Supplementary Information

Evaluation of Microwave-assisted Digestion Methods for ID-ICP-MS Characterization of KRISS Lake Sediment CRM 109-05-002

Jong Wha Lee[1,*], Youngran Lim[1], Hana Cho[1], Sung Woo Heo[1]

[1]Division of Chemical and Material Metrology, Korea Research Institute of Standards and Science (KRISS), Daejeon 34113, Republic of Korea

Table S1. Typical ICP-MS parameters for Thermo Element 2

Parameter	**Typical value**
RF power	1250 W
Cool gas	16 L/min
Auxiliary gas	(0.8 – 0.85) L/min
Sample gas	(0.88 – 0.99) L/min
Nebulizer	Glass concentric or PFA concentric
Spray chamber	Glass cyclonic or PFA cyclonic
Injector	Quartz or Pt
Sample tubing	0.76 mm ID PVC or viton
Peristaltic pump speed	(8 – 12) min^{-1}
Sampler cone	Pt
Skimmer cone	Pt 0.8X or 0.8H
Scanning mode	E-scan
Resolving power	Low resolution flat-top (Sn, Sb, and Pb) or medium resolution (Fe, Mg, Ti, Ca, Ba, Zn, Cr, Ni, and Cu)

Table S2. Typical ICP-MS parameters for Agilent 8800

Parameter	Typical value
RF power	1550 W
RF matching	1.8 V
Carrier gas	0.76 L/min
Makeup gas	0.45 L/min
Sampling depth	7.1 mm
Nebulizer	PFA concentric
Spray chamber	PFA Scott double path
Sample tubing	1.02 mm ID PVC
Injector	Pt
Nebulizer pump speed	0.10 s^{-1}
Sampler cone	Pt
Skimmer cone	Pt
Reaction cell gas flow	He 2.5 mL/min (Cd), He 6.0 mL/min + H_2 3.0 mL/min (Cd), or O_2 30 % (Se)

Table S3. Uncertainty budget for Fe, Mg, Ti, Ca, Ba, Zn, and Cr. Descriptions on the symbols can be found elsewhere.[1,2]

Quantity	Fe	Mg	Ti	Ca	Ba	Zn	Cr
w_z	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
m_x	2 %	< 1 %	2 %	< 1 %	1 %	< 1 %	9 %
$m_{y,xy}$	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
m_z	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
$m_{y,yz}$	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
M_x	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
M_z	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
R_x	10 %	2 %	14 %	1 %	1 %	2 %	16 %
R_z	3 %	< 1 %	26 %	< 1 %	3 %	3 %	35 %
R_y	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
R_{xy}	0	0	0	0	0	0	0
R_{yz}	0	0	0	0	0	0	0
x_x (ΣR_x)	22 %	< 1 %	< 1 %	46 %	15 %	45 %	2 %
x_z (ΣR_z)	22 %	< 1 %	< 1 %	44 %	15 %	44 %	2 %
f_{dry}	0	0	0	0	0	0	0
B	0	0	0	0	0	0	0
f_{cal}	< 1 %	< 1 %	6 %	< 1 %	< 1 %	< 1 %	4 %
f_{ran}	40 %	97 %	50 %	8 %	65 %	6 %	32 %

Table S4. Uncertainty budget for Ni, Pb, Cu, Sn, Sb, Cd, and Se. Descriptions on the symbols can be found elsewhere.[1,2]

Quantity	**Ni**	**Pb**	**Cu**	**Sn**	**Sb**	**Cd**	**Se**
w_z	< 1 %	< 1 %	< 1 %	< 1 %	2 %	< 1 %	< 1 %
m_x	2 %	24 %	7 %	3 %	5 %	< 1 %	< 1 %
$m_{y,xy}$	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
m_z	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
$m_{y,yz}$	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
M_x	< 1 %	3 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
M_z	< 1 %	2 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
R_x	10 %	28 %	10 %	2 %	3 %	48 %	59 %
R_z	3 %	5 %	32 %	< 1 %	< 1 %	26 %	6 %
R_y	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %	< 1 %
R_{xy}	0	0	0	0	0	0	0
R_{yz}	0	0	0	0	0	0	0
x_x (ΣR_x)	22 %	1 %	8 %	13 %	< 1 %	< 1 %	4 %
x_z (ΣR_z)	22 %	< 1 %	8 %	13 %	< 1 %	< 1 %	4 %
f_{dry}	0	0	0	0	0	0	0
B	0	0	0	0	0	0	0
f_{cal}	< 1 %	7 %	3 %	< 1 %	< 1 %	4 %	7 %
f_{ran}	40 %	29 %	32 %	68 %	88 %	22 %	21 %

References

1. J. W. Lee, *Metrologia*, 2022, **59**, 065010.
2. J. W. Lee, M. C. Lim, Y. Lim, G. B. Tegegn and K.-S. Lee, *Anal. Bioanal. Chem.*, 2024, **416**, 475-486.