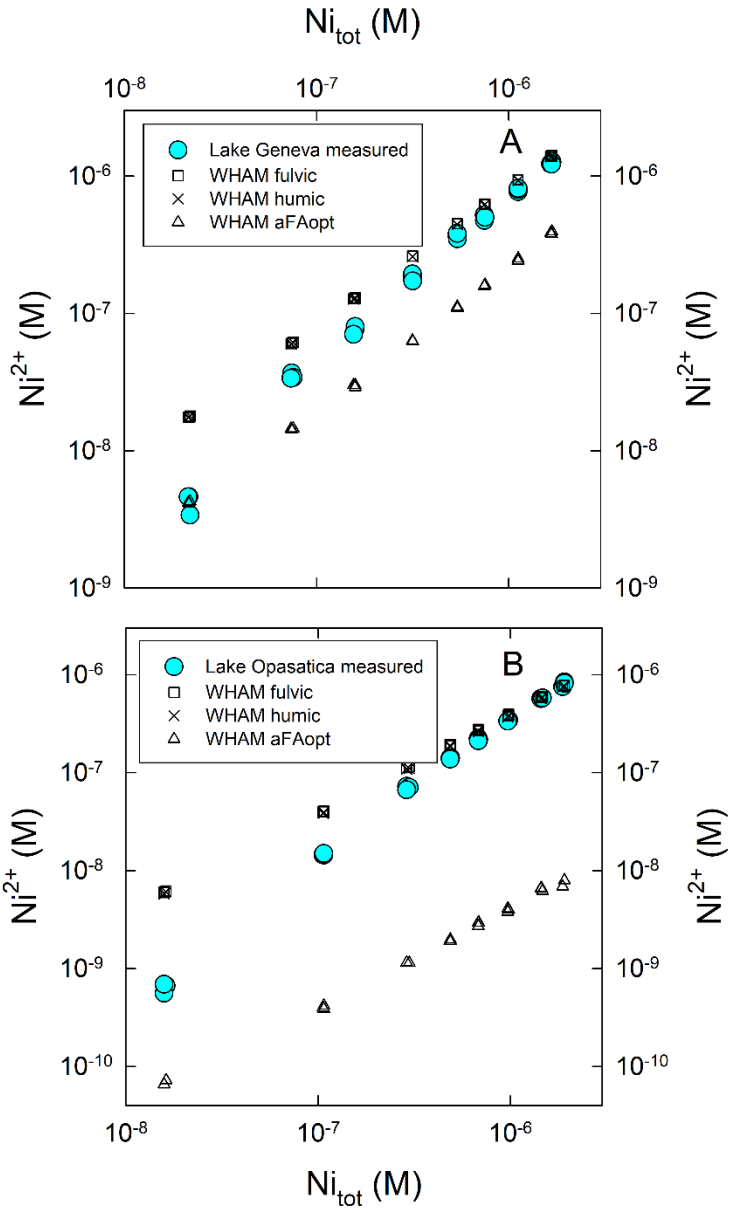

Fig. S1. Triplicate nickel titration curves for Lake Geneva (A) and Lake Opasatica (B). Measured values are shown in colour; values calculated with WHAM (ver. 7.05) are shown in black. Three scenarios were compared for WHAM calculations: using fulvic acid (open squares) as the default natural organic matter (as presented in Figure 2); using humic acid (X) as the default natural organic matter; or using optimised active fulvic acid (open triangles) as suggested by Mueller *et al.* (2012b). Some replicate data points are superimposed and therefore not completely visible.

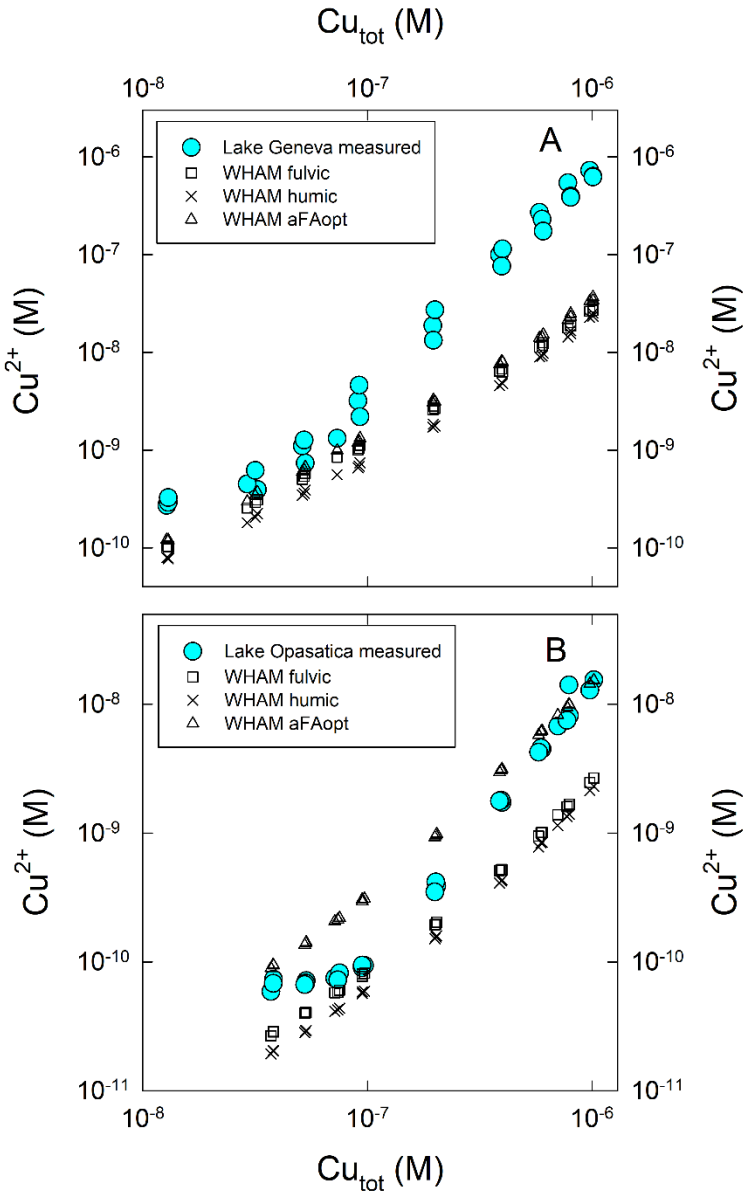

Fig. S2. Triplicate copper titration curves for Lake Geneva (A) and Lake Opasatica (B). Measured values are shown in colour; values calculated with WHAM (ver. 7.05) are shown in black. Three scenarios were compared for WHAM calculations: using fulvic acid (open squares) as the default natural organic matter (as presented in Fig. 2); using humic acid (X) as the default natural organic matter; or using optimized active fulvic acid (open triangles) as suggested by Mueller *et al.* (2012b). Some replicate data points are superimposed and therefore not completely visible.

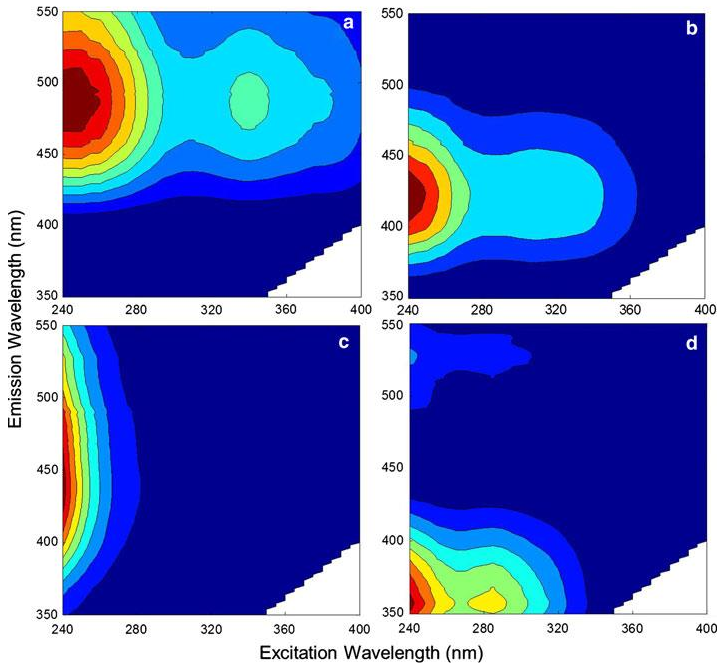

Fig. S3. Parallel factor analysis (PARAFAC) components 1 (a), 2 (b), 3 (c) and 4 (d) identified from the excitation–emission matrix (EEM) fluorescence spectra of DOM from the Sudbury and Rouyn-Noranda lakes studied by Mueller *et al.* (2012a). Figure reproduced with permission from Mueller *et al.* (2012a).

References

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