

# **Substituting HF by HBF<sub>4</sub> - An optimized digestion method for multi elemental sediment analysis via ICP-MS/MS**

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# Electronic Supplemental

**Table A1** Quantified elements, their analyzed *m/z*, as well as used detection modes.

<b>Element</b>	<b><i>m/z</i> (Q1)</b>	<b><i>m/z</i> (Q2)</b>	<b>cell mode</b>
Be		9	No Gas
Mg	24	24	H <sub>2</sub>
Al	27	27	H <sub>2</sub>
P	31	47	O <sub>2</sub>
K	39	39	H <sub>2</sub>
Ca		40	H <sub>2</sub>
Sc	45	61	O <sub>2</sub>
Ti	47	63	O <sub>2</sub>
V	51	67	O <sub>2</sub>
Cr		52	He
Mn	55	55	H <sub>2</sub>
Fe	56	56	H <sub>2</sub>
Co		59	He
Ni		60	He
Cu		63	He
Zn		66	He
Ga		71	He
As	75	91	O <sub>2</sub>
Rb		85	No Gas
Sr		88	He
Zr	90	106	O <sub>2</sub>
Mo	95	127	O <sub>2</sub>
Ag		107	He
Cd	111	111	H <sub>2</sub>
Sb		121	He
Te		125	No Gas
Cs		133	No Gas
Ba		137	He
La		139	No Gas
Ce		140	No Gas
Pr		141	No Gas
Nd		146	No Gas
Sm		147	No Gas
Eu		153	No Gas
Gd		157	No Gas
Tb		159	No Gas
Dy		163	No Gas
Ho		165	No Gas
Er		166	No Gas
Tm		169	No Gas
Yb		172	No Gas
Lu		175	No Gas

W	182	214	O <sub>2</sub>
Tl		205	He
Pb		208	No Gas
Bi		209	He
Th		232	He
U		238	He

**Table A2** Typical instrument settings and operating conditions for ICP-MS/MS measurements using the Agilent 8800.

<b>Instrument configurations and settings</b>				
Sample Introduction	Double-pass spray chamber			
Nebulizer	Self aspirating PFA MicroFlow (ESI)			
Interface cones	Nickel			
RF power	1550 W			
Carrier gas flow	1.12 L min <sup>-1</sup>			
Make-up gas flow	0.11 L min <sup>-1</sup>			
Used cell gases	He, O <sub>2</sub> , H <sub>2</sub>			

  

<b>Lens parameters</b>	<b>No Gas</b>			
	<b>Gas</b>	<b>He</b>	<b>H<sub>2</sub></b>	<b>O<sub>2</sub></b>
Extract 1	0 V	0 V	0 V	0 V
Extract 2	-180 V	-180 V	-180 V	-180 V
Omega Bias	-95 V	-95 V	-95 V	-95 V
Omega Lens	8 V	8 V	8 V	8 V
Q1 Entrance	0 V	-4 V	0 V	2 V
Q1 Exit	-3 V	-13 V	-6 V	-2 V
Cell Focus	0 V	5 V	4 V	5 V
Cell Entrance	-40 V	-50 V	-50 V	-50 V
Cell Exit	-50 V	-60 V	-60 V	-60 V
Deflect	13 V	-3 V	-5 V	3 V
Plate Bias	-50 V	-60 V	-60 V	-60 V

  

<b>Cell parameters</b>				
Cell gas flow	none	4.5 mL min <sup>-1</sup>	6.0 mL min <sup>-1</sup>	30%
OctP Bias	-8 V	-18 V	-18 V	-5 V
OctP RF	130 V	190 V	200 V	190 V
Energy Discrimination	5 V	5 V	0 V	-7 V