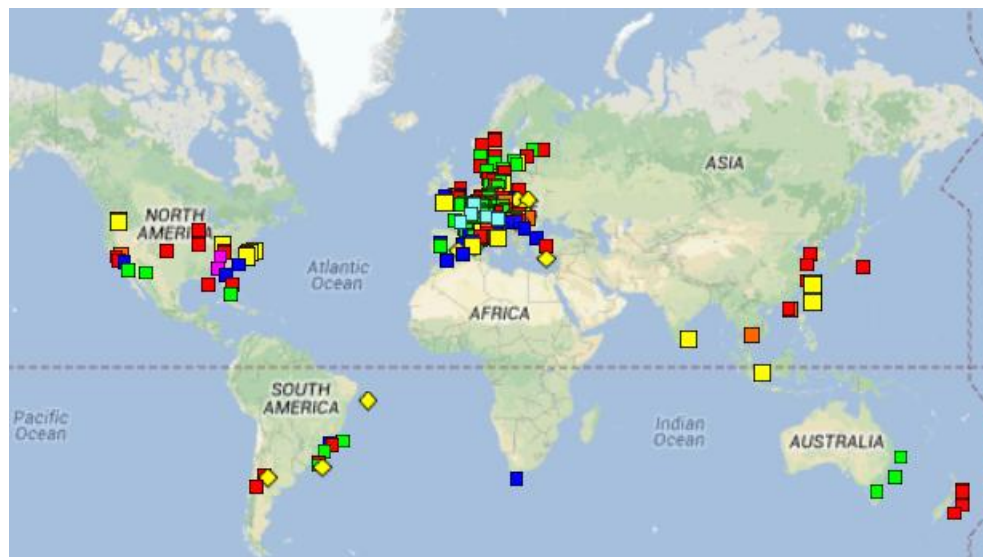


# Metal analysis of ground- and high matrix waters using ICP-MS

**Eurofins Analytico**

Wim Proper

- **Introduction Eurofins**
- **Method / Instrument setup**
- **Instrument performance**
- **MassHunter software**
- **Results evaluation (LIMS link)**



■ AGROSCIENCE | ■ ENVIRONMENT | ■ FOOD | ■ GENOMICS | ■ PHARMA | ■ PRODUCT TESTING | ◆ SERVICE CENTRES



## Company Overview

Eurofins Scientific is an international life sciences company which provides a unique range of analytical testing services to clients across multiple industries. The Group is the world leader in food and pharmaceutical products testing. It is also number one in the world in the field of environmental laboratory services, and one of the global market leaders in agrosience, genomics and central laboratory services.

## Short History

Eurofins Scientific was founded in 1987 with 10 employees. Today the Eurofins Group is a leading provider of analytical services with:

- an international network of over **180** laboratories across **35** countries in Europe, the USA, Asia and South America
- **over 14,000** staff
- a portfolio of over **100,000** reliable analytical methods
- more than **80 million** assays performed each year.



■ AGROSCIENCE | ■ ENVIRONMENT | ■



## Company Overview

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## Eurofins | Analytico

Barneveld (NL)

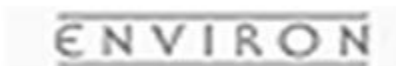


**Environmental samples like water,  
soil, waste water, ...**

**NEN-EN-ISO 17025**

**2x ICP-OES and 5x ICP-MS**

**(Agilent Partnerlab ICP-MS)**



- Nebulizer choice
- TDS dependency
- Interferences (C, Cl, Ca, ...)
- Selectivity
- Method validation (MDL, RSD%, REC%, linearity).



## NEN-EN-ISO 17294-2:

### 5 Interferences

#### 5.1 General

In certain cases, isobaric and non-isobaric interferences may occur. The most important interferences in this respect are coinciding masses and physical interferences from the sample matrix. For more detailed information, refer to ISO 17294-1.

Common isobaric interferences are given in Table 2 (for additional information see ISO 17294-1). In order to detect these interferences, it is recommended that several different isotopes of an element be determined. All the results should be similar. If they are not, mathematical correction is then necessary if, for a given element, there is no isotope which can be measured without interferences.

Small drifts or variations in intensities should be corrected by the application of the reference-element technique. In general, in order to avoid physical and spectral interferences, the mass concentration of dissolved matter (salt content) shall not exceed 2 g/l.



Feature▼ Type▶	Concentric (std. glass)	Concentric (PFA low flow)	Cross-Flow	High Solids (e.g. Burgener)
Aerosol Efficiency	Good	Excellent	Moderate	Fair
Ability for Ultra-Low Liquid Uptake (<200uL/min)	No	Yes	No	No
Dissolved Solids Tolerance	Moderate	Moderate-poor	Good	Good
Un-dissolved Solids (particulates) Tolerance	Poor	Poor	Moderate	Good
Self-Aspiration	Yes	Yes	Yes	No
HF Resistant	No	Yes	Usually	Yes (typically)
Use for Organic Solvents?	Yes	Most	Yes	No

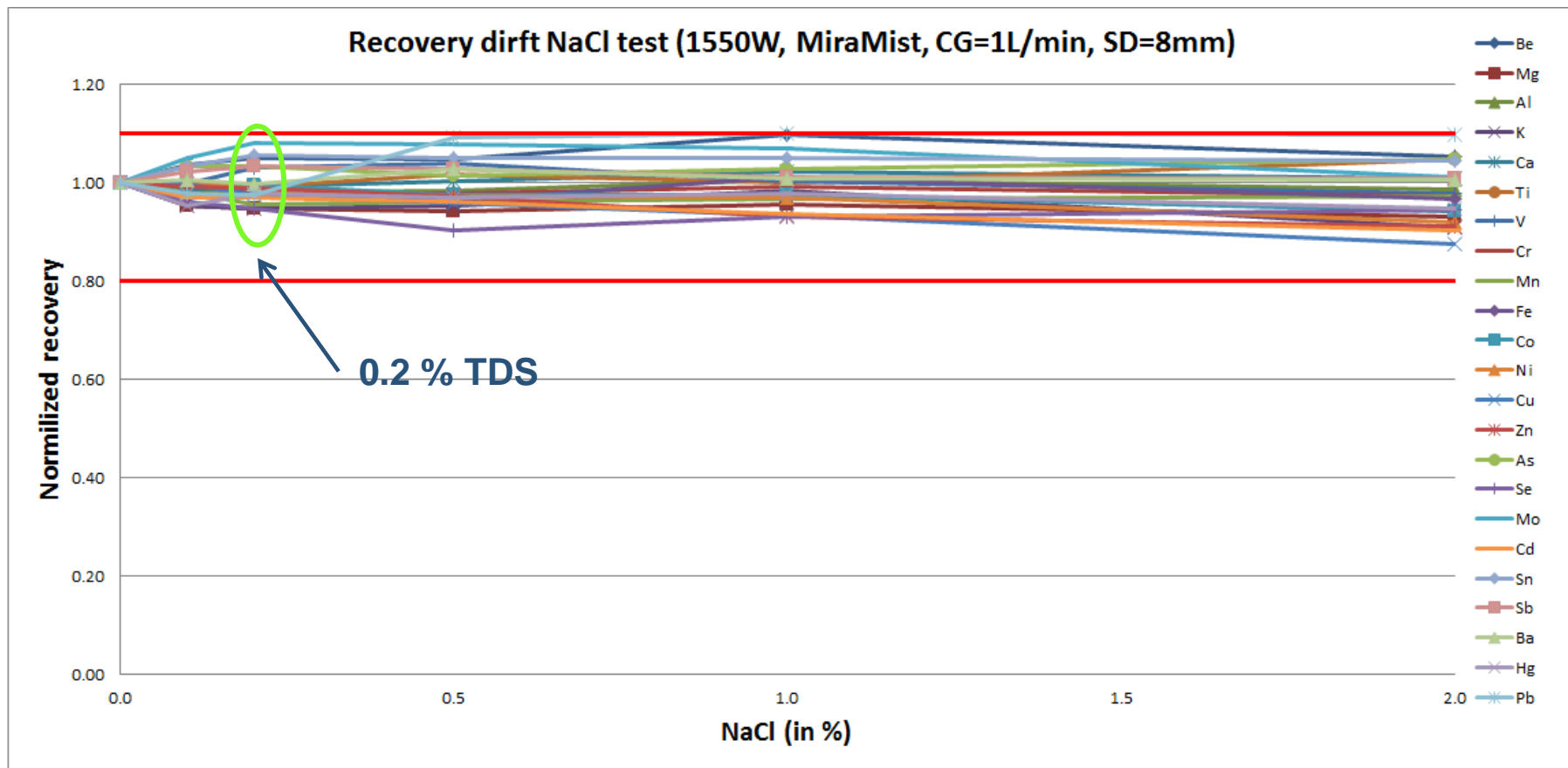


Standard Micro Mist



Mira Mist

# Method / Instrument setup (TDS)



# Method / Instrument setup (interference)



— analytico®

ISO 17294-1:2004(E)

## Annex A (informative)

### Spectral interferences, choice of isotopes and method detection limits for quadrupole ICP-MS instruments

Table A.1 — Spectral interferences, choice of isotopes and method detection limits for quadrupole ICP-MS instruments

Element	Isotope	Abundance %	Method detection limit <sup>a</sup> µg/l	Theoretical interferences		Interference with practical relevance		Best usable isotopes	
				Inter-element	Polyatomic ions	Preference	Reason	Preference	Reason
Ag	107	51,8	1	—	ZrO, YO	<sup>81</sup> Zr/ <sup>107</sup> Ag	x	least interference	
	109	48,2	1	—	ZrO, ZrOH, NbO	—	—	—	
Al	27	100	5	—	BeO, BO, CN, HCN	—	x	—	
As	75	100	1	<sup>5m</sup> 2 <sup>+</sup> , <sup>5l</sup> 2 <sup>+</sup> , <sup>5n</sup> 2 <sup>+</sup>	ArCl, CoO, Ar <sub>2</sub> H, Ar <sub>3</sub> , CaO <sub>2</sub> , NaClAr, CPO <sub>2</sub> , CaCl	<sup>45</sup> Ar/ <sup>75</sup> As	x	—	
Au	197	100	0,5	—	HfO, TaO	—	x	—	
	B	10	19,9	10	—	—	x	free of interference, low background	
Ba	11	80,1	10	—	BH	—	—	—	
	135	6,6	3	—	—	—	—	—	
	137	11,2	3	—	—	—	x	highest abundance, least interference	
Be	9	100	0,5	—	—	—	x	—	
	10	100	0,5	—	—	—	x	—	
Ca	43	0,14	100	S <sup>2+</sup>	MgO, BO, AlO, CaH, CNO, CO <sub>2</sub>	S <sup>2+</sup>	x	low background, least interference	
	44	2,1	50	S <sup>2+</sup>	CaH, MgO, AlO, BO, CNO, SiO, CO <sub>2</sub> , N <sub>2</sub> O	S <sup>2+</sup> , <sup>12</sup> C/ <sup>44</sup> Ca	x	lowest detection limit	
Cd	111	12,8	0,5	—	MoO, MoOH, ZrOH, K <sub>2</sub> O <sub>2</sub>	<sup>81</sup> Zr/ <sup>111</sup> Cd, <sup>90</sup> Mo/ <sup>111</sup> Cd	—	—	
	113	12,2	0,5	In	MoO, ZrOH, Ca <sub>2</sub> O <sub>2</sub> H, Al <sub>2</sub> O <sub>3</sub> , H <sub>2</sub> O	In, <sup>113</sup> Mo/ <sup>113</sup> Cd	x	for high Sn	
	114	28,7	0,3	Sn	MoO, MoOH, RuO	Sn, <sup>114</sup> Mo/ <sup>114</sup> Cd	x	lowest detection limit, least interference	
Ce	140	86,5	0,1	—	—	—	x	—	
Co	59	100	0,2	Sr <sup>2+</sup>	CaO, CaOH, MgCl, Ar <sub>2</sub> Ne, ArOH, ArF	<sup>43</sup> Ca/ <sup>59</sup> Co	x	—	
Cr	52	83,8	1	—	SO, ArO, ArC, Ar <sub>2</sub> N, ClO, HClO, ClN, ArNH	<sup>45</sup> Ar/ <sup>52</sup> Cr	x	for low Cr and high Cl	
	53	9,5	5	—	HBO, ArC, HClO, ClO, ArOH, Ar <sub>2</sub> N, ArNH, SO	<sup>53</sup> Cl/ <sup>53</sup> Cr	x	for high Cr and low Cl	
Cs	133	100	0,1	—	RuO <sub>2</sub>	—	x	—	

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ISO 17294-1:2004(E)

continued

Isotopic ions	Interference with practical relevance	Best usable isotopes	
		Preference	Reason
D, PO <sub>2</sub> , ArNa, I, NaCa, CaOH, NH, NiCl, ClO	<sup>47</sup> Ti/ <sup>110</sup> Na, <sup>49</sup> Ar/ <sup>23</sup> Na	x	for low Na and TI, lowest detection limit
O, PO <sub>2</sub> , SO <sub>2</sub> , H, ArMg, CaOH, N <sub>2</sub> H, S <sub>2</sub> , COCl	<sup>47</sup> Ti/ <sup>110</sup> Na, <sup>49</sup> Ar/ <sup>23</sup> Na, <sup>49</sup> Ar/ <sup>23</sup> Mg	x	for medium Mg, S and TI and high Na
NdO, SmO	—	x	—
SmO, NdO	—	x	—
BaO	—	—	—
BaO	—	x	—
IO, ArO, ArN, ArOH, SO, ClO	ArN Cr	x	abundance and background determine choice
D, ArO, ArOH, Ar <sub>2</sub> N, CaOH, CaOH, MgO, ArF	<sup>40</sup> Ar/ <sup>101</sup> H, <sup>40</sup> Ca/ <sup>101</sup> H	x	—
ArF, VO, ArS, SO <sub>2</sub> , S <sub>2</sub>	Be <sup>2+</sup>	—	—
CO <sub>2</sub> , ArCl, SO <sub>2</sub> , ArS, CrO	—	x	least interference
PhO, LaO, BF	—	x	least interference
IO, PhO, NaO	Dy	—	—
VO, Cl <sub>2</sub> , Ar <sub>2</sub>	Se	x	—
IO, DyO, ErO	—	x	—
WO	<sup>186</sup> W/ <sup>186</sup> W	—	—
WO	<sup>186</sup> W/ <sup>186</sup> W	x	least interference from WO
WO	<sup>186</sup> W/ <sup>186</sup> W	—	—
SmO	—	x	—
RuO	Sn	x	—
HfO, LuO	—	x	—
ArH	—	x	—
—	—	x	—
—	—	x	—
—	—	x	—
GdO, TbO	Hf	—	—
IO, NaH, C <sub>2</sub>	—	x	lowest detection limit, least interference
BeO, C <sub>2</sub> , C <sub>2</sub> H	—	—	—
BO, CN, C <sub>2</sub> H <sub>2</sub> , C <sub>2</sub> H	—	x	for higher Mg concentrations
ArN, ClO, NaS, Br, ArNH, KO, N, ArO, ArF	ArNH	x	—
ArO, BrO	—	—	—
BrO, K <sub>2</sub> O	Ru	x	lowest detection limit

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A.1 (continued)

Polyatomic ions	Interference with practical relevance	Best usable isotopes	
		Preference	Reason
LiO	—	x	—
BeO, RuO <sub>2</sub>	—	x	—
CaO, ArO, CaN, NaCl, MgS, CaOH, S <sub>2</sub> , ArOH	Fe	x	for low Fe
CaO, CaOH, MgCl, NiCl	<sup>44</sup> Ca/ <sup>40</sup> Ca	x	least interference
CaOH, NiCl	<sup>44</sup> Ca/ <sup>40</sup> Ca, <sup>48</sup> Ca/ <sup>40</sup> Ca	—	—
SiH, NO, NOH, N <sub>2</sub> H, CO, COH	NO	x	—
PIO	—	x	sum of 206, 207 and 208
YO	—	x	sum of 206, 207 and 208
PIO	—	x	sum of 206, 207 and 208
YO, ArCu	—	—	—
MoO, ZrO	Cd	x	—
—	—	x	—
HfO	—	x	—
—	—	x	—
TmO, ErO	—	x	least interference
TmO, YbO	Os	x	highest abundance
SrO, ArCl, RbO	—	x	—
ArH, NiCl	—	—	—
SiO	Pd	x	lowest detection limit, least interference
O <sub>2</sub> , BH, MOH, O <sub>2</sub> H	O <sub>2</sub>	x	—
PhO	—	x	least interference
ZrO	Te	—	—
CO, SiO, BO, AlO, CaH, ClO, CaCl, Cl <sub>2</sub> , Ar <sub>2</sub> , ArCl	<sup>110</sup> Ti/ <sup>110</sup> Ca, <sup>208</sup> Pb/ <sup>110</sup> Ca	x	—
Ar <sub>2</sub> , CaCl, ArCl	<sup>40</sup> Ar/ <sup>37</sup> Cl	x	for low Cl
Ar <sub>2</sub> H, BH, CO <sub>2</sub> , SO <sub>2</sub> , Ar <sub>2</sub> H, ArCl	K <sub>2</sub> , <sup>78</sup> Br/H	x	for low Br
CO, N <sub>2</sub> , SO, SiH, ArH, COH, N <sub>2</sub> H	—	x	—
RuO <sub>2</sub>	—	x	—
MoO, RuO, PdO	—	x	least interference
RuO, PdO	Te	—	—
RbH	—	—	—
—	—	x	lowest detection limit, least interference

1 (continued)

Polyatomic ions	Interference with practical relevance	Best usable isotopes	
		Preference	Reason
NdO, PrO	—	x	—
—	—	x	least interference
PdO	Xe	x	lowest detection limit
—	—	x	—
IO <sub>2</sub> , PO, SO, ClCl, NH, SiOH, Sn, N <sub>2</sub> , NO <sub>2</sub> H	<sup>31</sup> P/ <sup>10</sup> P	x	least interference
VO, ClO, SO, NO <sub>2</sub> , PO, Sn, N <sub>2</sub> , C <sub>2</sub>	Ca, <sup>32</sup> S/ <sup>16</sup> O	—	—
SOH	<sup>32</sup> S/ <sup>16</sup> O/H	—	—
WO, ReO, WHO	—	—	—
—	—	x	lowest detection limit, least interference
—	—	x	—
—	—	x	—
HfO, ClO, ClN, ArH, ArC, ArN, Sn, SO	<sup>36</sup> Cl/ <sup>36</sup> Cl	x	—
HoO, DyO, ErO	—	x	least interference
ErO, YbO	Cs	—	—
—	—	x	—
DyO, SmO, GdO	—	x	least interference
DyO, GdO	Hf	—	—
O, CaO, PO <sub>2</sub> , SO <sub>2</sub> , Cl, S <sub>2</sub> , Ph <sub>2</sub> H, Ar <sub>2</sub> , ArMg	Ni, <sup>63</sup> Ni/ <sup>60</sup> Ni, <sup>32</sup> S/ <sup>16</sup> S, <sup>40</sup> Ar/ <sup>20</sup> Ar	—	—
IO, VO, SO <sub>2</sub> , PCl, FeC, S <sub>2</sub> , SO <sub>2</sub> H	<sup>31</sup> P/ <sup>10</sup> P, <sup>34</sup> S/ <sup>16</sup> S	x	for medium TI and S
O, ClO <sub>2</sub> , SO <sub>2</sub> , TiO, rS, FeN, PCl, FeC, S <sub>2</sub> , Ar <sub>2</sub> , ArS	Be <sup>2+</sup> , <sup>40</sup> Ar/ <sup>20</sup> Ar	x	for low Be and Si
—	—	x	—

end-independent spectral interferences and relate to matrix element concentration  
a) variation of individual abundances

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# Method / Instrument setup (interference)

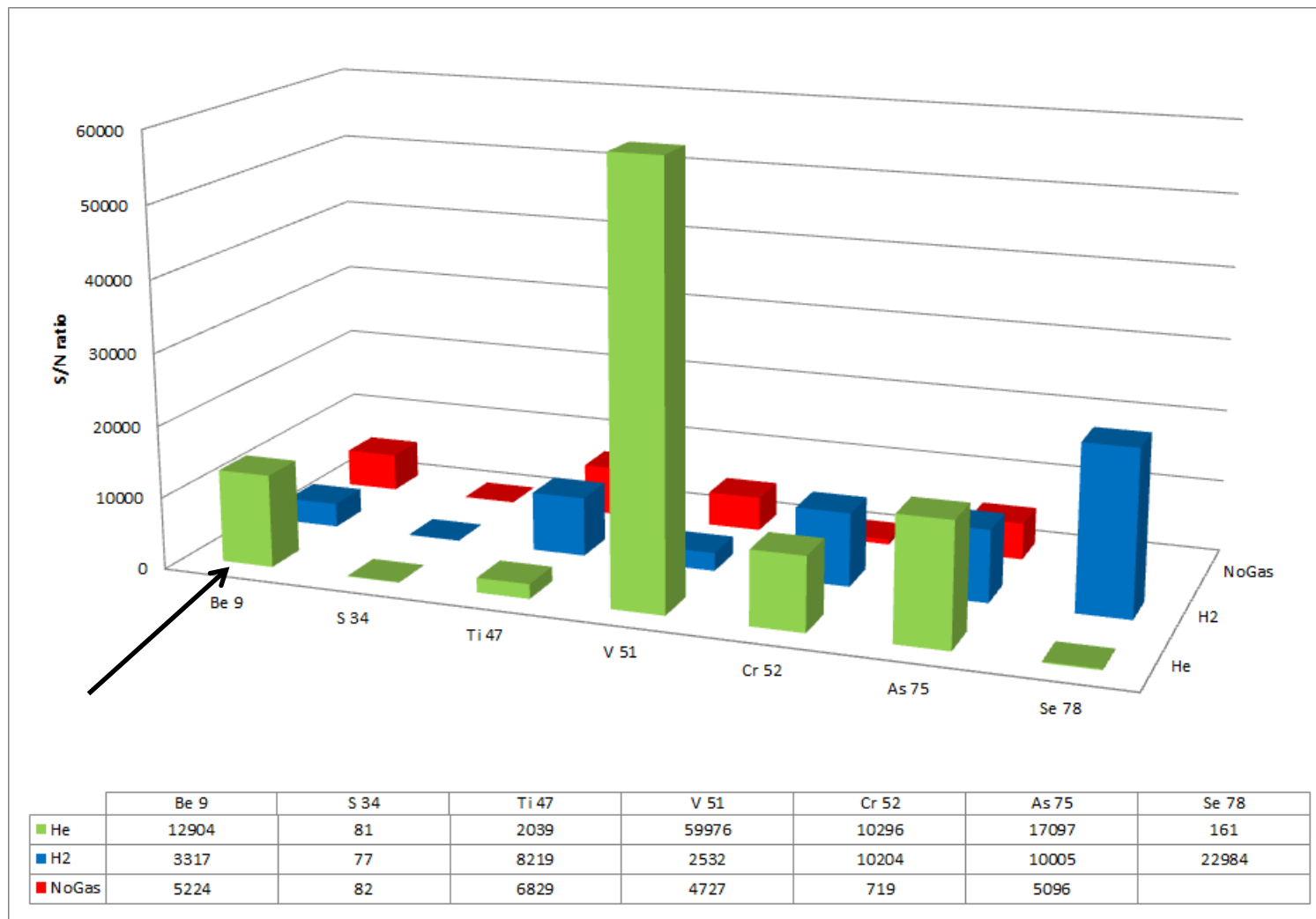
Element	Isotope	Abundance %	Method detection limit <sup>a</sup> µg/l	Theoretical interferences		Interference with practical relevance	Best usable isotopes	
				Inter-element	Polyatomic ions		Preference	Reason
Cu	63	69,2	1	—	TiO, PO <sub>2</sub> , ArNa, MgCl, NaCa, CaOH, ArCNH, NCCI, ClO	<sup>47</sup> Ti <sup>16</sup> O, <sup>40</sup> Ar <sup>23</sup> Na	x	for low Na and Ti, lowest detection limit
	65	30,8	2	Pb <sup>2+</sup>	TiO, PO <sub>2</sub> , SO	<sup>49</sup> Ti <sup>16</sup> O	y	for medium Mg, S

CI 10000mg/L (NaCl)									
		Results				Interference?	Lowest	In or decrease %	
Element	Unit	Reporting limit	He-mode	H2-mode	Nogas-mode	(ISO17294-2)			
Na / 23	mg/L	0.1	6028.13	6700.05	>				
V / 51	µg/L	1	1.33	40.82	94.02	Y	He	98.6	
Cr / 53	µg/L	1	3.66	269.34	264.69	Y	He	98.6	
Cu / 63	µg/L	5	0.52	18.73	87.48	Y	He	99.4	
As / 75	µg/L	3	0.27	1.26	96.84	Y	He	99.7	
Se / 77	µg/L	0.5	5.13	0.27	689.48	Y	H2	100.0	
Se / 78	µg/L	0.5	0.61	0.05	25.26	Y	H2	99.8	

Reaction gas flow: He 4.0 mL/min and H2 4.0 mL/min

In total 25 interference solutions were measured (like C, Cl, W, ... incl mixed)

# Method / Instrument setup (S/N)



# Method / Instrument setup (Overview)

ICP-MS Top - ANA.QCC / G\_WATER.M

Instrument AcquireData DataAnalysis Methods Sequence Chained Sequence Tools Offline Tools Run Information Help

Method G\_Water.m — C:\ICPMH1\METHODS\ Sequence w17do7.S — C:\ICPMH1\SEQUENCE\

ICP-MS Acquisition - G\_WATER.M / 10MINSTR.D

Spectrum (Multi Tune) Acquisition Parameters

Step 1 Step 2 Step 3

Tune File: start\_he.u h2.u he.u

Stabilization Time: 5 [sec] 30 [sec] 30 [sec]

Mass Elem.	Detector	per Point	per Mass	per Point	per Mass	per Point	per Mass
6 Li	Auto	...	...	...	...	0.50	1.5
7 Li	Auto	...	...	...	...	0.10	0.30
9 Be	Auto	...	...	...	...	0.50	1.5
13 C	Auto	...	...	...	...	0.010	0.030
23 Na	Auto	...	...	...	...	0.10	0.30
24 Mg	Auto	...	...	...	...	0.10	0.30
26 Mg	Auto	...	...	...	...	0.10	0.30
27 Al	Auto	...	...	...	...	0.10	0.30
31 P	Auto	...	...	...	...	0.10	0.30
34 S	Auto	...	...	...	...	0.10	0.30
35 Cl	Auto	...	...	...	...	0.10	0.30
39 K	Auto	...	...	...	...	0.10	0.30
40 Ca	Auto	...	...	0.10	0.30	...	...
44 Ca	Auto	...	...	0.10	0.30	...	...
45 Sc	Auto	...	...	0.10	0.30	0.10	0.30
47 Ti	Auto	...	...	0.10	0.30	0.10	0.30

Integration time: per Point: 0.500 [sec] ( 500.00 [msec])

Detector: Auto

Acquisition Time: Repetition: 3

Number of Masses: 71

AMU Select File: DEFAULT.AMU

Show Interference Equation

Periodic Table Mass Scale

Clear All Mass Table OK Cancel Help

ICP-MS	7500ce
Nebulizer	Burgener MiraMist
RF Power	1550 W
Sampling Depth	8.0 mm
Carrier gas	1.0 L/min
KED voltage	3 V
He flow rate	4 mL/min
H2 flow rate	4 mL/min

## Calibration ranges:

- 0 – 2 µg/L Hg
- 0 – 250 µg/L Ag
- 0 – 500 µg/L Li, B, Be, Ti, V, Cr, **Mn\***, Ni, Co, Cu, Zn, As, **Se\***, Sr, Mo, Cd, Sn, Sb, Te, Ba, Tl, Pb
- 0 – 1 mg/L Br, Zr, W
- 0 – 50 mg/L Na, **Fe\***, K, **Ca\***, Al, Mg
- 0 – 100 mg/L C, Cl, P, S

\* ) Measured in Hydrogen mode

- **Method detection limit**  
(level between 1 – 3x required reporting limit)
- **Reproducibility**  
(low level, high level and NIST 1640)
- **Recovery**  
(same as reproducibility)
- **Linearity and working range**

Artificial ground water was used

# Method validation (MDL)

## Method detection limit according AS3000 regulation

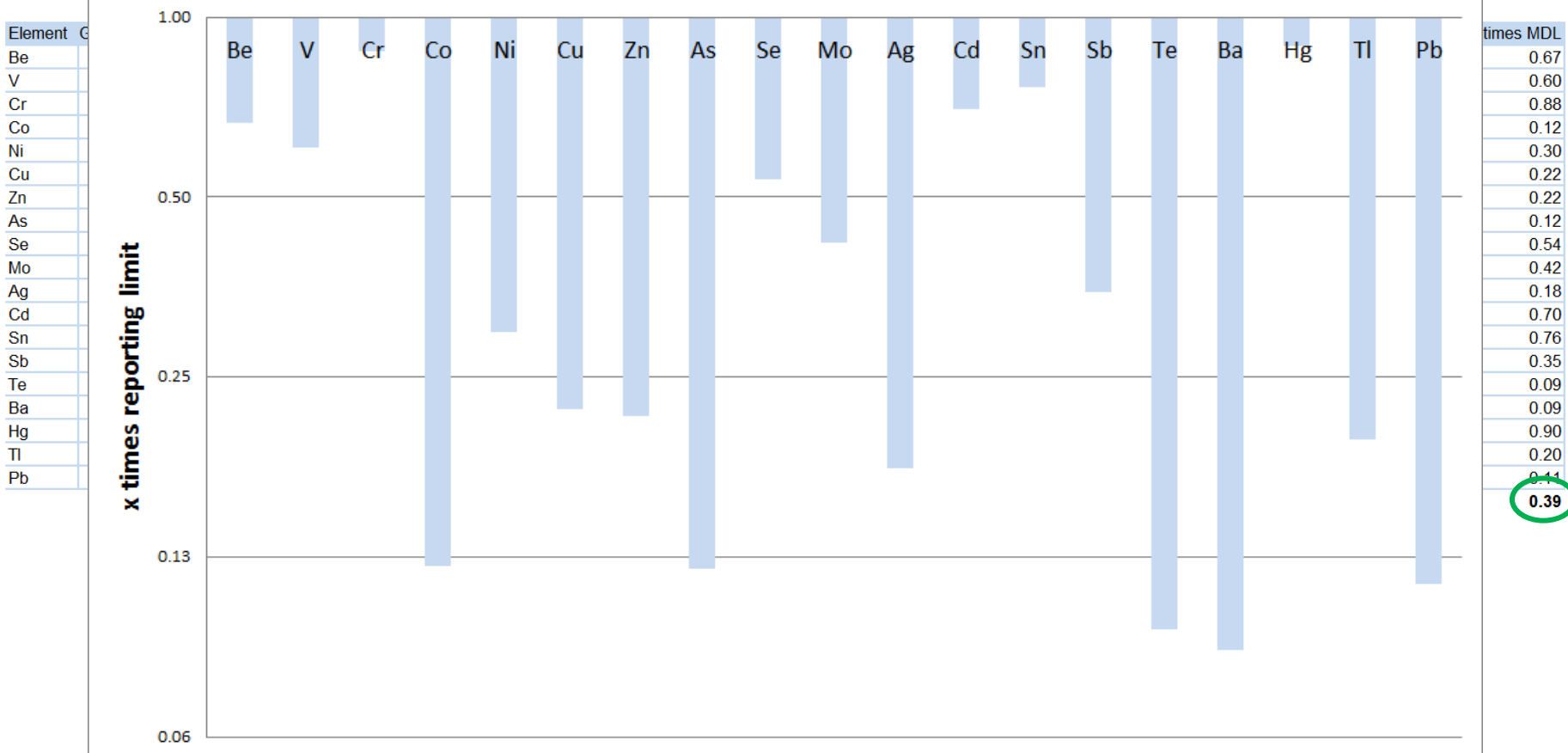
Results in µg/L

Element	GW_MDL_01	GW_MDL_02	GW_MDL_03	GW_MDL_04	GW_MDL_05	GW_MDL_06	GW_MDL_07	GW_MDL_08	GW_MDL_09	GW_MDL_10	Conc	MDL (3σ)	MDL_required	x times MDL
Be	0.964	1.083	1.244	1.212	1.015	1.048	0.958	0.900	1.095	0.983	1.050	0.333	0.5	0.67
V	3.981	3.928	4.186	3.888	3.732	3.714	3.549	3.610	3.749	3.587	3.792	0.603	1	0.60
Cr	3.148	2.822	2.985	3.537	2.934	2.758	2.645	2.802	3.122	3.434	3.019	0.878	1	0.88
Co	9.432	9.559	9.873	9.234	9.352	9.495	9.258	9.547	9.197	9.362	9.431	0.603	5	0.12
Ni	24.841	28.063	26.222	24.758	25.889	25.733	25.215	25.927	25.169	24.824	25.664	2.974	10	0.30
Cu	9.950	10.432	10.638	10.082	10.040	10.299	10.085	10.338	9.708	9.362	10.093	1.104	5	0.22
Zn	26.451	28.116	28.189	27.921	27.394	26.922	23.548	28.490	26.860	26.344	27.023	4.307	20	0.22
As	5.100	4.934	5.097	5.180	4.934	5.108	4.881	4.951	5.129	5.227	5.054	0.357	3	0.12
Se	0.583	0.510	0.677	0.433	0.450	0.387	0.420	0.431	0.471	0.417	0.478	0.268	0.5	0.54
Mo	2.761	2.455	2.665	2.362	2.468	2.408	2.322	2.399	2.439	2.374	2.465	0.419	1	0.42
Ag	25.198	21.637	21.534	21.388	22.037	21.633	21.531	21.641	21.479	21.129	21.921	3.522	20	0.18
Cd	1.991	2.078	2.193	2.047	2.049	2.013	1.962	2.042	2.051	1.490	1.992	0.560	0.8	0.70
Sn	2.183	1.983	2.085	1.771	1.494	2.292	1.903	2.134	2.254	1.757	1.986	0.764	1	0.76
Sb	0.665	0.501	0.597	0.529	0.515	0.495	0.471	0.509	0.534	0.499	0.531	0.173	0.5	0.35
Te	46.098	46.024	49.898	47.826	46.756	47.570	47.339	48.696	48.944	48.465	47.762	3.788	40	0.09
Ba	26.826	25.754	27.092	26.842	26.606	26.855	26.691	26.582	25.863	26.368	26.548	1.308	15	0.09
Hg	0.107	0.122	0.089	0.103	0.098	0.110	0.121	0.127	0.084	0.091	0.105	0.045	0.05	0.90
Tl	24.739	24.169	25.068	23.750	24.122	23.586	23.551	23.523	22.984	23.211	23.870	1.969	10	0.20
Pb	24.302	23.958	24.568	23.565	23.701	23.938	23.624	24.162	23.355	23.631	23.880	1.129	10	0.11
														0.39



# Method validation (MDL)

Method detection limit vs reporting limit (1 means M.D.L. = R.L.)

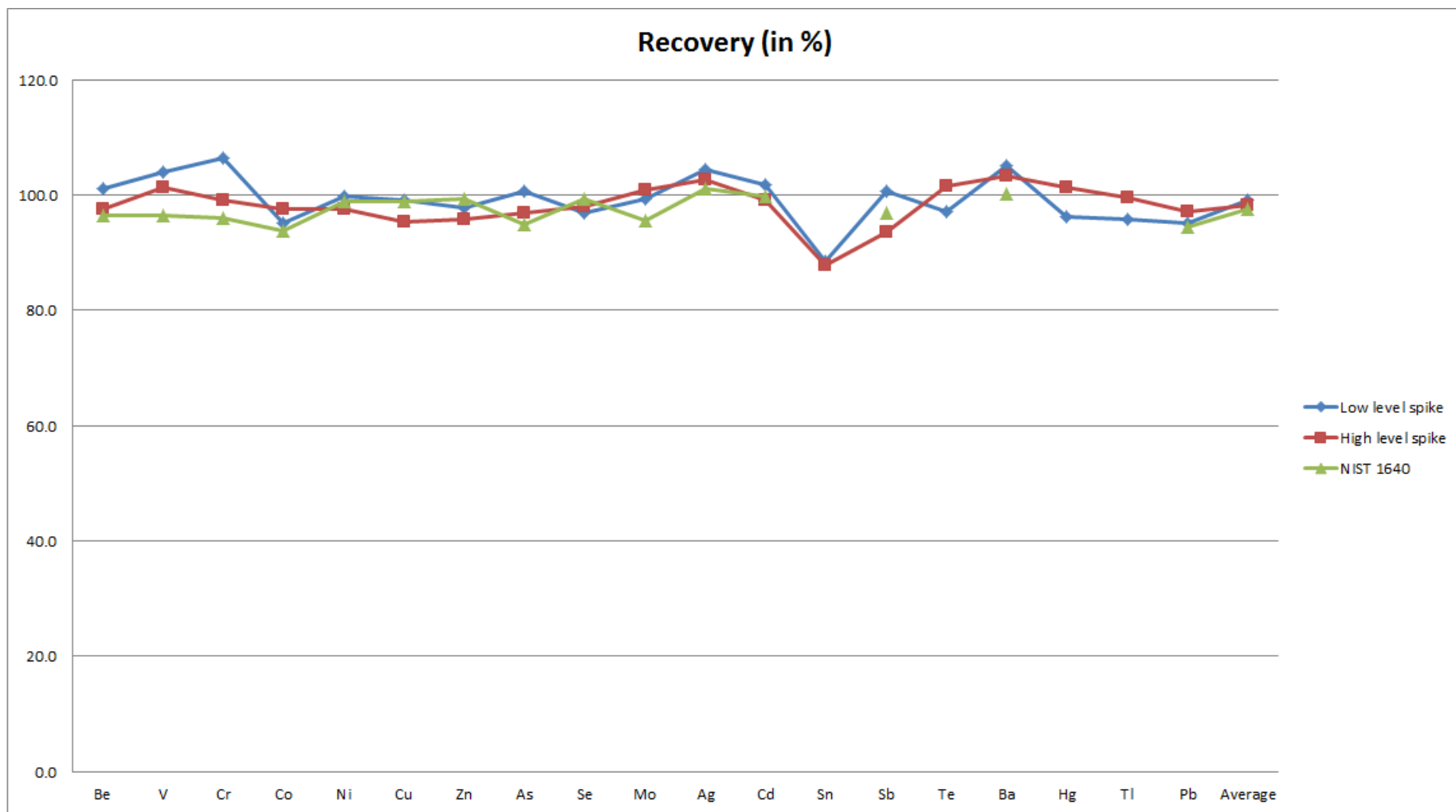


# Method validation (precision and recovery)

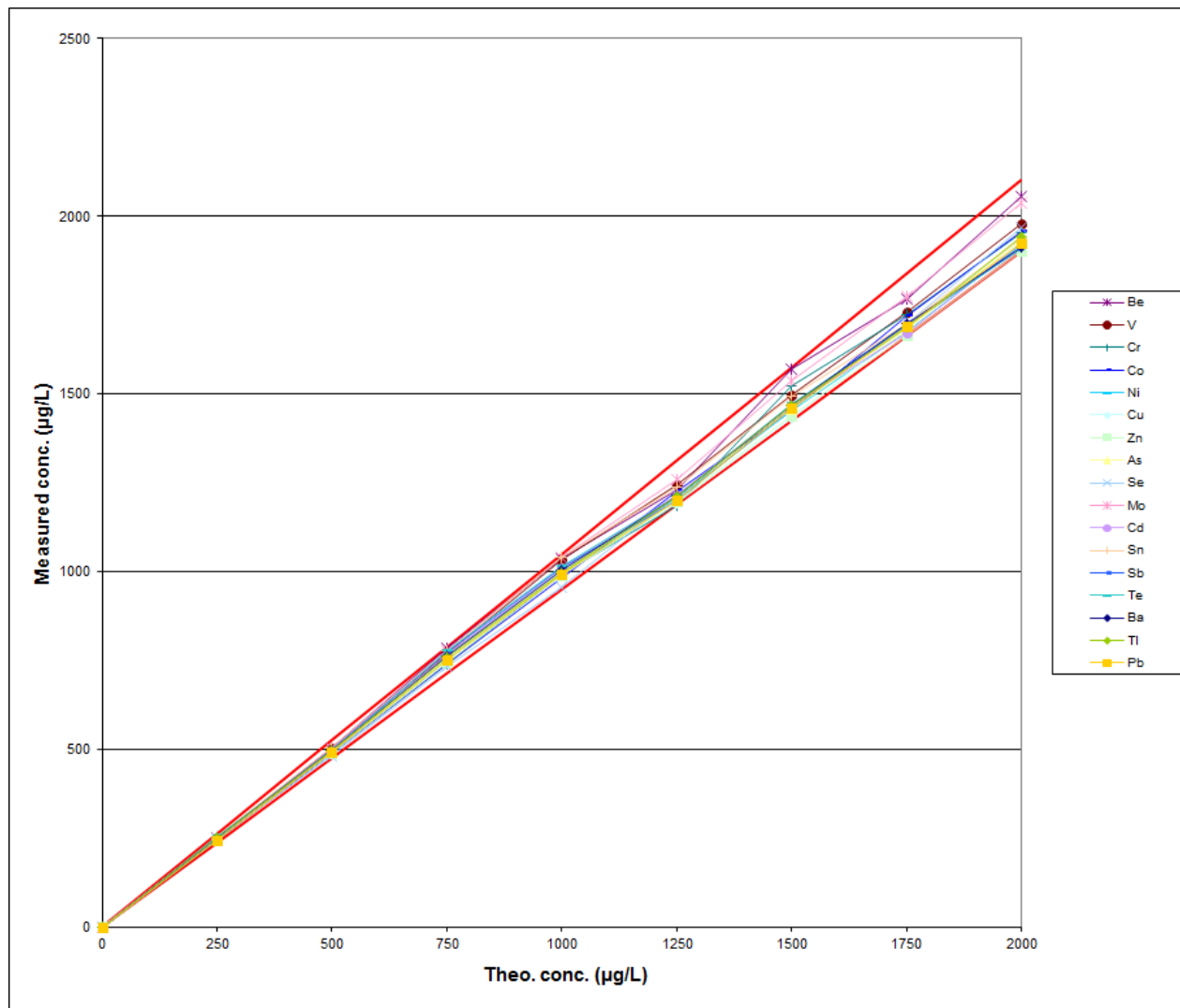


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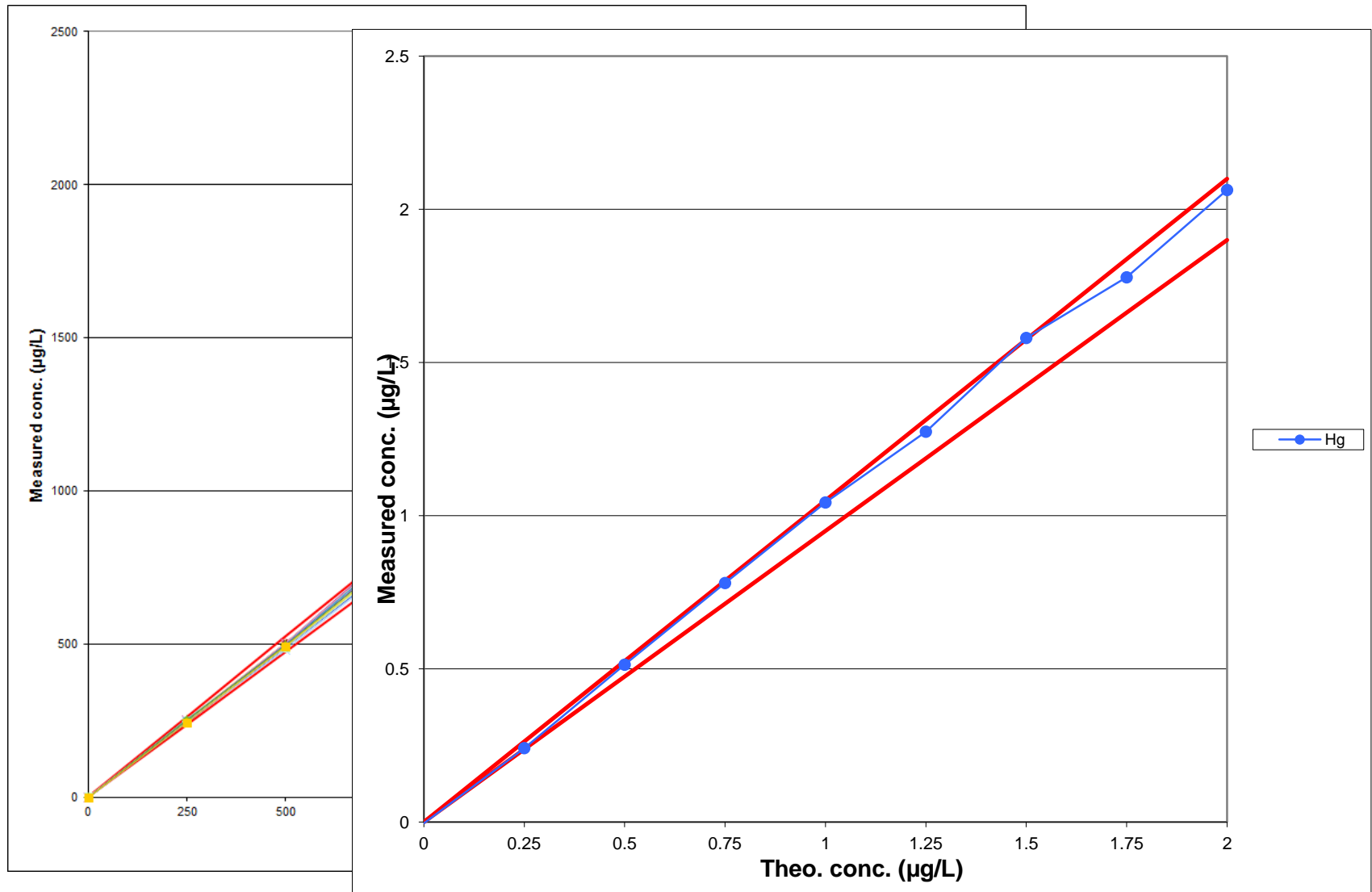
Element	Low level spike			High level spike			NIST 1640		
	Spike added (µg/L)	Reproducibility CV%	Recovery %	Spike added (µg/L)	Reproducibility CV%	Recovery %	Concentration (µg/L)	Reproducibility CV%	Recovery %
Be	20.2	3.3	101.2	97.6	3.7	97.6	33.7	2.9	96.4
V	20.8	2.9	104.0	101.4	3.2	101.4	12.5	2.1	96.5
Cr	21.3	2.5	106.4	99.1	2.5	99.1	37.0	2.0	96.0
Co	19.0	2.5	95.1	975.6	1.8	97.6	19.0	1.5	93.7
Ni	99.8	2.3	99.8	975.5	2.1	97.5	27.1	1.5	98.9
Cu	19.8	2.2	99.2	95.2	2.5	95.2	84.2	1.8	98.8
Zn	97.8	2.0	97.8	958.8	2.5	95.9	52.9	3.1	99.4
As	20.1	2.6	100.7	96.9	1.6	96.9	25.3	1.7	94.9
Se	19.4	4.9	96.9	979.2	3.7	97.9	21.8	3.4	99.2
Mo	19.9	2.3	99.4	1008.1	1.7	100.8	44.7	1.8	95.5
Ag	52.2	2.0	104.4	102.7	1.8	102.7	7.7	2.6	101.2
Cd	20.4	2.3	101.8	99.1	2.3	99.1	22.7	1.7	99.7
Sn	17.7	3.3	88.4	87.9	2.5	87.9			
Sb	20.1	3.1	100.7	93.5	7.3	93.5	13.4	1.4	96.8
Te	97.2	2.3	97.2	1014.9	2.1	101.5			
Ba	105.1	1.7	105.1	1033.2	1.4	103.3	148.2	1.5	100.1
Hg	0.5	7.5	96.3	2.0	7.5	101.3			
Tl	95.7	2.2	95.7	994.9	1.4	99.5			
Pb	95.1	2.0	95.1	972.1	1.4	97.2	26.4	1.8	94.5
Average		2.8	99.2		2.8	98.2		2.0	97.4



# Method validation (Linearity 5% rule)

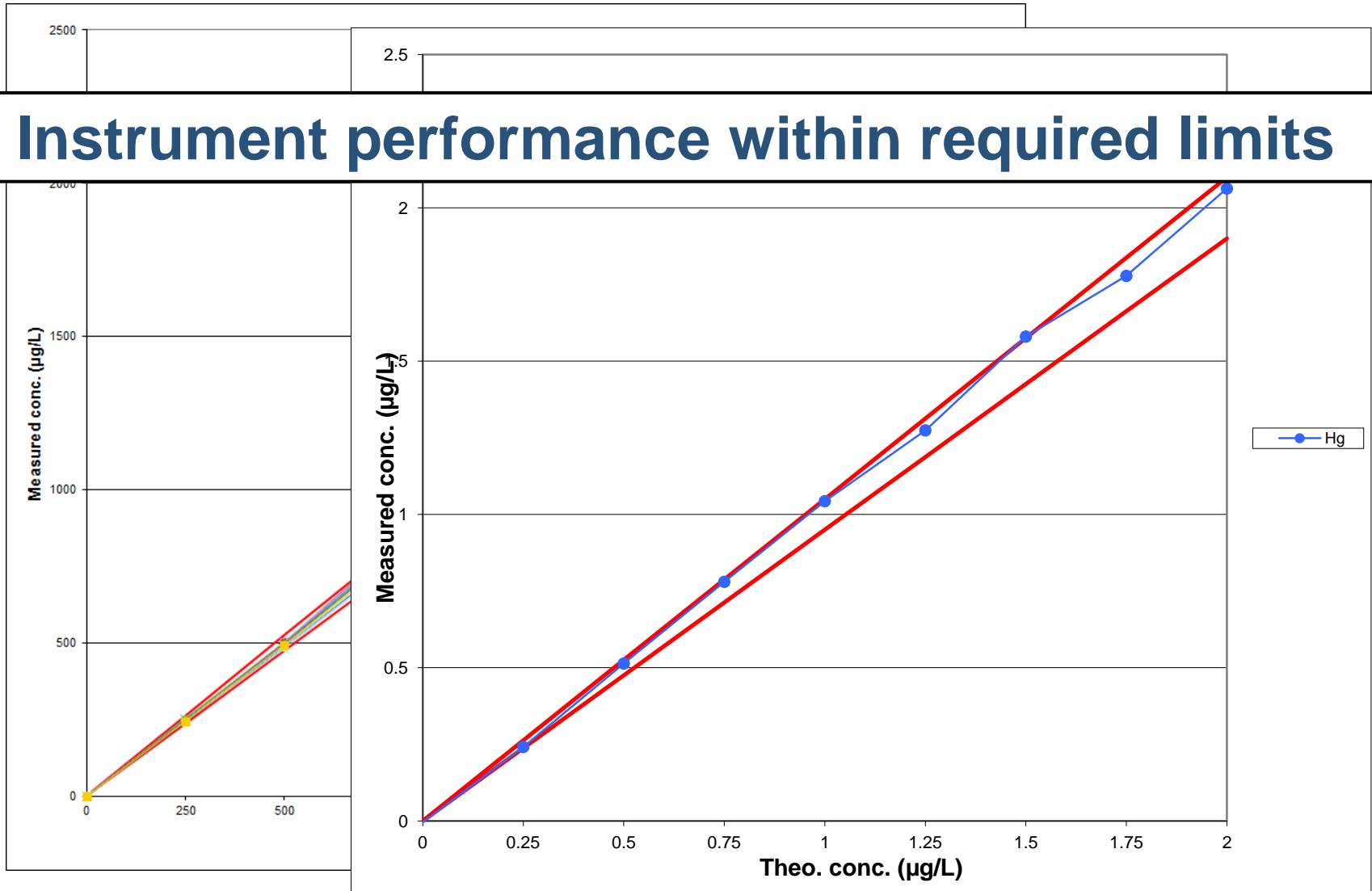


# Method validation (Linearity 5% rule)



# Method validation (Linearity 5% rule)

**Instrument performance within required limits**



# Running samples (sequence)

Edit Sample Log Table - G\_Water.S

SMPL Configure Columns...

	Method	Type	Vial	Data File	Sample	Comment	Dil/Lvl	ISTD Conc	on	Skip	LC/G Vial
1	THODSVG_Water.M	Blanco	1101		Blank water		1.000				
2	THODSVG_Water.M	Sample	1102		1st Line control		1.000				
3	THODSVG_Water.M	Sample	1103		LOF		1.000				
4	THODSVG_Water.M	Sample	1104		LOF 10vv		1.000				
5	THODSVG_Water.M	Sample	1105	6821628	6821628	20 Mo Onbekend	1.000				
6	THODSVG_Water.M	Sample	1106	6821915	6821915	20 Ba,Cd,Co,Cu,Hg,Mo,Ni,Pb,Zn Onbekend	1.000				
7	THODSVG_Water.M	Sample	1107	6821914	6821914	20 Ba,Cd,Co,Cu,Hg,Mo,Ni,Pb,Zn Onbekend	1.000				
8	THODSVG_Water.M	Sample	1108	6821913	6821913	20 Ba,Cd,Co,Cu,Hg,Mo,Ni,Pb,Zn Onbekend	1.000				
9	THODSVG_Water.M	Sample	1109	6823318	6823318	20 Ba,Cd,Co,Cu,Hg,Mo,Ni,Pb,Zn Onbekend	1.000				
10	THODSVG_Water.M	Sample	1110	6820993	6820993	20 Ba,Cd,Co,Cu,Hg,Mo,Ni,Pb,Zn Onbekend	1.000				
11	THODSVG_Water.M	Sample	1111	6821627	6821627	20 Mo Onbekend	1.000				
12	THODSVG_Water.M	Sample	1112	6821625	6821625	20 As,Ba,Be,Cd,Co,Cr,Cu,Hg,Mo,Ni,Pb,Sb,Se,Sn,V,Zn Onbekend	1.000				
13	THODSVG_Water.M	Sample	1201	6821624	6821624	20 Mo Onbekend	1.000				
14	THODSVG_Water.M	Sample	1202	6822039	6822039	20 As,Ba,Cd,Co,Cu,Hg,Mo,Ni,Pb,Zn Onbekend	1.000				
15	THODSVG_Water.M	Sample	1203	6821626	6821626	20 As,Ba,Be,Cd,Co,Cr,Cu,Hg,Mo,Ni,Pb,Sb,Se,Sn,V,Zn Onbekend	1.000				
16	THODSVG_Water.M	Sample	1204	6821629	6821629	20 Mo Onbekend	1.000				
17	THODSVG_Water.M	Sample	1205	6821964	6821964	20 As,Ba,Cd,Co,Cu,Hg,Mo,Ni,Pb,Zn Onbekend	1.000				
18	THODSVG_Water.M	Sample	1206	6821630	6821630	20 Mo Onbekend	1.000				
19	THODSVG_Water.M	Sample	1207	6820987	6820987	20 Ba,Cd,Co,Cu,Hg,Mo,Ni,Pb,Zn Onbekend	1.000				
20	THODSVG_Water.M	Sample	1208	6816744	6816744	12 As,Cd,Cr,Cu,Hg,Ni,Pb,Zn Onbekend	1.000				
21	THODSVG_Water.M	Sample	1209	6816745	6816745	12 As,Cd,Cr,Cu,Hg,Ni,Pb,Zn Onbekend	1.000				
22	THODSVG_Water.M	Sample	1210	6817908	6817908	12 Pb Onbekend	1.000				
23	THODSVG_Water.M	Sample	1211	6817907	6817907	12 Pb Onbekend	1.000				
24	THODSVG_Water.M	Sample	1212	6817910	6817910	12 Pb Onbekend	1.000				
25	THODSVG_Water.M	Sample	1301	6817909	6817909	12 Pb Onbekend	1.000				
26	THODSVG_Water.M	Sample	1302	6817911	6817911	12 Pb Onbekend	1.000				
27	THODSVG_Water.M	Sample	1303	6818529	6818529	12 Al,As,Ba,Ca,Cd,Cr,Cu,Fe,Hg,K,Mg,Mn,Na,Ni,P,Pb,Sb,Se,Zn Onbek	1.000				
28	THODSVG_Water.M	Sample	1304	6819541	6819541	12 Ba,Cd,Co,Cu,Hg,Mo,Ni,Pb,Zn Onbekend	1.000				
29	THODSVG_Water.M	Sample	1305	6818578	6818578	12 Ba,Cd,Co,Cu,Hg,Mo,Ni,Pb,Zn Onbekend	1.000				

Edit Sample Log Table - G\_Water.S

Periodic Block

	Block	Period	Unit	Reset
1	CCV	10	samples	QC_1
2	USER	40	samples	QC_6
3	ICS	40	samples	ICS
4				

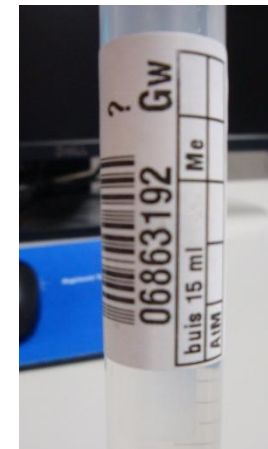
  

Import DA Method from Existing Batch  
 DA Method Only  DA method and Std Data

Source Data Batch Directory  
 C:\ICPMHYT\DATA\DaMeth\_A.BV DaMeth\_A.batch.xml Browse

Print OK Cancel Help

Sample: 6818578



**Water samples are filtered in the field and acidified with 0.5% HNO<sub>3</sub>. In the lab 0.6% HCl will be added to stabilize mercury.**

# Running samples (DA method)

Offline ICP-MS Data Analysis - (Method Editor) - w17d06

File Edit View Process DA Method Report Tools Global Help

DA Method Editor Process Batch Default Layout Conc Count Default Columns

Method Development Tasks

Method Table: QC Parameters

DA Method Task:

Sample Type	Analyte	ISTD (Method Name: IS)
1 Sample	Main Error1 Flag	Main Error Flag
2 CalBlk	LDB hoog	LDB hoog
3 CalStd		IS Fout

Report Template:

Action Failure		
Title	Action	#Allowed Failure
1st Error by ISTD check	NextSmpl	0
1st Error1 by QC check	NextSmpl	0
1st Error2 by QC check	NextSmpl	0

Advanced Info

QC Parameters

Tune Step	Mass	Name	QC Check	Report	Main Criteria			
					RSD Min. CPB	LDR	Upper Error1 Lim.	Upper Error2 Lim.
56	3	137 Ba	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		2000	1	1
57	3	182 W	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		10	1	1
58	3	200 Hg	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		2	1	1
59	3	201 Hg	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		2	1	1
60	3	202 Hg	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		2	1	1
61	3	203 Tl	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		2000	1	1
62	3	205 Tl	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		2000	1	1
63	3	206 Pb	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		2000	1	1
64	3	207 Pb	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		2000	1	1
65	3	208 Pb	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		2000	1	1
66	1	220	<input type="checkbox"/>	<input checked="" type="checkbox"/>			1	1

ISTD (Method Name: IS)								
Tune Step	Mass	Name	QC Check	Report	Main Criteria			
					Lower Exp.	Lower Error Lim.	Upper Exp.	Upper Error Lim.
1	3	6 Li	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
2	2	45 Sc	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
3	3	45 Sc	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
4	2	74 Ge	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
5	3	74 Ge	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
6	3	103 Rh	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
7	3	193 Ir	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25

66 Analytes - 7 ISTD



# Running samples (DA method)

Offline ICP-MS Data Analysis - (Method Editor) - w17d6

File Edit View Process DA Method Report Tools Global Help

Method Development Tasks

Method Table: QC Parameters

DA Method Task: [Icon]

Sample Type

Analyte	ISTD (Method Name : IS)
1 Sample	Main Error Flag
2 CalBlk	Main Error Flag
3 CalStd	QC Fout
4 Bkgnd	IS Fout

Report Template: [Dropdown]

Action Failure

Title	Action	#Allowed Failure
1st Error by ISTD check	NextSmpl	0
1st Error by QC check	NextSmpl	0

Method Development Tasks

- New
  - Reset DA Method
  - Import DA Method Only...
  - Import DA Method and Standard Data...
  - Import FQ Parameters from CS Cal...
- Set up Basic Information
  - Data Analysis Method
- Set up Analyte
  - Analyte List
- Set up Analysis Parameters
  - FullQuant
  - SemiQuant
  - Isotope Ratio
  - Advanced Info
    - FullQuant Outlier
    - QC Parameters**
    - Worklist Actions
- Validate/Return
  - Validate
  - Return to Batch at a Glance

Method Table: QC Parameters

Sample Type	Analyte	ISTD (Method Name : IS)
1	Sample	Main Error Flag
2	CalBlk	Main Error Flag
3	CalStd	QC Fout
4	Bkgnd	IS Fout
5	FQBlk	
6	SQBlk	
7	SQStd	
8	SQISTD	
9	IsoStd	
10	CICSpk	
11	DilStd	
12	DriRChk	
13	QC1	
14	QC2	
15	QC3	
16	BlkVrfy	
17	QC_1	
18	Blank	
19	1st Line	

Analyte

Tune Step	Mass	Name	QC Check	Report	RSD Min. CPS	Main Criteria			
						Lower Exp.	Lower Error Lim.	Upper Exp.	Upper Error Lim.
55	3	135 Ba	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		50	0.9	50	1.1
56	3	137 Ba	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		50	0.9	50	1.1
57	3	182 W	<input type="checkbox"/>	<input checked="" type="checkbox"/>					
58	3	200 Hg	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		1	0.9	1	1.1
59	3	201 Hg	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		1	0.9	1	1.1
60	3	202 Hg	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		1	0.9	1	1.1
61	3	203 Tl	<input type="checkbox"/>	<input checked="" type="checkbox"/>					
62	3	205 Tl	<input type="checkbox"/>	<input checked="" type="checkbox"/>					
63	3	206 Pb	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		50	0.9	50	1.1
64	3	207 Pb	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		50	0.9	50	1.1
65	3	208 Pb	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		50	0.9	50	1.1

ISTD (Method Name : IS)

Tune Step	Mass	Name	QC Check	Report	Lower Exp.	Lower Error Lim.	Upper Exp.	Upper Error Lim.
1	3	6 Li	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
2	2	45 Sc	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
3	3	45 Sc	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
4	2	74 Ge	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
5	3	74 Ge	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
6	3	103 Rh	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25
7	3	193 Ir	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	100	0.75	100	1.25

66 Analytes - 71STD

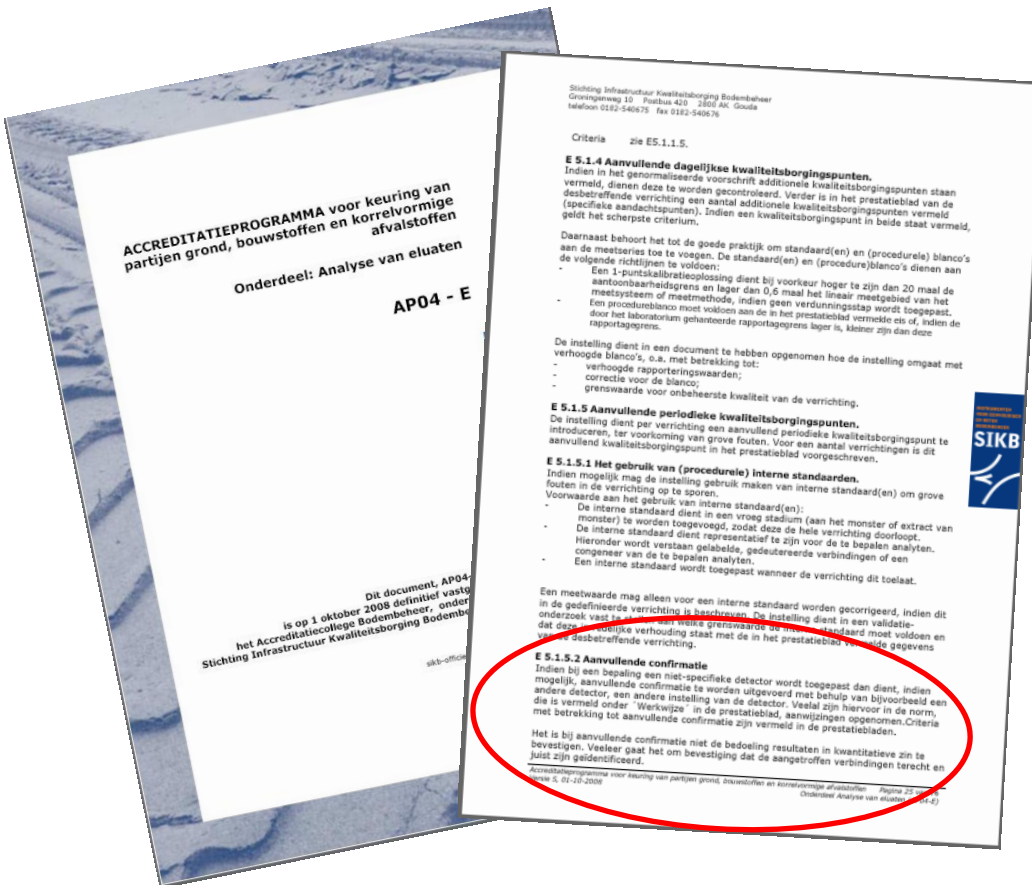


## Section E 5.1.5.2: Aanvullende confirmatie (Additional confirmation)

“If a non-specific detector is used, the result should, if possible, be confirmed using another detector, or a different setting of the detector.”

“Non-specific” refers to the fact that more than 1 ion may be present at each mass – i.e. the analyte measurement may be affected by the presence of interferences

“This additional confirmation is not intended to provide a second quantitative result. ***Rather it is confirmation that the compounds detected using the first measurement are correctly identified.***”



Dutch accreditation program  
AP-04 - regulated methods  
for soils and other materials

# Running samples (LIMS link)

**Protocol [X:\ICPMS\AGILENT7500CE\PROTOCOL\Agilent7500CE.MDB]**

File Options

Element: **Ni** Interferents **Result**

Report limit: 2 Blanc corr.: 0

RSD: 20 % Int. Std.: Ge 74 >...

Send results to LIMS Sorter: 4

Remarks:

**Interferencies Ni**

Mass	Element	Value
58	Fe	0.91
60	Ca	8892
60	Sn	3273
61	Ca	24
61	Ti	22479
61	Sn	905
62	Sn	2771

If all five conditions per mass are false, the mass will be included in the calculation of the average.

OK

- Blank check and correction
- CCV check 'in-line'
- ISTD check nebulization
- LDR check
- Isotope confirmation

# Running samples (LIMS link)

Processing ICP-MS data v2.1

Protocol [X:\ICPMS\AGILENT7500CE\PROTOCOL\Agilent7500CE.MDB]

File Options

Element:  Interferents

Report limit:  Blanc corr.:

RSD:  % Int. Std.:   >...

Send results to LIMS Sorter:

Remarks:

mass:	Result
58	
60	
61	
62	

Fr Ra Ac

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw

Interferents visible

Interferents visible

Mass: 61

Ca	>	24
Sn	>	905
	>	
	>	
	>	

Mass: 62

Ti	>	22479
Sn	>	2771
	>	
	>	
	>	

If all five conditions per mass are false, the mass will be included in the calculation of the average.

OK

# Running samples (LIMS link)

The screenshot shows a software window titled "Interferenties Ni" with a close button (X). It contains four panels for different mass values:

- Mass: 58**: Fe > 0.91
- Mass: 60**: Ca > 8892, Sn > 3273
- Mass: 61**: Ca > 24, Sn > 905
- Mass: 62**: Ti > 22479, Sn > 2771

In the background, another window titled "Processing ICP-MS data v2.1" is visible, showing a "Protocol" dropdown set to "X:\ICPMS\AGILENT 7500CE\PROTOCOL\Agilent7500CE.MDB". Below this, there are fields for "Element:", "Report limit: 2", "Blanc corr.: 0", "RSD: 20 %", "Int. Std.: Ge 74", and a checked box for "Send results to LIMS".

Element	Isotope	Abundance %	Method detection limit <sup>a</sup> µg/l	Theoretical interferences		Interference with practical relevance	Best usable isotopes	
				Inter-element	Polyatomic ions		Preference	Reason
Ni	58	68,1	1	Fe	CaO, ArO, CaN, NaCl, MgS, CaOH, Si <sub>2</sub> , ArOH	Fe	x	for low Fe
	60	26,2	3	—	CaO, CaOH, MgCl, NaCl	<sup>44</sup> Ca <sup>16</sup> O	x	least interference
	61	1,1	5	—	CaOH, ScO	<sup>44</sup> Ca <sup>16</sup> O <sup>1</sup> H, <sup>45</sup> Sc <sup>16</sup> O		—

# Running samples (LIMS link)

Processed

El	Eenheid	Gem conc.	Gem rsd	R	I	W	Q	B	LIMS
Cd	ug/l	0.1357	120.3697						VER
Cr	ug/l	9.5139	0	●					VER
Cu	ug/l	0.9905	12.0296						VER
Ni	ug/l	17.8403	0	●			●		VER
Pb	ug/l	-0.4359	5.2442						VER
Zn	ug/l	14.4245	2.6717	●					VER
Hg	ug/l	0.1583	0	●					VER
As	ug/l	25.3996	0						VER
Se	ug/l	5.481	65.3961	●					VER
Sb	ug/l	0.2619	10.1517						VER
Sn	ug/l	-0.3224	28.7756						VER
Ba	ug/l	193.953	0.1633						VER
Co	ug/l	8.0682	0						VER
Mo	mg/l	0.0007	84.8528						VER
Mn	mg/l	2.5542	0			●		●	VER
Ca	mg/l	1195.8921	2.1291	●	●	●		●	VER
Mg	mg/l	293.2472	0.4103			●		●	VER
Al	mg/l	0.0054	0						VER
Fe	mg/l	41.0951	1.5285						VER
Na	mg/l	598.0349	0			●		●	VER
K	mg/l	57.1115	0						VER
Ti	ug/l	4.2739	0	●	●	●		●	VER
V	ug/l	3.9917	0						VER

Nr	Omschrijving	Tijd	Rep	vv	Dilution
163	06821400	11:31 pm	3	1	1
164	06821401	11:36 pm	3	1	1
165	06821402	11:42 pm	3	1	1
166	06821403	11:47 pm	3	1	1
167	06821404	11:52 pm	3	1	1
168	06821405	11:57 pm	3	1	1
169	06821406	12:03 am	3	1	1
170	06821407	12:08 am	3	1	1

Gebruik	R	W	Q	B	Mas.	Conc.	RSD	Interferenties
●			●		58	52.2000	1.011	Fe>0.91
●					60	17.4500	5.720	Geen interferentie gevonden.
●					61	40.8200	12.398	Ca>24

Opmerkingen:

- Mn 55 LDB hoog
- Ca 40 LDB hoog
- Ca 44 LDB hoog
- Mg 24 LDB hoog
- Mg 26 LDB hoog
- Na 23 LDB hoog
- Ti 48 LDB hoog
- Sr 86 LDB hoog
- Sr 88 LDB hoog

# Running samples (LIMS link)

The screenshot displays the StarLIMS 9 software interface with the following components:

- Processed Table:** A list of elements and their concentrations. The value for Ni (17.8403) is highlighted with a red box.
- Certificaatgegevens Table:** A table with columns: Flag, Certificaatnr, Status, Validatiestatus, Spoedcode, ClientID, Contactpersoon. Row 1: 0, 2012068748, Active, 12, 2144, L. Ensing.
- Monstergegevens Table:** A table with columns: Monsternr, Status, Validatiestatus, Komm, Monsteromschrijving 1, Monsteromschrijving 2. Row 1: 6821405, Done, -, fors01-1-1 fors01 (-).
- Analyses Table:** A table with columns: Bottle, Reps, Profile#, Test Name, Status, Validatie, Serv. G, Instrument. Row 1: 1, 680, 1795, Vb Met. ex filt/aanz, Done, Released, 45, 82.
- Resultaten Table:** A table with columns: Analyte, Rapportage, Unit, Rapportage-naam, Resultaat, Norm1, Norm2, Rep, Status. Row 1: Ni, 18, µg/L, Nikkel (Ni), 17.8403, 1, Done, F.



- Proven method since 2004.
- Tuned with robust settings, high matrix samples can be measured.
- No need to correct for interferences, only isobaric overlay.
- Instrument performance within required limits (He / H<sub>2</sub> mode).
- Replaced ICP-OES + AAS + Hg analyzer.
- Fully implemented in the lab.

## Excellent work horse!