Supporting Information

Quantitative Determination of Polyphosphate in Sediment using Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) Spectroscopy and Partial Least Squares

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Table 1S. Summary of PLS regression results performed on sediment and sediment extracts

Concentration range (mg/g)	Spectra data detail	Range of selected Factors	Range of R-squared	Range of RMSEP*
0-5	River sediment, 1200-1400 Cm^{-1}, 1st derivative, Reduced Average	7-1	0.986-0.150	0.22-1.7 (6)**
0-2	River sediment, 1200-1400 Cm^{-1}, 1st derivative, Reduced Average	7-1	0.898-0.220	0.21-0.2 (2.5)
	outliers removed	6-2	0.961-0.410	0.136-0.5 (1.4)
0-1	River sediment, 1200-1400 Cm^{-1} Max-Normalized, baseline corrected	7-1	0.999-0.984	001-0.04
0-1	River sediment, 1200-1400 Cm^{-1}, 1st derivative, outliers removed	3-1	0.95-0.695	0.014-0.03 (0.2)
0-0.5	River sediment, 1200-1400 Cm^{-1}, 1st derivative, Reduced Average, outliers removed	4-1	0.92-0.61	0.048-0.1 (0.5)
0-100	Wetland sediment, Reduced Average, all range ", outliers removed	4-2	0.965-0.86	13.8 -27.9 (250)
0-50	Wetland sediment extract, no outliers removed, 1200-1400 Cm^{-1}range	4-1	0.9890.270	1.85 (55)
0-50	Wetland sediment extract 1 st derivative, Outliers removed, 1200-1400 Cm^{-1}range	6-1	0.985-0.941	8.76-18.4 (250)
0-20	1st derivative, 1200-1400 Cm^{-1}range	5-1	0.99-0.731	0.37-4.32 (26)
0-10	1st derivative, 1200-1400 Cm^{-1}range	7-1	0.99-0.942	7.7-18.4 (250)

* Root Mean Square Error of Prediction; **out of full scale predicted versus Reference plots