

## Supplementary materials

**Table S1** Single extraction procedures used

Extracting agent	Liquid/ solid ratio	Equilibration time	Reference
0.01 mol/L CaCl <sub>2</sub>	1 to 10	3 h	Novozamsky et al. (1993)
0.005 mol/L DTPA, 0.01 mol/L CaCl <sub>2</sub> and 0.1 mol/L TEA	1 to 2	2 h	Lindsay and Norvell (1978)
0.05 mol/L EDTA	1 to 10	1 h	Quevauviller et al. (1996)
0.5 mol/L HNO <sub>3</sub>	1 to 5	2h	Van Ranst et al. (1999)
1 mol/L MgCl <sub>2</sub>	1 to 8	2 h	Tessier et al. (1979)
0.1 mol/L NaNO <sub>3</sub>	1 to 2.5	2 h	Gupta and Aten (1993)
1 mol/L NH <sub>4</sub> NO <sub>3</sub>	1 to 2.5	2 h	DIN (1995), Legislation Germany
1 mol/L NH <sub>4</sub> OAc	1 to 30	2 h	Van Ranst et al. (1999)

**Table S2** Statistical parameters of physicochemical properties and total trace element content of soils (*n*=25)

Parameter	Mean	Median	Minimum	Maximum	Standard deviation
pH	7.4	7.4	6.5	8.2	0.4
EC (dS/m)	0.170	0.150	0.070	0.340	0.070
CEC (cmole/kg)	15.4	15.0	9.4	26.8	5.2
OM (%)	1.3	0.9	0.01	4.9	1.2
CaCO <sub>3</sub> (%)	11.5	10.2	4.0	24.0	6.2
Clay (%)	21.1	23.8	7.0	42.5	10.7
Silt (%)	27.5	18.7	4.7	72.7	20.7
Sand (%)	51.4	53.5	1.1	85.5	27.3
Total Cd (mg/kg)	1.3	1.3	0.8	2.0	0.4
Total Co (mg/kg)	10.1	10.1	7.9	11.9	1.5
Total Cu (mg/kg)	22.7	20.8	11.9	43.9	9.5
Total Ni (mg/kg)	41.2	37.8	30.1	65.8	9.5
Total Zn (mg/kg)	37.0	37.7	23.8	47.1	5.6

EC, Electrical conductivity; CEC, Cation exchange capacity; OM, Organic matter; CaCO<sub>3</sub>, Equivalent calcium carbonate.

**Table S3** Correlation coefficients between Cd, Co, Cu, Ni and Zn extracted by different extracting agents and soil properties

Metal	Method	pH	EC	CEC	OM	CaCO <sub>3</sub>	Clay	Silt	Sand
Cd	CaCl <sub>2</sub>	-0.27	0.35	-0.46*	-0.57***	-0.25	-0.73***	-0.53***	0.69***
	DTPA	-0.29	0.28	-0.20	-0.18	-0.14	-0.37	-0.30	0.37
	EDTA	-0.15	0.41*	-0.26	-0.21	0.01	-0.46*	-0.24	0.36
	HNO <sub>3</sub>	0.10	0.57***	-0.42*	-0.24	0.21	-0.24	-0.03	0.12
	MgCl <sub>2</sub>	0.28	-0.22	0.35	0.38	0.38	0.38	0.69***	-0.68***
	NaNO <sub>3</sub>	0.02	-0.57***	0.76***	0.49*	0.07	0.59***	0.41*	-0.54***
	NH <sub>4</sub> NO <sub>3</sub>	0.11	-0.54***	0.67***	0.51***	0.16	0.71***	0.40*	-0.58***
	NH <sub>4</sub> OAc	-0.46*	0.46*	-0.32	-0.38	-0.16	-0.56***	-0.64***	0.71***
Co	CaCl <sub>2</sub>	-0.40*	-0.45*	0.18	0.25	-0.45*	0.24	-0.21	0.06
	DTPA	-0.51*	0.30	-0.30	-0.04	-0.25	-0.33	-0.40	0.43*
	EDTA	-0.11	0.10	-0.26	-0.06	-0.22	-0.25	-0.26	0.30
	HNO <sub>3</sub>	-0.69***	0.28	-0.42*	-0.32	-0.54**	-0.43*	-0.69***	0.69***
	MgCl <sub>2</sub>	-0.31	-0.08	0.11	0.37	-0.07	0.22	0.08	-0.15
	NaNO <sub>3</sub>	0.03	-0.54**	0.61***	0.51**	0.08	0.68***	0.32	-0.51**
	NH <sub>4</sub> NO <sub>3</sub>	-0.34	-0.43*	0.18	0.19	-0.42*	0.25	-0.19	0.05
	NH <sub>4</sub> OAc	-0.39	-0.14	-0.19	-0.11	-0.41*	-0.33	-0.38	0.42*
Cu	CaCl <sub>2</sub>	-0.32	0.66***	-0.61**	-0.50*	-0.15	-0.75***	-0.56**	0.72***
	DTPA	-0.42*	0.71***	-0.46*	-0.34	0.00	-0.60**	-0.40*	0.54**
	EDTA	-0.43*	0.46*	-0.43*	-0.41*	-0.22	-0.67***	-0.53**	0.67***
	HNO <sub>3</sub>	-0.61**	0.35	-0.35	-0.42*	-0.37	-0.59**	-0.62**	0.70***
	MgCl <sub>2</sub>	-0.11	0.24	-0.04	0.01	-0.06	-0.05	-0.10	0.10
	NaNO <sub>3</sub>	-0.38	0.20	0.13	0.29	-0.14	-0.22	-0.10	0.16
	NH <sub>4</sub> NO <sub>3</sub>	-0.16	0.59**	-0.23	-0.21	0.06	-0.29	-0.25	0.30
	NH <sub>4</sub> OAc	-0.29	0.55**	-0.41*	-0.42*	-0.06	-0.54**	-0.51*	0.60**
Ni	CaCl <sub>2</sub>	-0.19	0.47*	-0.54**	-0.46*	-0.14	-0.69***	-0.51**	0.65***
	DTPA	-0.02	-0.20	-0.14	0.03	-0.21	0.36	-0.12	-0.05
	EDTA	-0.02	-0.31	0.07	-0.16	-0.41*	-0.06	-0.01	0.03
	HNO <sub>3</sub>	-0.38	-0.18	-0.12	-0.36	-0.59**	-0.23	-0.35	0.36
	MgCl <sub>2</sub>	-0.09	0.30	-0.04	0.05	0.15	-0.03	0.01	-0.06
	NaNO <sub>3</sub>	0.08	-0.04	0.37	0.22	0.12	0.48*	0.16	-0.31
	NH <sub>4</sub> NO <sub>3</sub>	0.21	0.00	0.46*	0.44*	0.50*	0.42*	0.67***	-0.68***
	NH <sub>4</sub> OAc	-0.51**	0.30	-0.22	-0.18	-0.29	-0.48*	-0.61**	0.65***
Zn	CaCl <sub>2</sub>	-0.18	0.38	-0.25	-0.28	0.01	-0.42*	-0.34	0.42*
	DTPA	-0.03	0.16	-0.46*	-0.15	-0.27	-0.21	-0.07	0.14
	EDTA	-0.12	0.28	-0.44*	-0.36	-0.23	-0.56**	-0.43*	0.54**
	HNO <sub>3</sub>	-0.50*	0.50*	-0.47*	-0.40*	-0.23	-0.64**	-0.53**	0.65***
	MgCl <sub>2</sub>	-0.51**	0.52*	-0.18	-0.14	0.03	-0.21	-0.24	0.26
	NaNO <sub>3</sub>	-0.06	-0.40*	0.61**	0.37	0.09	0.58**	0.24	-0.41*
	NH <sub>4</sub> NO <sub>3</sub>	-0.50*	0.40*	0.00	-0.14	-0.01	-0.22	-0.14	0.19
	NH <sub>4</sub> OAc	-0.30	0.32	-0.23	-0.14	0.06	-0.15	-0.06	0.10

\*p &lt; 0.05, \*\* p &lt; 0.01, \*\*\* p &lt; 0.001

**Table S4** Average saturation indices of trace elements using different extracting agents

Trace elements	Extracting agents																
	CaCl <sub>2</sub>	SI	MgCl <sub>2</sub>	SI	DTPA	SI	EDTA	SI	HNO <sub>3</sub>	SI	NaNO <sub>3</sub>	SI	NH <sub>4</sub> NO <sub>3</sub>	SI	NH <sub>4</sub> OAc	SI	
Cd	Cd(OH) <sub>2</sub> (s)	-7.35	Cd(OH) <sub>2</sub> (s)	-8.13	Cd(OH) <sub>2</sub> (s)	-14.19	Cd(OH) <sub>2</sub> (s)	-19.71	Cd(OH) <sub>2</sub> (s)	-17.80	Cd(OH) <sub>2</sub> (s)	-3.55	Cd(OH) <sub>2</sub> (s)	-8.37	Cd(OH) <sub>2</sub> (s)	-8.98	
	CdCl <sub>2</sub> (s)	-10.94	CdCl <sub>2</sub> (s)	-8.03	-	-	-	-	-	-	-	-	-	-	-	-	
	CdCl <sub>2</sub> ·1H <sub>2</sub> O(s)	-9.91	CdCl <sub>2</sub> ·1H <sub>2</sub> O(s)	-7.02	-	-	-	-	-	-	-	-	-	-	-	-	-
	CdCl <sub>2</sub> ·2.5H <sub>2</sub> O(s)	-9.69	CdCl <sub>2</sub> ·2.5H <sub>2</sub> O(s)	-6.84	-	-	-	-	-	-	-	-	-	-	-	-	-
	CdOHCl(s)	-6.19	CdOHCl(s)	-5.12	-	-	-	-	-	-	-	-	-	-	-	-	-
Co	Otavite	-2.26	Otavite	-2.50	Otavite	-9.86	Otavite	-12.05	Otavite	-9.91	Otavite	0.71	Otavite	-1.16	Otavite	-2.92	
	Co(OH) <sub>2</sub> (am)	-6.22	Co(OH) <sub>2</sub> (am)	-4.82	Co(OH) <sub>2</sub> (am)	-13.19	Co(OH) <sub>2</sub> (am)	-18.93	Co(OH) <sub>2</sub> (am)	-16.09	Co(OH) <sub>2</sub> (am)	-3.07	Co(OH) <sub>2</sub> (am)	-7.64	Co(OH) <sub>2</sub> (am)	-6.11	
	Co(OH) <sub>2</sub> (c)	-5.41	Co(OH) <sub>2</sub> (c)	-4.02	Co(OH) <sub>2</sub> (c)	-12.38	Co(OH) <sub>2</sub> (c)	-18.13	Co(OH) <sub>2</sub> (c)	-15.29	Co(OH) <sub>2</sub> (c)	-2.27	Co(OH) <sub>2</sub> (c)	-6.83	Co(OH) <sub>2</sub> (c)	-5.30	
	CoCO <sub>3</sub> (s)	-2.49	CoCO <sub>3</sub> (s)	-0.55	CoCO <sub>3</sub> (s)	-10.17	CoCO <sub>3</sub> (s)	-12.63	CoCO <sub>3</sub> (s)	-9.56	CoCO <sub>3</sub> (s)	-0.17	CoCO <sub>3</sub> (s)	-1.79	CoCO <sub>3</sub> (s)	-1.40	
	CoO(s)	-6.71	CoO(s)	-5.29	CoO(s)	-13.68	CoO(s)	-19.43	CoO(s)	-16.58	CoO(s)	-3.56	CoO(s)	-8.11	CoO(s)	-6.58	
Cu	CoCl <sub>2</sub> (s)	-19.28	CoCl <sub>2</sub> (s)	-14.20	-	-	-	-	-	-	-	-	-	-	-	-	
	CoCl <sub>2</sub> ·6H <sub>2</sub> O(s)	-13.56	CoCl <sub>2</sub> ·6H <sub>2</sub> O(s)	-8.61	-	-	-	-	-	-	-	-	-	-	-	-	
	Cu(OH) <sub>2</sub> (s)	-4.84	Cu(OH) <sub>2</sub> (s)	-2.06	Cu(OH) <sub>2</sub> (s)	-13.74	Cu(OH) <sub>2</sub> (s)	-19.42	Cu(OH) <sub>2</sub> (s)	-12.42	Cu(OH) <sub>2</sub> (s)	-1.41	Cu(OH) <sub>2</sub> (s)	-4.54	Cu(OH) <sub>2</sub> (s)	-5.36	
	CuCO <sub>3</sub> (s)	-4.62	CuCO <sub>3</sub> (s)	-1.29	CuCO <sub>3</sub> (s)	-14.23	CuCO <sub>3</sub> (s)	-16.63	CuCO <sub>3</sub> (s)	-9.40	CuCO <sub>3</sub> (s)	-2.01	CuCO <sub>3</sub> (s)	-2.20	CuCO <sub>3</sub> (s)	-	
	Malachite	-6.20	Malachite	-0.09	Malachite	-24.71	Malachite	-32.79	Malachite	-18.56	Malachite	-0.16	Malachite	-3.47	Malachite	-	
Ni	Tenorite(am)	-4.04	Tenorite(am)	-1.23	Tenorite(am)	-12.94	Tenorite(am)	-18.62	Tenorite(am)	-11.62	Tenorite(am)	-0.61	Tenorite(am)	-3.72	Tenorite(am)	-4.56	
	Tenorite(c)	-3.19	Tenorite(c)	-0.38	Tenorite(c)	-12.09	Tenorite(c)	-17.77	Tenorite(c)	-10.77	Tenorite(c)	0.24	Tenorite(c)	-2.87	Tenorite(c)	-3.71	
	Melanothallite	-18.86	Melanothallite	-13.23	-	-	-	-	-	-	-	-	-	-	-	-	
	-	-	Azurite	-0.95	-	-	Azurite	-48.99	Azurite	-27.52	Azurite	-1.75	Azurite	-5.24	-	-	
	-	-	-	-	-	-	-	-	-	-	Cu <sub>2</sub> (OH) <sub>2</sub> NO <sub>3</sub> (s)	-2.71	Cu <sub>2</sub> (OH) <sub>2</sub> NO <sub>3</sub> (s)	-6.01	-	-	
Zn	Ni(OH) <sub>2</sub> (am)	-5.50	Ni(OH) <sub>2</sub> (am)	-4.37	Ni(OH) <sub>2</sub> (am)	-13.76	Ni(OH) <sub>2</sub> (am)	-20.17	Ni(OH) <sub>2</sub> (am)	-15.78	Ni(OH) <sub>2</sub> (am)	-2.75	Ni(OH) <sub>2</sub> (am)	-7.11	Ni(OH) <sub>2</sub> (am)	-6.72	
	Ni(OH) <sub>2</sub> (c)	-3.40	Ni(OH) <sub>2</sub> (c)	-2.27	Ni(OH) <sub>2</sub> (c)	-11.66	Ni(OH) <sub>2</sub> (c)	-18.07	Ni(OH) <sub>2</sub> (c)	-13.68	Ni(OH) <sub>2</sub> (c)	-0.65	Ni(OH) <sub>2</sub> (c)	-5.01	Ni(OH) <sub>2</sub> (c)	-4.62	
	NiCO <sub>3</sub> (s)	-1.98	NiCO <sub>3</sub> (s)	-0.30	NiCO <sub>3</sub> (s)	-10.95	NiCO <sub>3</sub> (s)	-14.07	NiCO <sub>3</sub> (s)	-9.46	NiCO <sub>3</sub> (s)	-0.05	NiCO <sub>3</sub> (s)	-1.47	NiCO <sub>3</sub> (s)	-2.22	
	Zn(OH) <sub>2</sub> (am)	-5.06	Zn(OH) <sub>2</sub> (am)	-5.01	Zn(OH) <sub>2</sub> (am)	-11.43	Zn(OH) <sub>2</sub> (am)	-17.61	Zn(OH) <sub>2</sub> (am)	-15.18	Zn(OH) <sub>2</sub> (am)	-2.43	Zn(OH) <sub>2</sub> (am)	-6.76	Zn(OH) <sub>2</sub> (am)	-6.20	
	Zn(OH) <sub>2</sub> (beta)	-4.34	Zn(OH) <sub>2</sub> (beta)	-4.29	Zn(OH) <sub>2</sub> (beta)	-10.71	Zn(OH) <sub>2</sub> (beta)	-16.89	Zn(OH) <sub>2</sub> (beta)	-14.46	Zn(OH) <sub>2</sub> (beta)	-1.71	Zn(OH) <sub>2</sub> (beta)	-6.04	Zn(OH) <sub>2</sub> (beta)	-5.48	
Zn	Zn(OH) <sub>2</sub> (delta)	-4.43	Zn(OH) <sub>2</sub> (delta)	-4.38	Zn(OH) <sub>2</sub> (delta)	-10.80	Zn(OH) <sub>2</sub> (delta)	-16.98	Zn(OH) <sub>2</sub> (delta)	-14.55	Zn(OH) <sub>2</sub> (delta)	-1.80	Zn(OH) <sub>2</sub> (delta)	-6.13	Zn(OH) <sub>2</sub> (delta)	-5.57	
	Zn(OH) <sub>2</sub> (epsilon)	-4.12	Zn(OH) <sub>2</sub> (epsilon)	-4.07	Zn(OH) <sub>2</sub> (epsilon)	-10.49	Zn(OH) <sub>2</sub> (epsilon)	-16.67	Zn(OH) <sub>2</sub> (epsilon)	-14.24	Zn(OH) <sub>2</sub> (epsilon)	-1.49	Zn(OH) <sub>2</sub> (epsilon)	-5.82	Zn(OH) <sub>2</sub> (epsilon)	-5.26	
	Zn(OH) <sub>2</sub> (gamma)	-4.32	Zn(OH) <sub>2</sub> (gamma)	-4.27	Zn(OH) <sub>2</sub> (gamma)	-10.69	Zn(OH) <sub>2</sub> (gamma)	-16.87	Zn(OH) <sub>2</sub> (gamma)	-14.44	Zn(OH) <sub>2</sub> (gamma)	-1.69	Zn(OH) <sub>2</sub> (gamma)	-6.02	Zn(OH) <sub>2</sub> (gamma)	-5.46	
	Zn <sub>2</sub> (OH) <sub>2</sub> Cl(s)	-9.32	Zn <sub>2</sub> (OH) <sub>2</sub> Cl(s)	-7.36	-	-	-	-	-	-	-	-	-	-	-	-	
	Zn <sub>3</sub> (OH) <sub>4</sub> Cl <sub>2</sub> (s)	-19.35	Zn <sub>3</sub> (OH) <sub>4</sub> Cl <sub>2</sub> (s)	-15.37	-	-	-	-	-	-	-	-	-	-	-	-	
Zn	ZnCl <sub>2</sub> (s)	-17.53	ZnCl <sub>2</sub> (s)	-13.79	-	-	-	-	Zn(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O(s)	-9.40	Zn(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O(s)	-11.73	Zn(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O(s)	-10.22	-	-	
	ZnCO <sub>3</sub> (s)	-2.35	ZnCO <sub>3</sub> (s)	-1.76	ZnCO <sub>3</sub> (s)	-9.43	ZnCO <sub>3</sub> (s)	-12.33	ZnCO <sub>3</sub> (s)	-9.67	ZnCO <sub>3</sub> (s)	-0.55	ZnCO <sub>3</sub> (s)	-1.93	ZnCO <sub>3</sub> (s)	-2.52	
	ZnCO <sub>3</sub> ·1H <sub>2</sub> O(s)	-2.89	ZnCO <sub>3</sub> ·1H <sub>2</sub> O(s)	-2.32	ZnCO <sub>3</sub> ·1H <sub>2</sub> O(s)	-9.97	ZnCO <sub>3</sub> ·1H <sub>2</sub> O(s)	-12.87	ZnCO <sub>3</sub> ·1H <sub>2</sub> O(s)	-10.21	ZnCO <sub>3</sub> ·1H <sub>2</sub> O(s)	-1.09	ZnCO <sub>3</sub> ·1H <sub>2</sub> O(s)	-2.49	ZnCO <sub>3</sub> ·1H <sub>2</sub> O(s)	-3.08	
	Hydrozincite	-12.78	Hydrozincite	-11.41	Hydrozincite	-46.01	Hydrozincite	-70.38	Hydrozincite	-57.76	Hydrozincite	-1.28	Hydrozincite	-17.01	Hydrozincite	-16.53	
	Smithsonite	-2.25	Smithsonite	-1.66	Smithsonite	-9.33	Smithsonite	-12.23	Smithsonite	-9.57	Smithsonite	-0.45	Smithsonite	-1.83	Smithsonite	-2.42	
Zincite	-3.82	Zincite	-3.74	Zincite	-10.18	Zincite	-16.37	Zincite	-13.94	Zincite	-1.19	Zincite	-5.50	Zincite	-4.94		