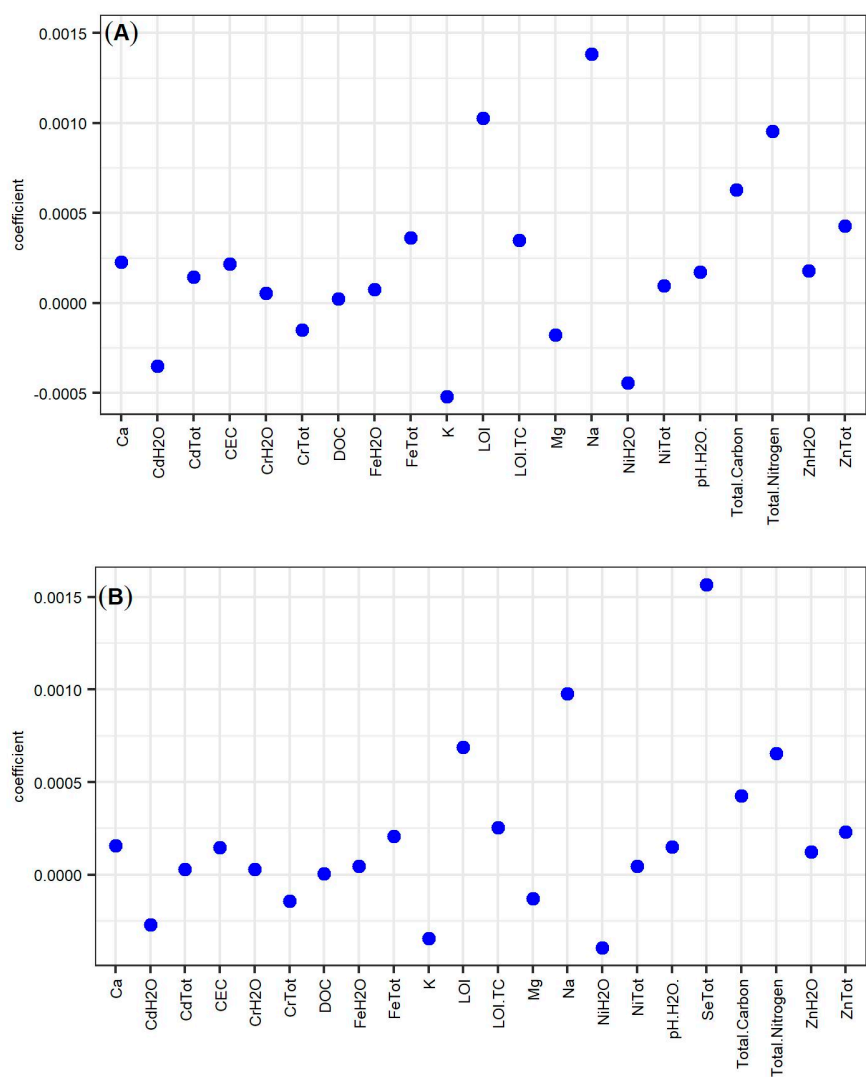Supplementary table S1. Communalities (correlations between original variables and PCs) from principal component analysis

	PC1	PC2	PC3
pH (H_2O)	−0.68	−0.68	−0.05
DOC	0.05	0.76	0.39
LOI	−0.73	0.47	0.38
Tot. C	−0.79	0.17	0.52
LOI/TC	0.51	0.26	−0.45
Tot. N	−0.68	0.52	0.41
Na	−0.56	−0.22	0.09
K	−0.63	−0.27	−0.18
Ca	−0.86	−0.41	0.14
Mg	−0.43	−0.39	−0.33
CEC	−0.87	−0.37	0.18
Cr_{H2O}	0.02	0.62	−0.61
Fe_{H2O}	0.54	0.69	0.06
Ni_{H2O}	−0.19	0.71	−0.46
Cd_{H2O}	0.43	0.65	0.26
Zn_{H2O}	0.39	0.71	0.28
Se_{H2O}	−0.73	0.31	0.17
Cr_{Tot}	−0.55	0.38	−0.64
Fe_{Tot}	−0.72	0.27	−0.49
Ni_{Tot}	−0.71	0.33	−0.53
Zn_{Tot}	−0.65	0.51	−0.14
Cd_{Tot}	−0.50	0.46	0.24
Se_{Tot}	−0.74	0.42	0.06

Supplementary figure S1. Coefficients of calibrated PLS models A and B from figure 6 in the main text.