

Appendix A

Table A1. Summary of certified values used in the matching library for XRF analysis. All units in mg kg⁻¹

Certified reference materials				
Element	GBW07403	GBW07405	ISE 921	BAM-U110
Al	64800	114247	56800 ±1440	*50382 ±1081
Ca	9071	679	43000 ±1180	*40638 ±2105
Cu	11.4	144	93.8 ±5.84	263 ±12
Cr	32	118	130 ±10.6	230 ±13
Fe	13989	88269	31900 ±1130	*28229 ±663
K	25226	12447	19100 ±640	*20381 ±4560
Mg	3498	3679	11100 ±370	*8380 ±735
Mn	304	1360	1190 ±43	621 ±20
Ni	12	40	42.4 ±3.21	101 ±5
P	320	390	1400 ±69	*3648 ±49
Pb	26	552	167 ±7.5	197 ±14
S	120	410	702 ±79.8	*10593
Si	349290	245746	271000 ±4600	*258125
Zn	31	494	522 ±19.9	1000 ±50

* reference value only not certified

Table A2. Measurement conditions for analysis of the elemental composition of soil samples prepared as pressed pellet with binder using benchtop energy dispersive X-ray fluorescence spectrometer. All samples were run under vacuum atmosphere

Element	Voltage (kv)	Secondary target	Peak detected (KeV)	Measurement time (s)
Cu	50	Mo	K α , 8.047	100
Cr	50	Cu	K α , 5.414	100
Mn	50	Mo	K α , 5.898	100
Ni	50	Mo	K α , 7.477	100
Zn	50	Mo	K α , 8.638	100
Pb	50	Mo	L β 1, 12.611	100
Al	25	Rx9	K α , 1.487	100
S	25	Rx9	K α , 2.308	100
P	25	Rx9	K α , 2.015	100
Mg	25	Si	K α , 1.254	300
Ca	50	Cu	K α , 3.691	100
K	50	Cu	K α , 3.313	100
Fe	50	Mo	K α , 6.403	100

Table A3 Average recovery of elements based on the concentration threshold of the ISE samples analysed with the fundamental parameters (FP) and matching library (ML) methods on the EDXRF

Elements	Concentration threshold (mg kg ⁻¹)	Average recovery including sand (%)	Average recovery (%) minus sand	Calibration method
Al	40760	-	106 ±10.2 (n=12)	ML
Ca	3750	120 ±29 (n=17)	106 ±12 (n=14)	ML
Cr	77.3	101±21 (n=14)	97±14.9 (n=12)	ML
Cu	39.66	125 ±14 (n=5)	122±14.5 (n=4)	ML
Fe	6040	106 ±10.4 (n=17)	102±4.5 (n=14)	FP
K	5988	108 ±10.1 (n=20)	-	FP
Mg	4844	107 ±22.8 (n=12)	102 ± 15.3 (n=11)	ML
Mn	238	114 ±18.3 (n=15)	107 ±4.9 (n=13)	FP
Ni	21.27	117 ±11.9 (n=14)	113 ±5.8 (n=12)	ML
P	727	130 ±87.04 (n=12)	85±14.17 (n=9)	ML
Pb	19.16	113±6.2 (n=16)	-	ML
S	603.5	164±130 (n=9)	100±10 (n=7)	ML
Zn	56.45	109±7.3 (n=13)	107± 3.6 (n=12)	FP



Figure A1. Common methods for soil sample preparation using low and high pressure for analysis on X-ray fluorescence spectroscopy (a) loose powder (LP)-200 inch lbs pressure added for 30s, (b) pressed powder pellet (PP)-15 tons pressure added for 30s, (c) pressed powder pellet with wax binder (PPB)-20 tons pressure added for 30s.

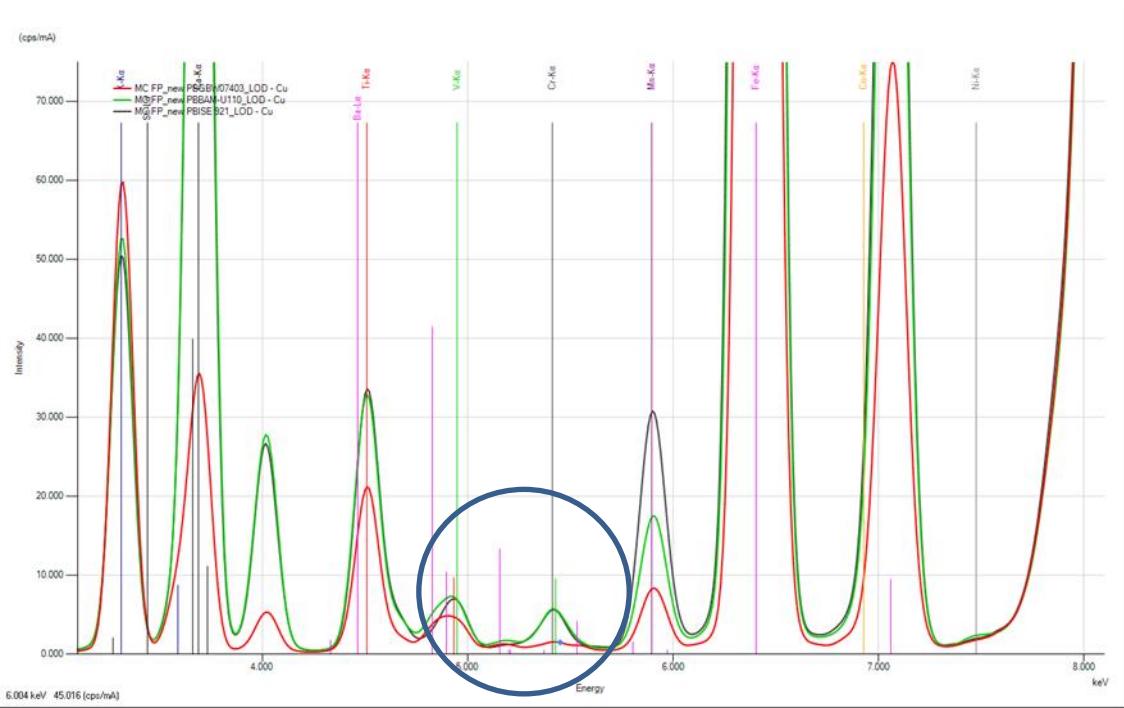


Figure A2. Spectrum of Cu target on EDXRF showing the elements on the target using three CRMs with different concentrations, whereby the red line (GBW07403) signifies elements at low concentrations, the black line (ISE 921) signifying elements at medium concentrations and the green line (BAM-U110) indicating a contaminated soil