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Field and laboratory evaluation of a high time resolution x-ray fluorescence instrument for determining the elemental composition of ambient aerosols

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S1. Map of the United Kingdom with sampling locations

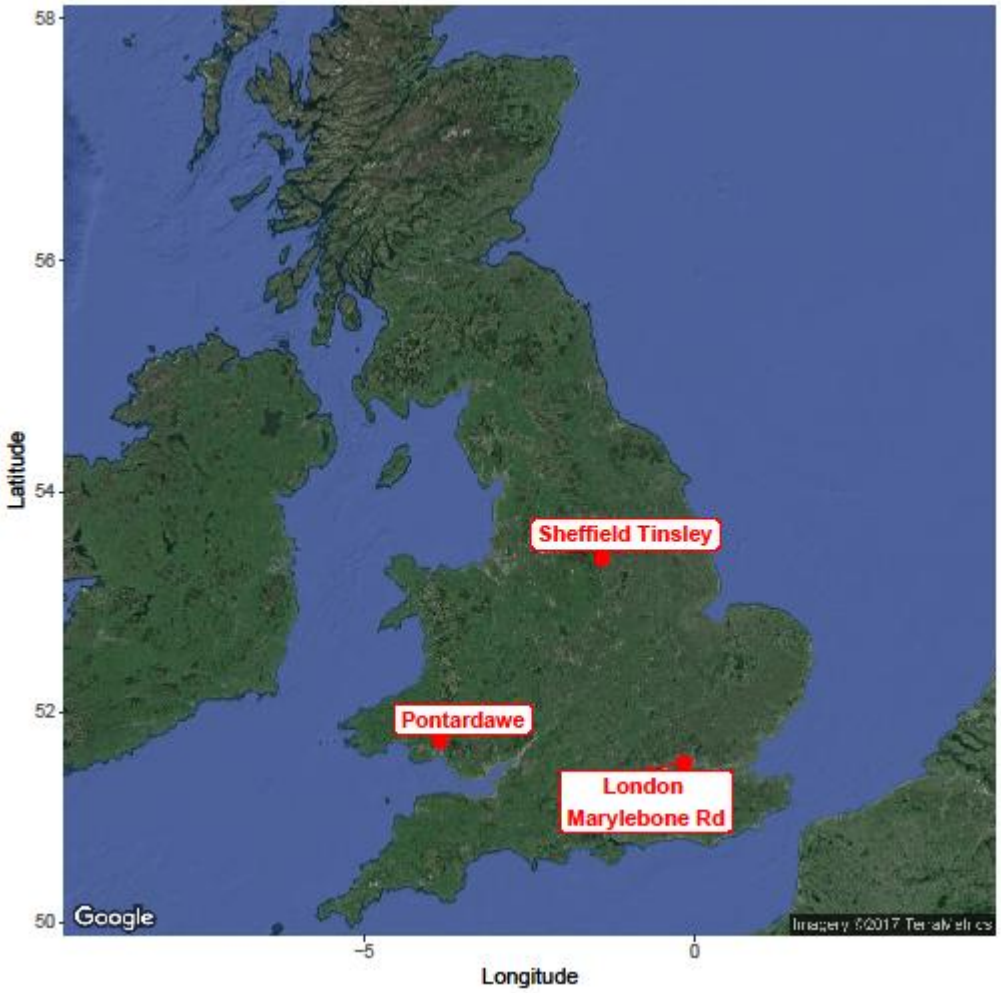

Figure S1: Sampling locations in the field experiments

S2. Deming Regression graphs of full range of tested aerosol concentrations measured with XACT and calculated from TEOM measurements

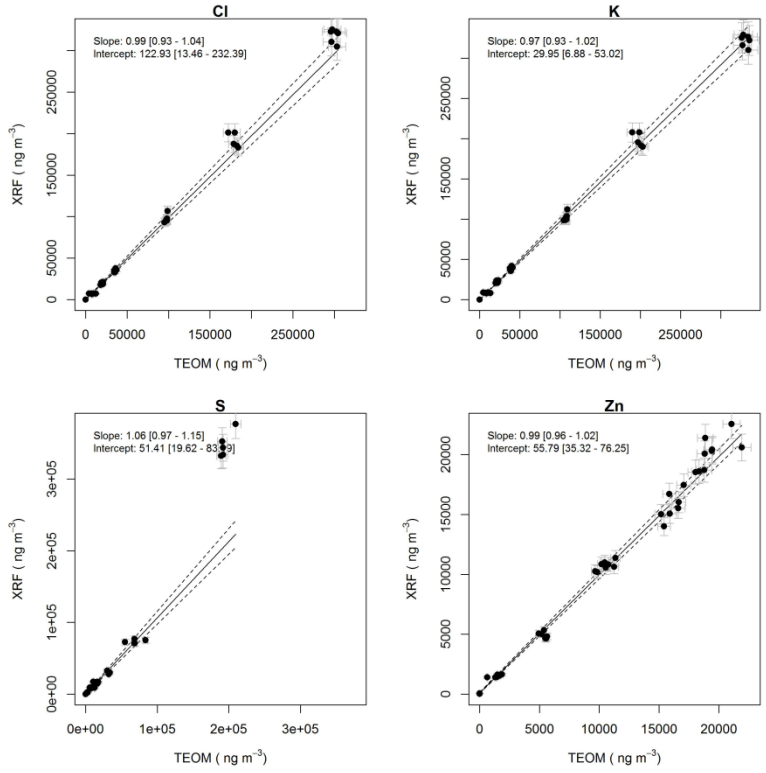

Figure S2: Deming regression of full range of tested aerosols; Cl (top left), K (top right), S (bottom left) and Zn (bottom right) mass concentrations measured with the XACT and calculated from TEOM mass measurements

S3. Deming regression graphs for all elements compared by XACT and ICP-MS

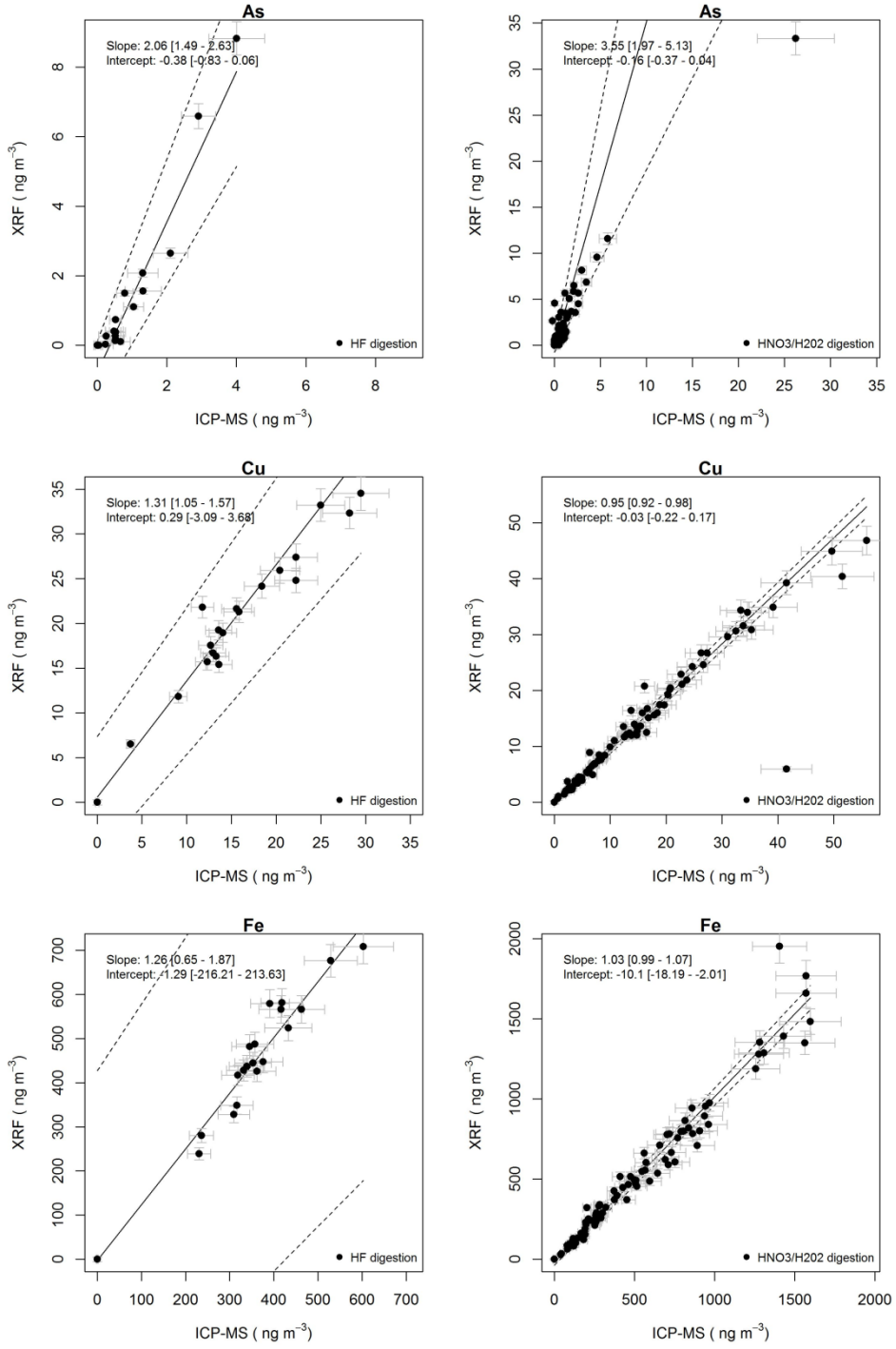

Figure S3: Deming regression of As, Cu and Fe as measured by ICP-MS (split into $HF/HClO_4$ (left) and HNO_3/H_2O_2 (right)) and XACT (ng m^{-3})

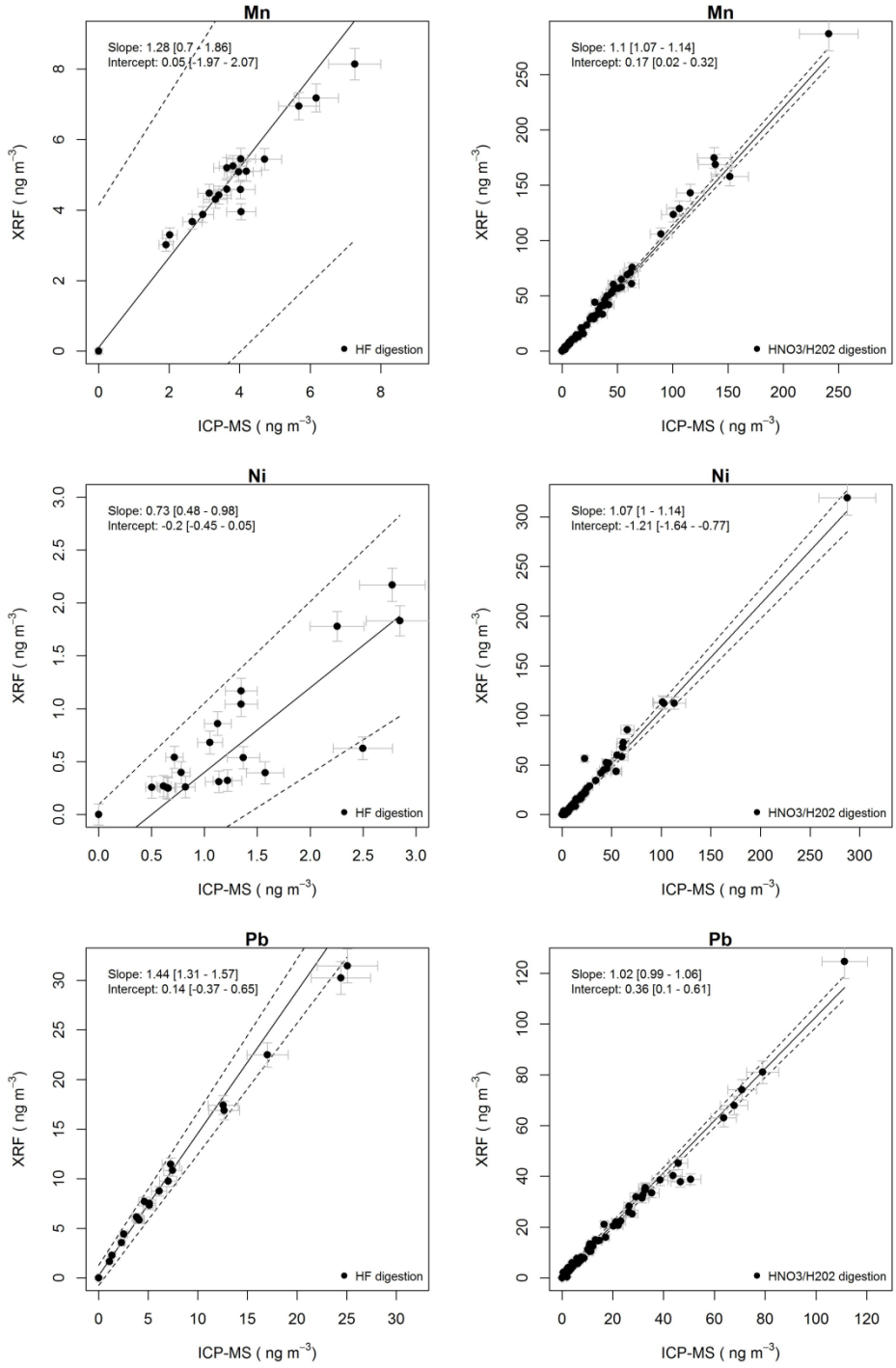

Figure S4: Deming regression of Mn, Ni, Pb as measured by ICP-MS (split into HF/$HClO_4$ (left) and HNO_3/H_2O_2 (right)) and XACT (ng m^{-3})

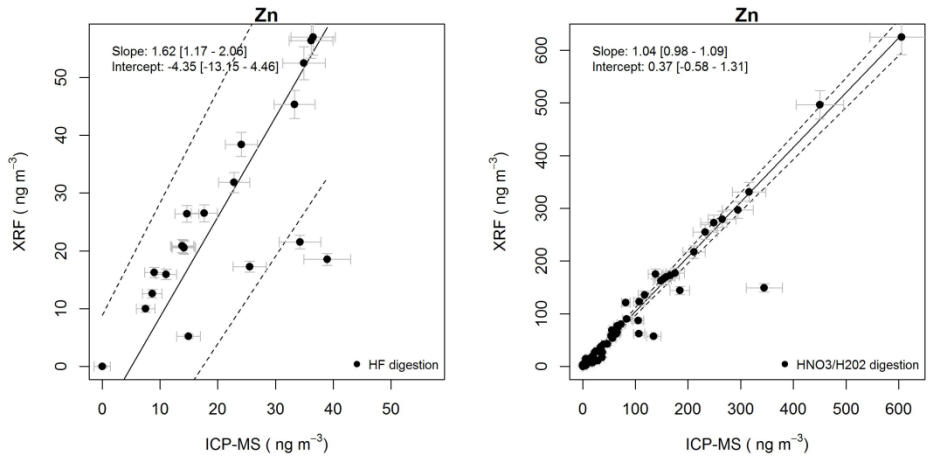

Figure S5: Deming regression of Zn as measured by ICP-MS (split into HF/$HClO_4$ (left) and HNO_3/H_2O_2 (right)) and XACT (ng m^{-3})

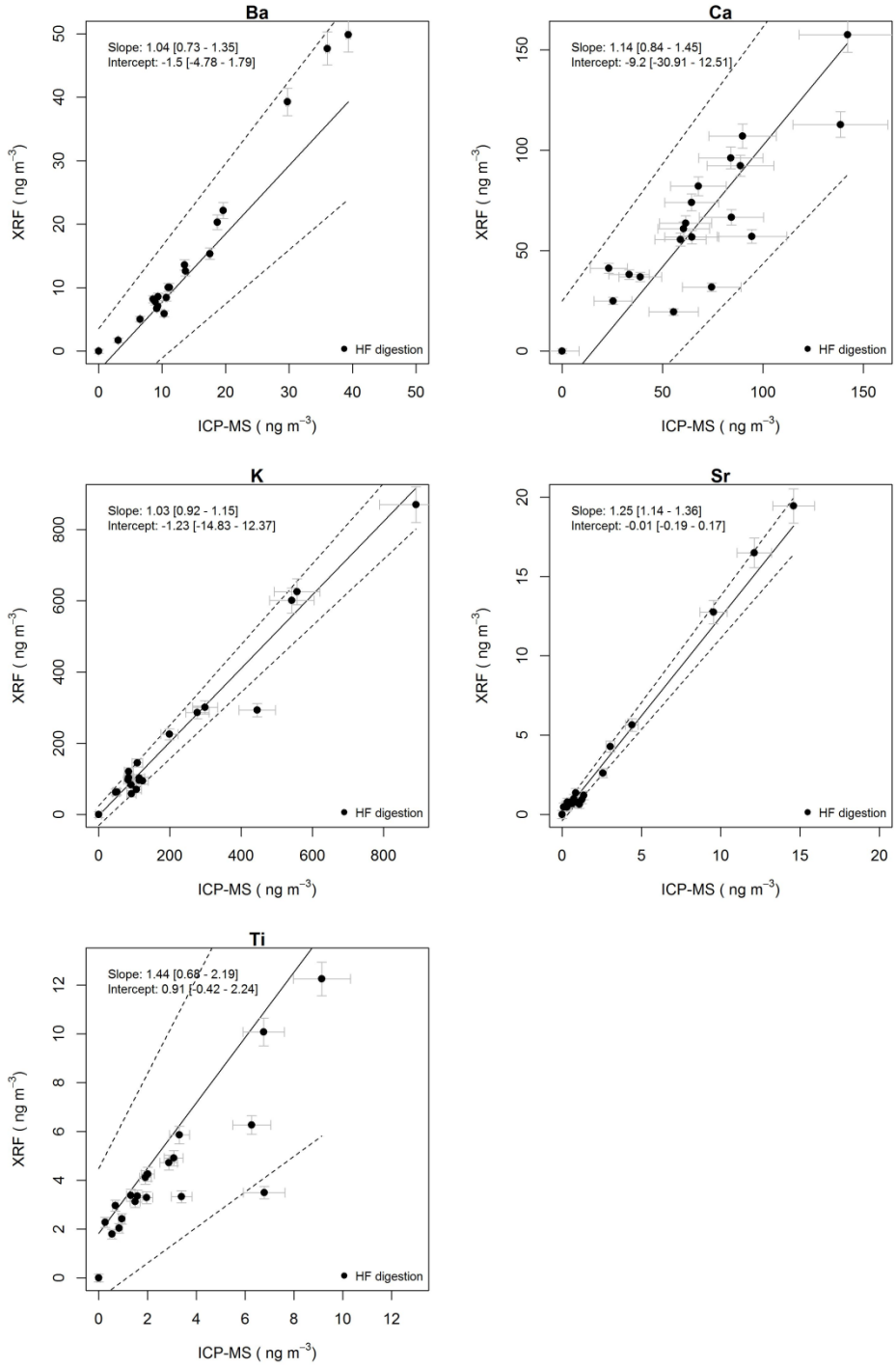

Figure S6: Deming regression of Ba, Ca, K, Sr and Ti as measured by ICP-MS (HF/$HClO_4$ only) and XACT (ng m^{-3})

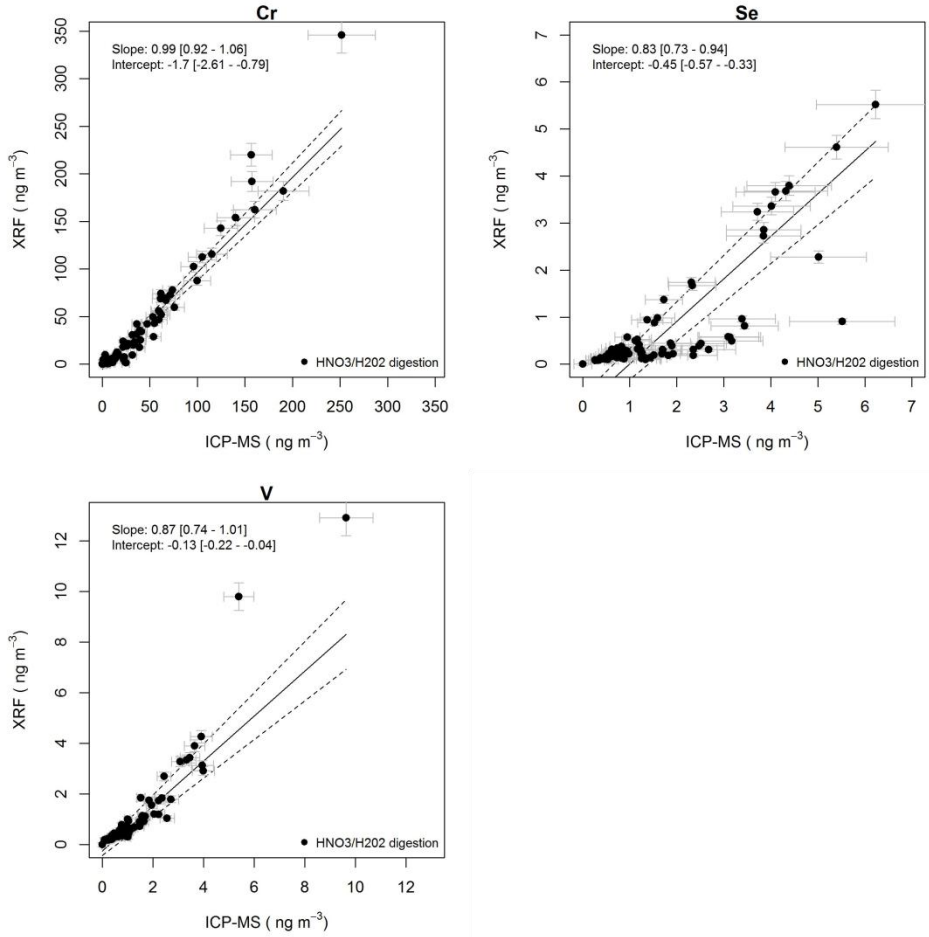

Figure S7: Deming regression of Cr, Se and V as measured by ICP-MS (HNO_3/H_2O_2 only) and XACT (ng m^{-3})

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S4. Deming regression graphs for all elements compared by XACT and XACT (filter)

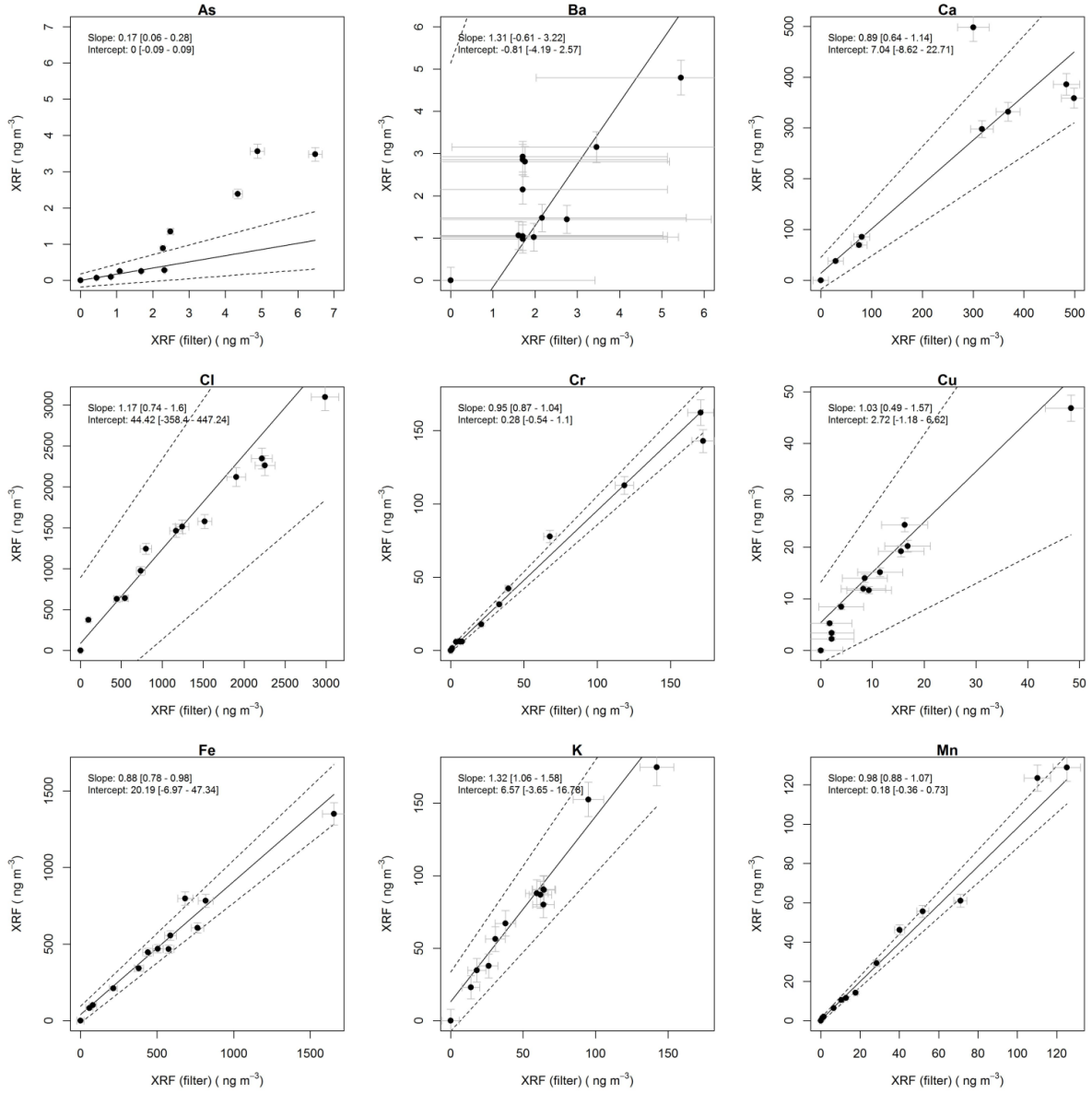

Figure S8: Deming regression of As, Ba, Ca, Cl, Cr, Cu, Fe, K and Mn as measured by XACT (filter) and XACT (in-situ) (ng m^{-3})

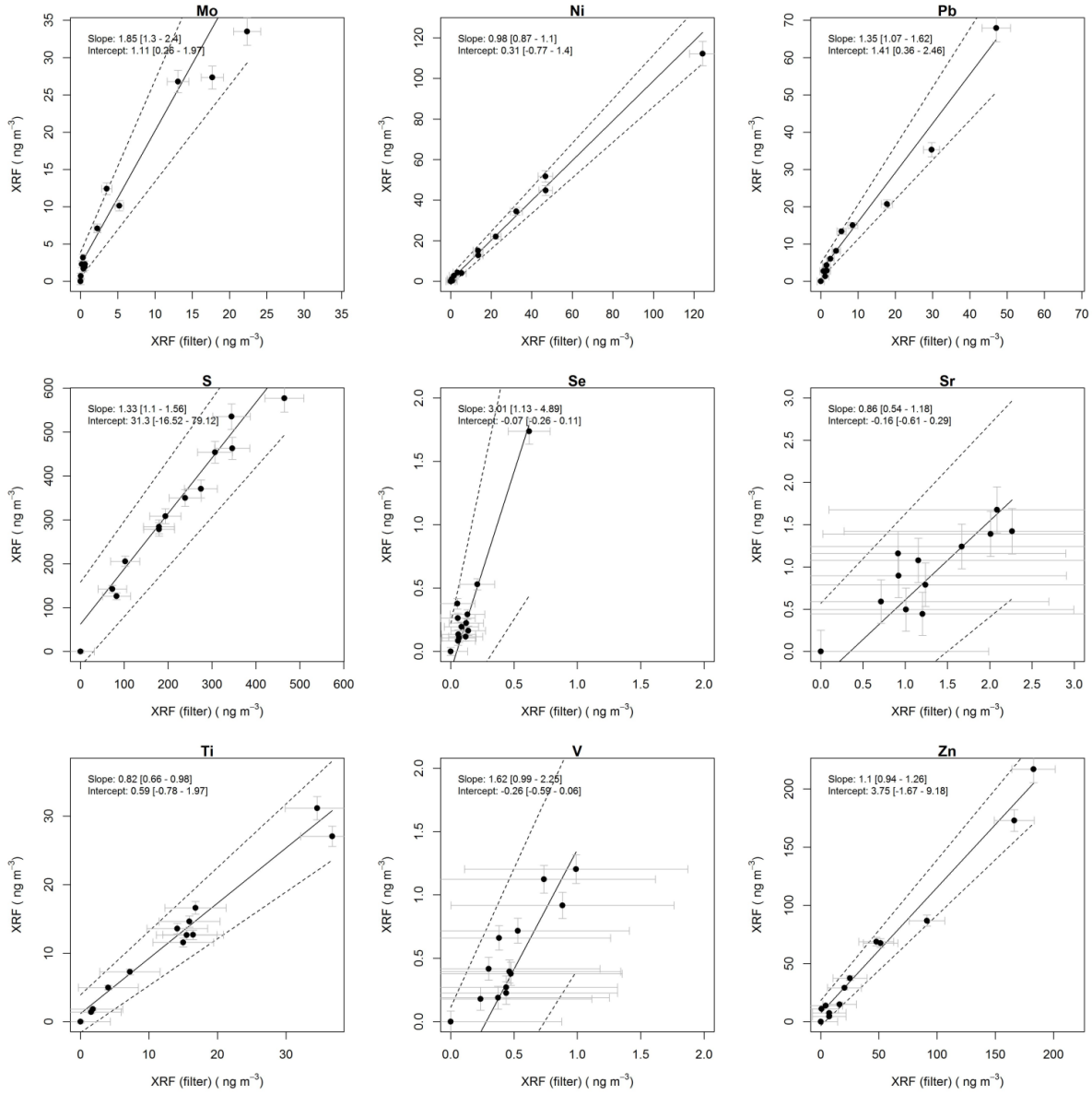

Figure S9: Deming regression of Mo, Ni, Pb, S, Se, Sr, Ti, V and Zn as measured by XACT (filter) and XACT (in-situ) (ng m^{-3})

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Table S1: Deming regression results and coefficient of determination for XACT comparison XACT (filter)

Element	Slope	Intercept	R^2
As	0.2 (0.1-0.3)	0 (-0.1-0.1)	0.91
Ba	1.3 (-0.6-3.2)	-0.8 (-4.2-2.6)	0.50
Ca	0.8 (0.7-0.8)	13.5 (-1.3-28.3)	0.98
Cl	0.4 (-1.6-2.5)	-0.2 (-16.1-15.8)	0.98
Cr	0.5 (-0.5-1.4)	0 (-0.9-0.9)	0.99
Cu	1.2 (0.7-1.6)	44.4 (-358-447)	0.96
Fe	1 (0.9-1)	0.3 (-0.5-1.1)	0.96
K	1 (0.5-1.6)	2.7 (-1.2-6.6)	0.95
Mn	0.9 (0.8-1)	20.2 (-7-47.3)	0.99
Mo	1.3 (1.1-1.6)	6.6 (-3.7-16.8)	0.96
Ni	1 (0.9-1.1)	0.2 (-0.4-0.7)	0.99
Pb	1.9 (1.3-2.4)	1.1 (0.3-2)	0.98
S	1 (0.9-1.1)	0.3 (-0.8-1.4)	0.96
Se	1.4 (1.1-1.6)	1.4 (0.4-2.5)	0.93
Sr	1.3 (1.1-1.6)	31.3 (-16.5-79.1)	0.61
Ti	3 (1.1-4.9)	-0.1 (-0.3-0.1)	0.97
V	0.9 (0.5-1.2)	-0.2 (-0.6-0.3)	0.76
Zn	0.8 (0.7-1)	0.6 (-0.8-2)	0.98

S5. Typical recovery rates for acid digestions

Table S2: Recovery rates for available elements, split by digestion method

Element	$HF/HClO_4$	HNO_3/H_2O_2
As		102%
Ca	99%	
Cr		71%
Cu	91%	97%
Fe	103%	100%
Mn	102%	100%
Ni	87%	93%
Pb	87%	103%
Se		98%
Sr	86%	
V		88%
Zn	89%	108%

S6. Deming regression of ICP-MS using different digestion methods

ICP/MS results were compared for the elements, which were available for both digestion methods (As, Cu, Fe, Mn, Ni, Pb and Zn). No simultaneous samples were available for the two digestion methods. In order to compare the two digestion methods and subsequent ICP-MS, the samples were grouped using the XACT element concentration and the resulting concentrations were compared using Deming regression. Uncertainties were estimated using the relationship between the existing concentrations/uncertainties over the concentration

range. ICP-MS results compared well between the two digestion methods with R^2 of 0.99, 0.98, 0.92, 0.96, 0.93, 0.996 and 0.93, for As, Cu, Fe, Mn, Ni, Pb and Zn, respectively. Samples digested with $HF/HClO_4$ resulted in significantly higher concentration for the element As, but in significantly lower concentration for the elements Cu, Pb and Zn. For the elements Fe, Mn and Ni no significant difference was found.

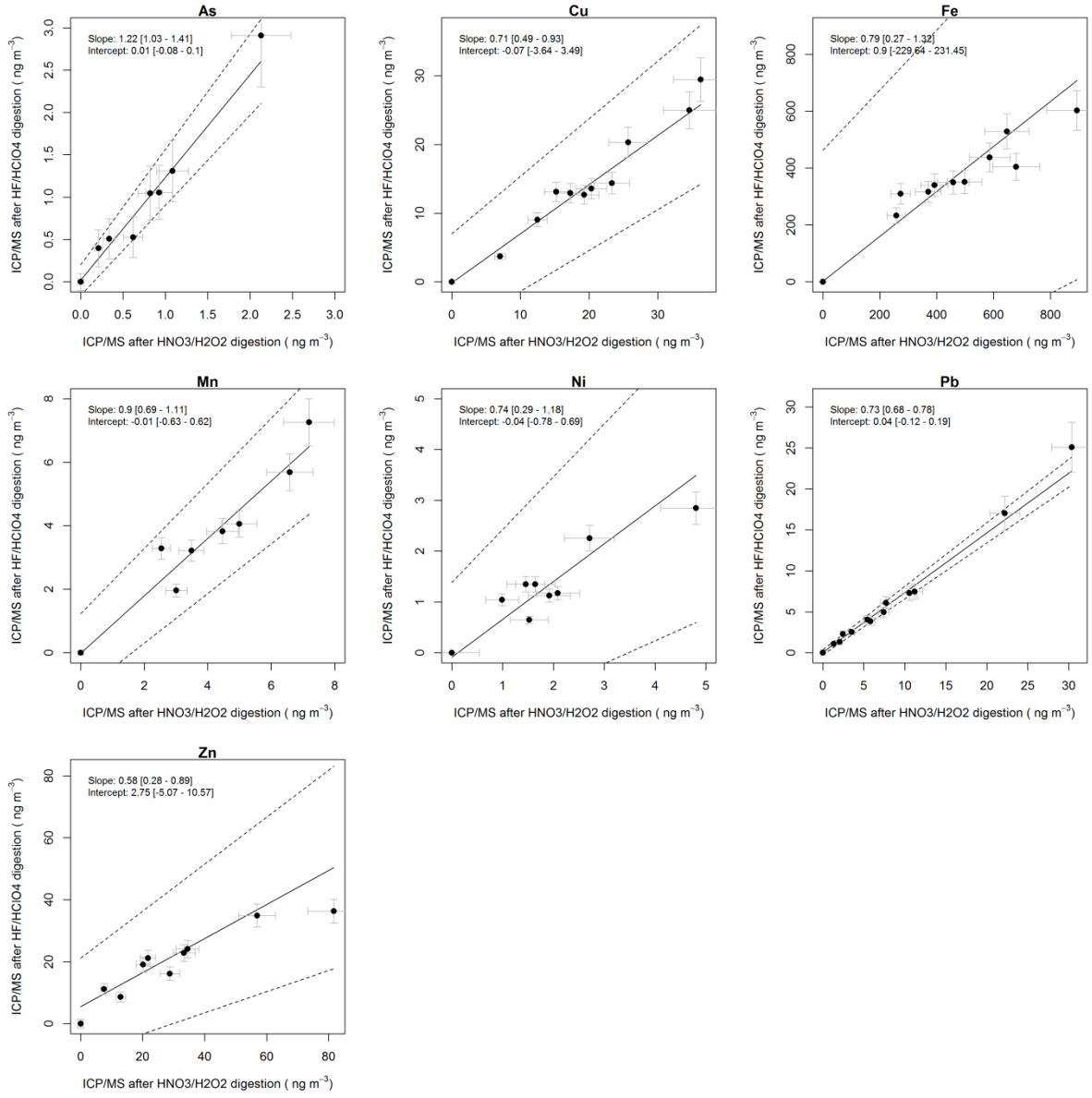

Figure S10: Deming regression of As, Cu, Fe, Mn, Ni, Pb and Zn as measured by ICP-MS (HNO_3/H_2O_2) and ICP-MS ($HF/HClO_4$) (ng m^{-3})