Elemental Scientific
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Automated Analysis of Environmental and Water Samples for Total Metals and Elemental Species

C. Derrick Quarles Jr., Patrick Sullivan, and Nick Bohlim

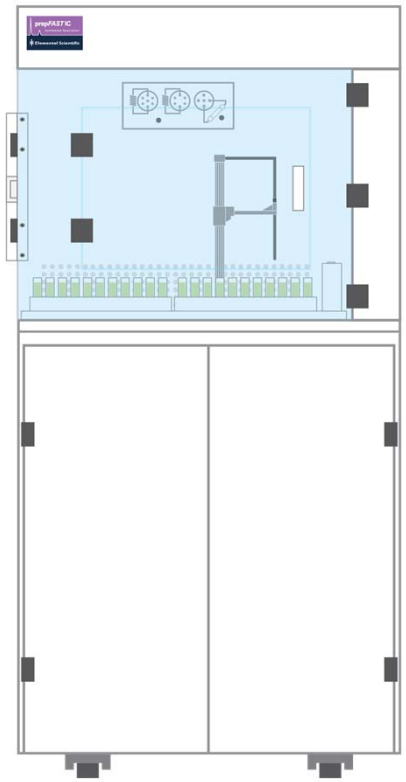
Elemental Scientific, Inc.

2021 NEMC, Metals Analysis and Remediation Session - August 10, 2021

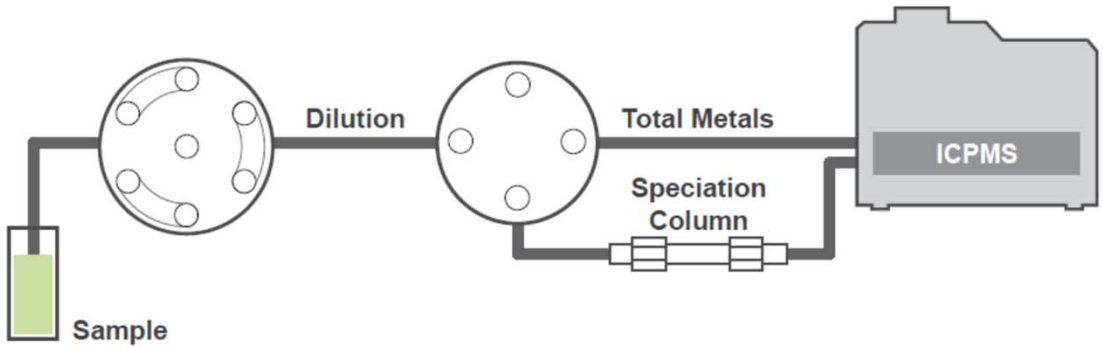
Goals

- Develop software that automates the elemental speciation of samples that exceed a set threshold during the total metals analysis.
- Utilize the ability of the prep*FAST* IC to operate in total metals (adopted 6020B EPA method) and speciation mode (chromium speciation) in combination with an ICPMS.
- Analyze samples from around the Omaha, NE, USA area for total metals and Cr speciation.

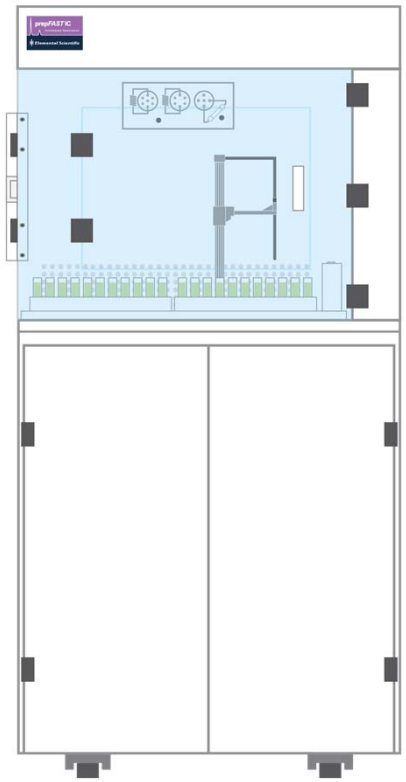
prep*FAST* IC



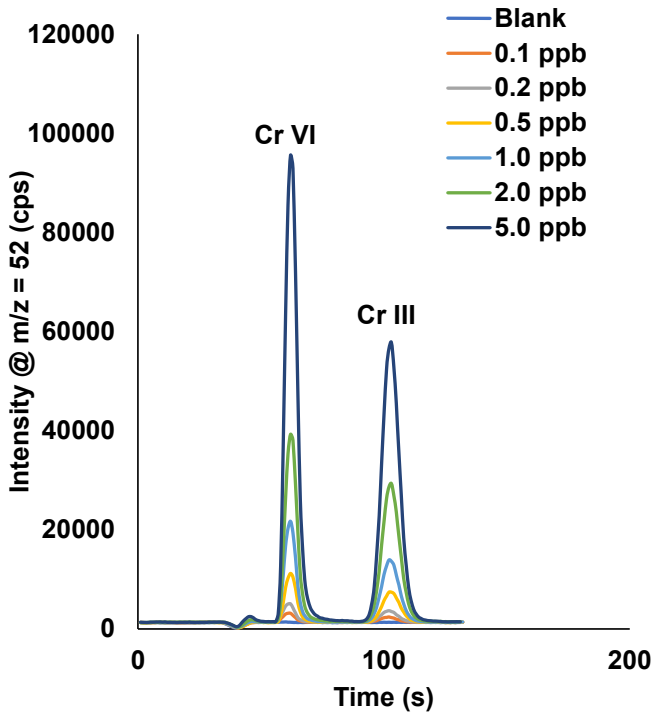
- Completely metal-free liquid and sample flow path from pump to nebulizer
- Inline autodilution and autocalibration functions
- Ability to operate in total metals or chromatography mode with a single instrument
- Syringe-driven, post-column standard addition, dilution, or derivatization
- Compatible with acids and organic solvents
- Micro-volume sampling (≥ 50 µL)
- Xceleri - full online control and data analysis software package



prep*FAST* IC - Metal Free



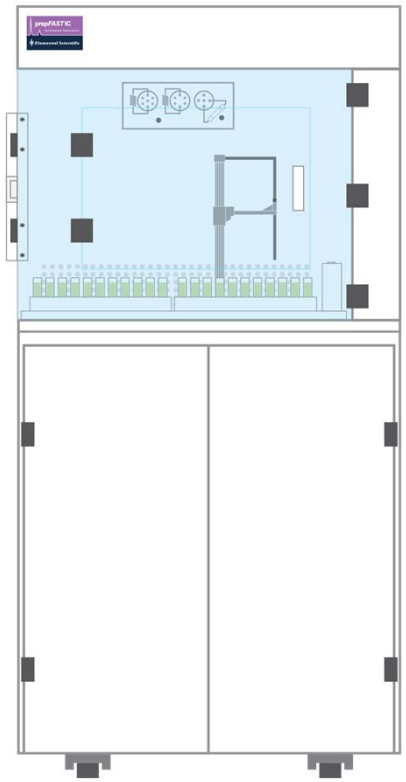
- Completely metal-free liquid and sample flow path from pump to nebulizer



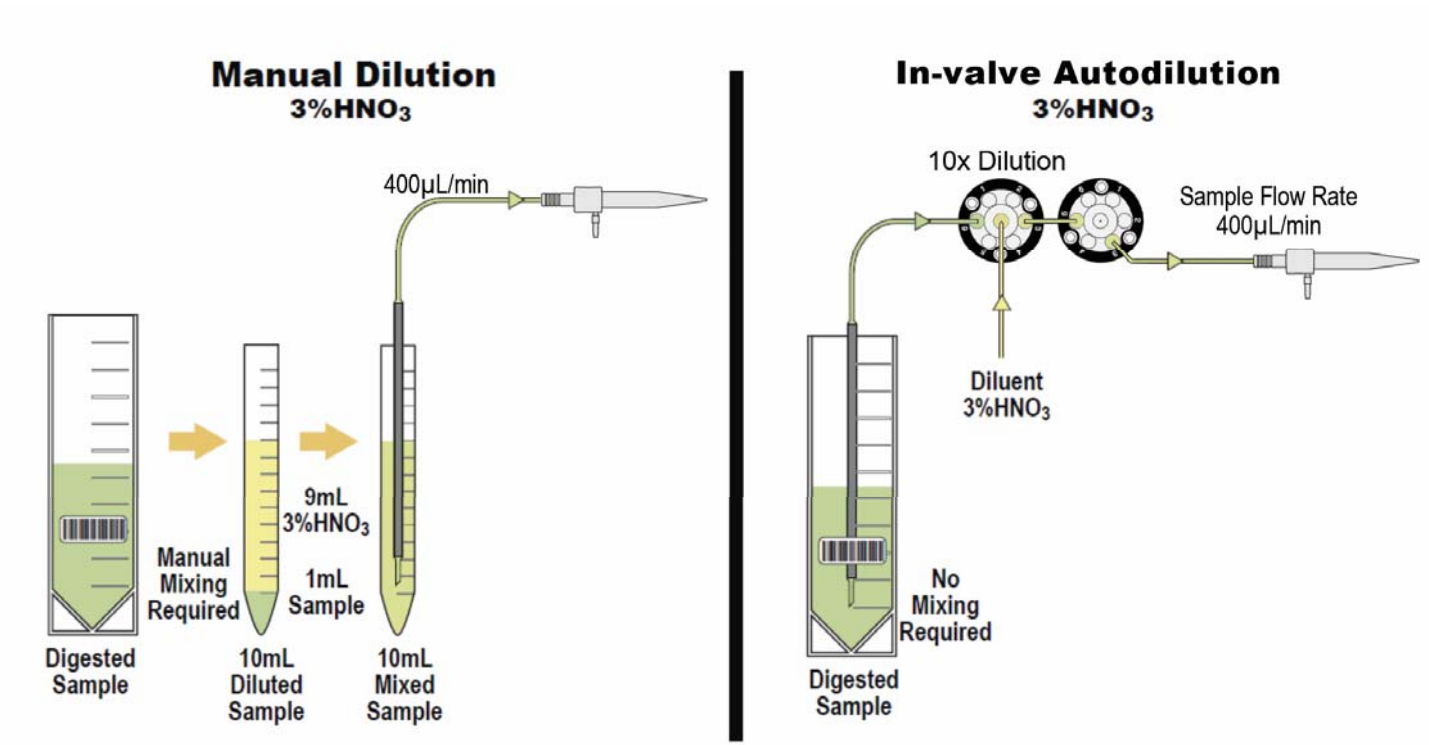
Improved LODs for Cr VI
- No metal components in prepFAST IC
- More suitable eluents for ICP plasma

	Cr VI	
	LOD	LOQ
HPLC + ICPMS	0.3 µg/L	1.0 µg/L
prepFAST IC + ICPMS	0.007 µg/L	0.023 µg/L

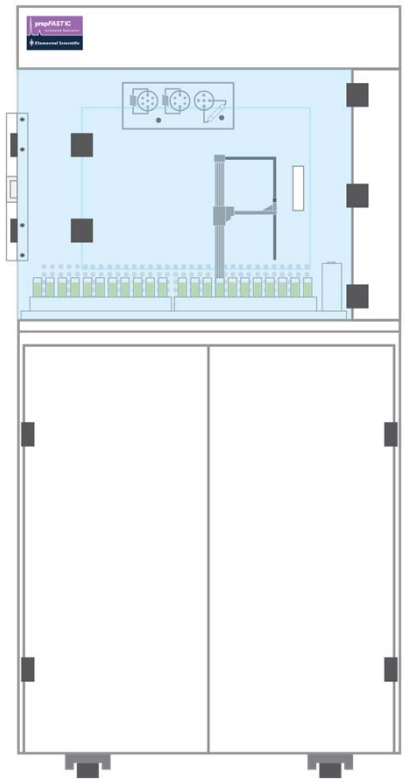
prep*FAST* IC - Inline Sample Preparation



- Inline autodilution and autocalibration functions



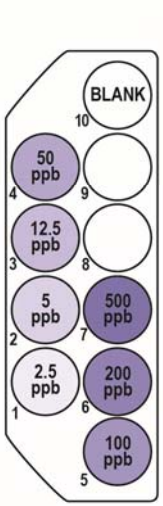
prep*FAST* IC - Inline Sample Preparation



- Inline autodilution and autocalibration functions

Conventional Calibration
(seven points)

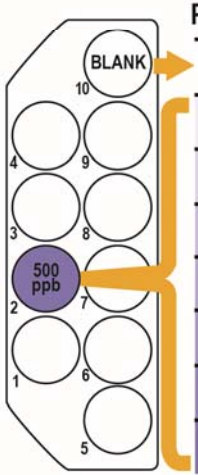
Offline Prep: 1 Blank + 7 Standards



STD Position	Concentration
10	0
1	2.5
2	5
3	12.5
4	50
5	100
6	200
7	500

prepFAST Autocalibration
(seven points)

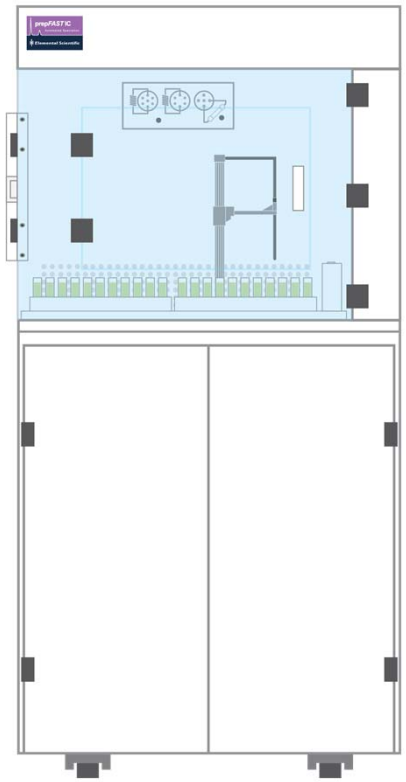
Inline Prep: 1 Blank + 1 Standard



STD Position	Inline Dilution Factor	Dilution Rate			Concentration
		Std	Diluent	Total	
10	200x	50	9950	10000	0
2	200x	50	9950	10000	2.5
2	100x	100	9900	10000	5
2	40x	250	9750	10000	12.5
2	10x	1000	9000	10000	50
2	5x	2000	8000	10000	100
2	2.5x	4000	6000	10000	200
2	1x	10000	0	10000	500

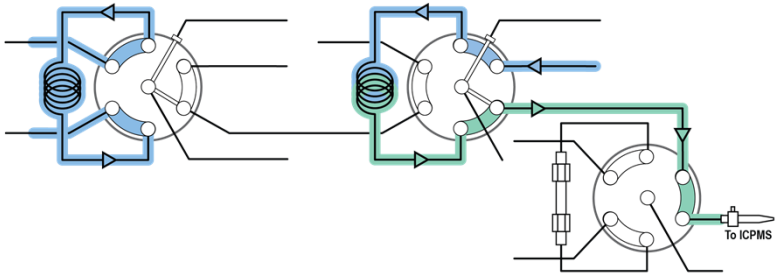
prep*FAST* Calibration: Blank can be analyzed diluted or undiluted.

prep*FAST* IC - Total Metals or Speciation Mode

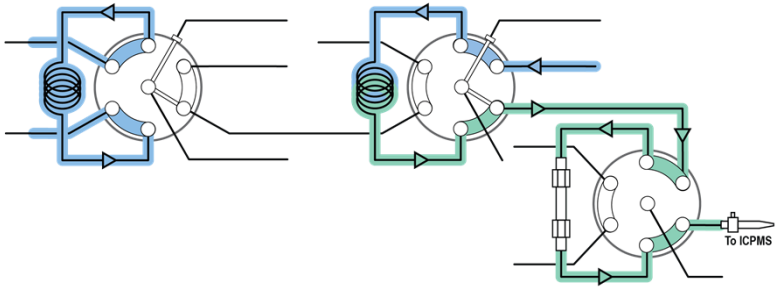


- Ability to operate in total metals or chromatography mode with a single instrument

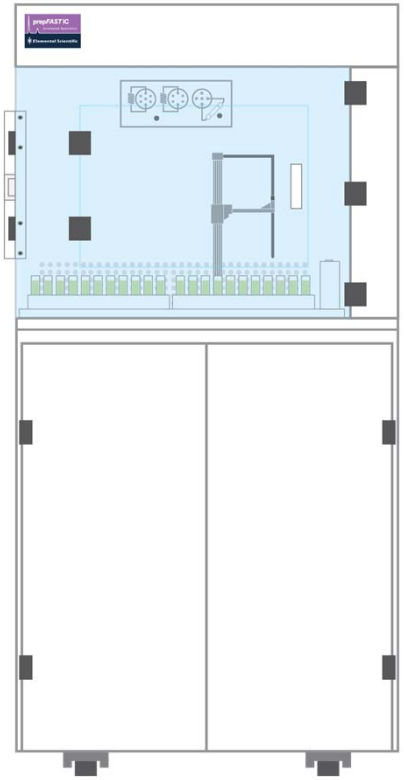
Total Metals Mode



Speciation Mode



prep*FAST* IC - Xceleri Software



- Xceleri - full online control and data analysis software package

Xceleri

- Instrument control software, triggers ICPMS, retrieves and processes data
- Automated data processing for total metals and speciation (transient data)
- Multiple options available for over-range samples
  - Re-analyze sample for confirmation
  - Intelligent dilution - analyze at dilution factor that will fall within calibration curve
  - Run speciation on sample
- Easy export of data via .csv or .xlsx

Xceleri Offline

- Offline version for data processing
- Load data files from ICPMS and software automates the data processing
- Automated peak finding, peak integration, and data reporting

prep*FAST* IC - Published Work Example

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Cite this: J. Anal. At. Spectrom., 2019, 34, 284

A fully automated total metals and chromium speciation single platform introduction system for ICP-MS†

C. Derrick Quarles, Jr,*[a] Michael Szoltysik,[b] Patrick Sullivan[a] and Maurice Reijnen[c]

Measuring chromium species in drinking water has become of particular interest due to daily environmental contamination that is caused by industrial processes. Agencies such as the US Environmental Protection Agency and the European Union continue to investigate the maximum to which Cr(vi) contaminant levels should be set; thus laboratories must seek more efficient ways of performing routine analyses. In this work a single platform, automated speciation and total metals method is presented for chromium speciation in drinking water, waste water, industrial waters, and recipient waters, and for total metals in sludges, soils, organic waste, ashes, biological samples, or paint. Samples were measured using a prepFAST IC system for Cr(iii) and Cr(vi) and the results were compared to the HPLC results. In addition, samples from the aqua regia total method were compared to those of the total metals method performed using the prepFAST IC. Sample comparisons resulted in linear regression plots with very good correlations, greater than 0.97 for total metals over a dynamic range of 0.010–100 000 μg L^{-1} for 63 elements and greater than 0.98 for Cr(vi) speciation. The limits of detection for Cr(vi) and Cr(iii) using the prepFAST IC and ICP-MS combination are 7 ng L^{-1} and 12 ng L^{-1}, respectively. The new method resulted in an ~43× improvement in detection limits as compared to the previous method employed in our laboratory. The accurate results for quality control samples of Cr(vi) were in good agreement with the historical values collected using the old method.

Received 13th October 2018
Accepted 30th November 2018

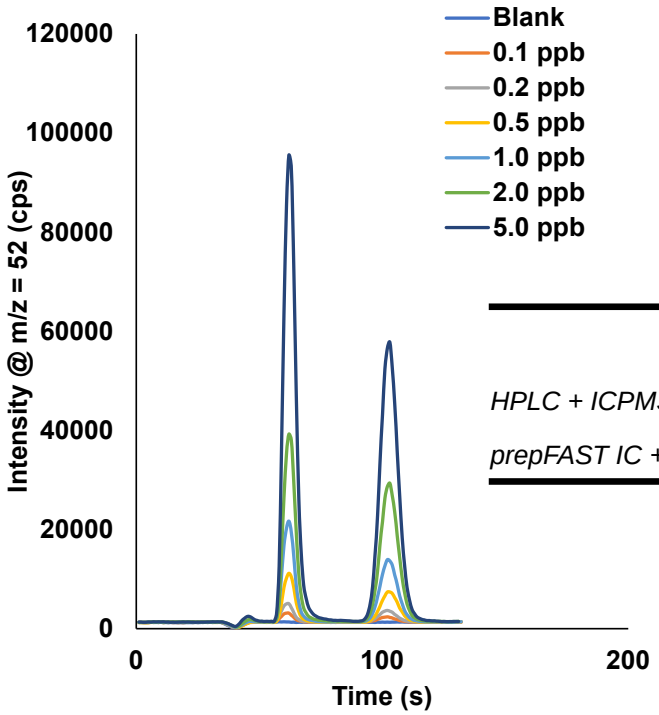
DOI: 10.1039/c8ja00342d

rsc.li/jaas

1. Introduction

Due to the recommendations and guidance of the European Union (EU) and the United States Environmental Protection Agency (EPA), the importance of chromium testing of soil, drinking water, and waste water has grown substantially in recent years.[1,2] The increase of information regarding the effects of chromium on humans has shed light on the fact that chromium has different biochemical behaviors which affect the human body in very different ways.[3] Chromium(iii) is considered an essential element, found in vegetables, fruits, meats, and/or nutritional supplements, and has been linked to Cr(iii) to Cr(vi). For example, Lindsay *et al.* showed that during chlorination of drinking water, which is a popular disinfection process in water treatment facilities, any present Cr(iii) in the water can be oxidized to Cr(vi).[4] Therefore, laboratory testing should include the identification of the chromium species (Cr(iii) and Cr(vi)) and not just the total chromium value to assess the overall exposure impact.

The most common way to measure elemental species is by liquid chromatography-inductively coupled plasma-mass spectrometry (LC-ICP-MS). Many reports exist in the literature on how to measure Cr(iii) and Cr(vi) using LC-ICP-MS.[1–3,8,10–28] However, most of these reports measure chromium using HPLC



	Cr VI	
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HPLC + ICPMS	0.3 μg/L	1.0 μg/L
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Improved LODs for Cr VI

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prep*FAST* IC - Published Work Example

Talanta Open 1 (2020) 100002

Contents lists available at ScienceDirect

Talanta Open

journal homepage: www.elsevier.com/locate/talo

Automated ICP-MS method to measure bromine, chlorine, and iodine species and total metals content in drinking water

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ARTICLE INFO

Keywords:
Chloride
Bromide
Iodide
Water
Elemental speciation

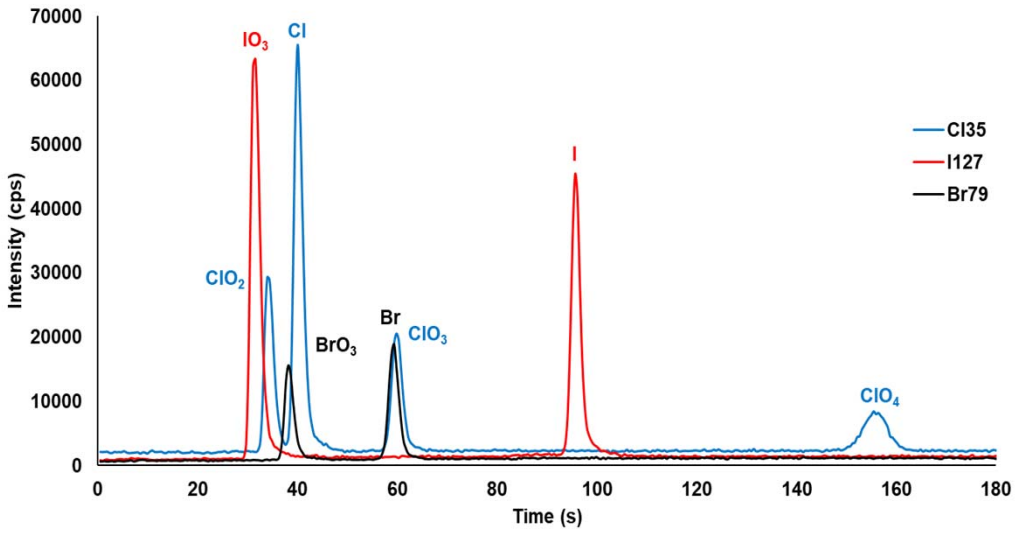
ABSTRACT

The disinfection of drinking water is an important aspect to human health. However, this process leads to potentially harmful disinfection by-products that should be monitored prior to drinking water reaching homes and businesses. Agencies such as the World Health Organization and United States Environmental Protection Agency set recommended levels for disinfection by-products and trace elements to keep the consumer healthy. In this work a single platform, automated total metals (adapted EPA 6020B method) and halogen speciation method is presented for water analysis that can help laboratories become more efficient while providing new capabilities. Samples from around the Atlanta, GA, USA region were collected and analyzed to investigate the effects of the local counties' water before and after the water treatment processes. The detection limits for this method were found to be 29 ng L^{-1} bromide, 31 ng L^{-1} bromate, 5.5 ng L^{-1} iodide, 1.8 ng L^{-1} iodate, 0.7 µg L^{-1} chloride, 2.6 µg L^{-1} chlorite, 6.8 µg L^{-1} chlorate, and 9.5 µg L^{-1} perchlorate. This halogen speciation method is completed in under 3 min per sample and can be automated into a single analytical run with trace elemental analysis when combined with an ICP-MS.

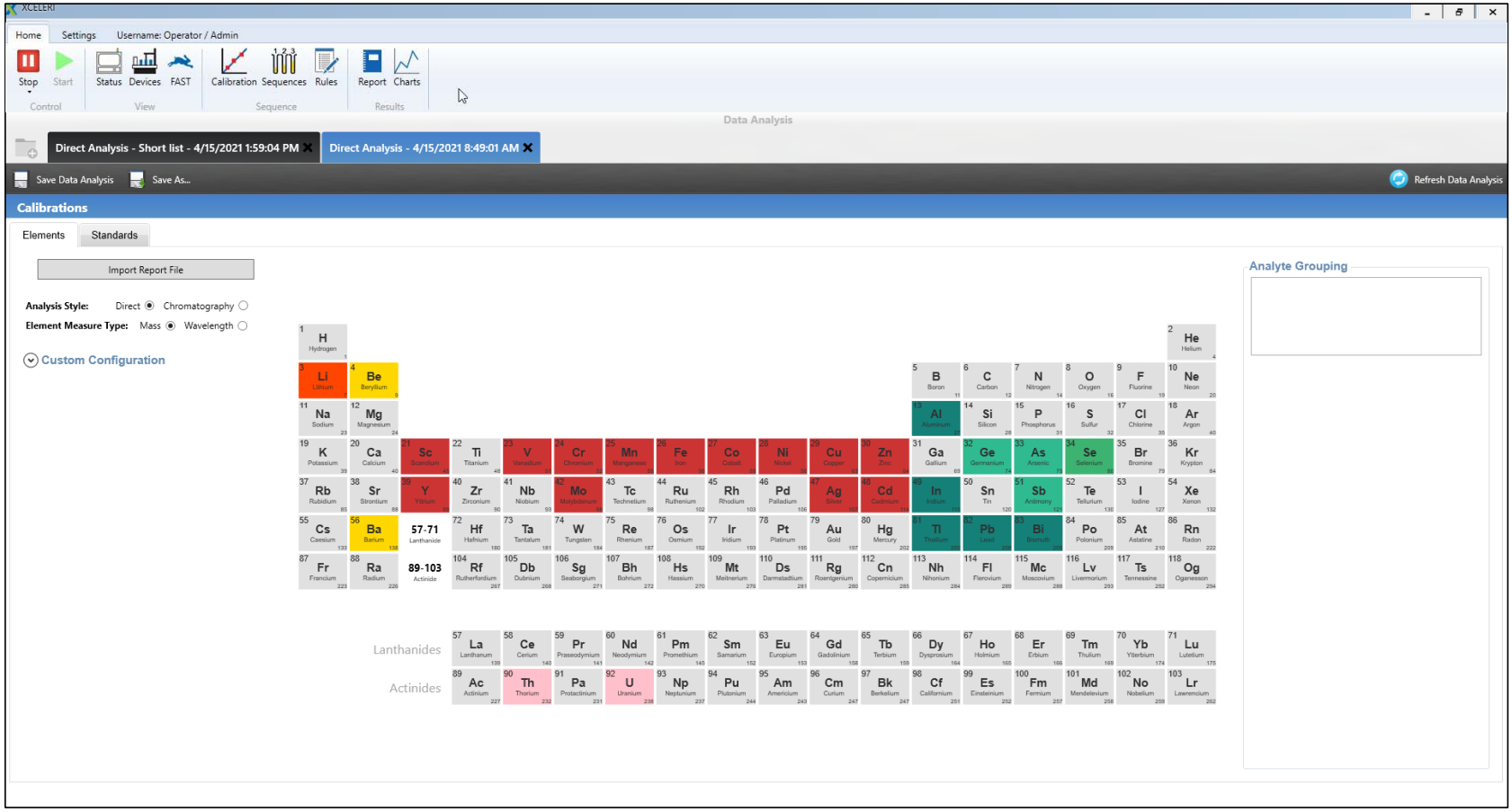
1. Introduction

The wide-spread provision of safe drinking water has been a significant piece of public health. While the earliest water treatment systems focused only on taste and aesthetics, increased knowledge and understanding of how water-borne diseases spread led to more sophisticated microbial disinfection processes. The most common disinfection techniques for drinking water involve chlorination, ozonation, and/or filtration [1–4]. In the 1970's, the disadvantage in using chemical disinfection agents was realized, and the public became aware of the formation of disinfection by-products (DBPs) [2]. The first known DBP, chloroform, was linked to cancer by the National Cancer Institute in 1976 [2]. Currently, > 700 DBPs have been identified but only a small quantity are regulated around the world [3]. These DBPs have been EPA) and 25 µg L^{-1} (World Health Organization, WHO) [9-14]. Iodide is another element that is naturally occurring in water that can form potentially harmful DBPs, these iodine containing DBPs have been recently identified as emerging contaminants of concern [1,15,16]. The process of chlorination involves the addition of chlorine bleach (sodium hypochlorite), which can create Cl-based DBPs such as chlorite, chlorate, and perchlorate. The US EPA has set the MCL as 1.0 mg L^{-1} chlorite and is seeking public input on the proposed MCL of 56 µg L^{-1} perchlorate [3, 9], whereas the WHO has set provisional guideline values of 0.7 mg L^{-1} for chlorite and chlorate [14].

In addition to the halogenated DBPs there is also great concern for monitoring the inorganic chemical contaminants that may be present in drinking water. The US EPA has set MCLs for antimony (0.006 mg L^{-1}), arsenic (0.010 mg L^{-1}), barium (2 mg L^{-1}), beryllium (0.004 mg L^{-1}),



Xceleri - Building Total Metals Method



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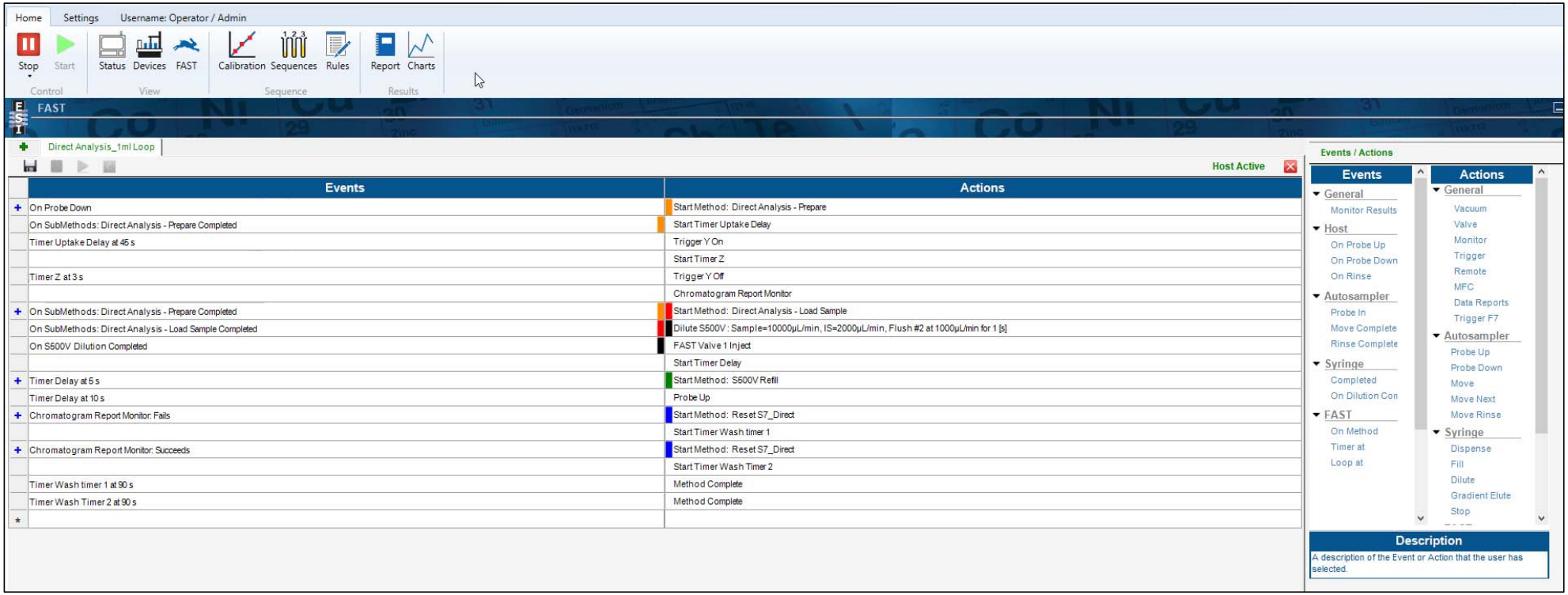


Xceleri - Building Total Metals Calibration

Calibrations

Standards Panel

Add Standard | Remove Standard

Internal Standards

107Ag (No Gas)	115In (Helium Gas)
111Cd (Helium Gas)	115In (No Gas)
121Sb (Helium Gas)	209Bi (No Gas)
137Ba (Helium Gas)	45Sc (Helium Gas)
	72Ge (Helium Gas)

>> <<

Multi Row Configuration

Line Fit

Forcing: None

Unit

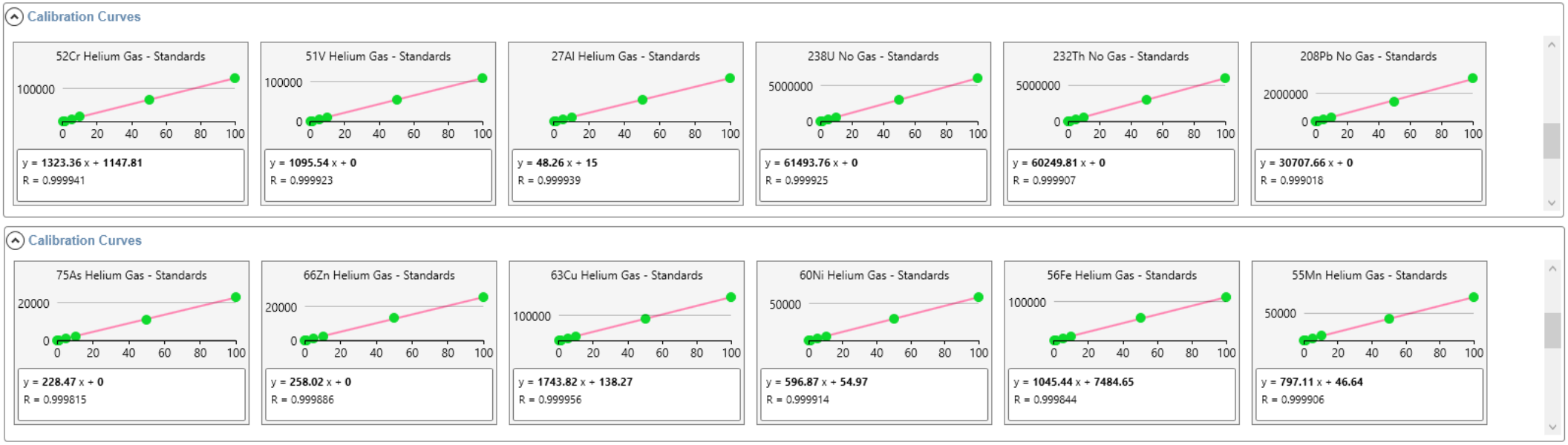
Apply

Standards

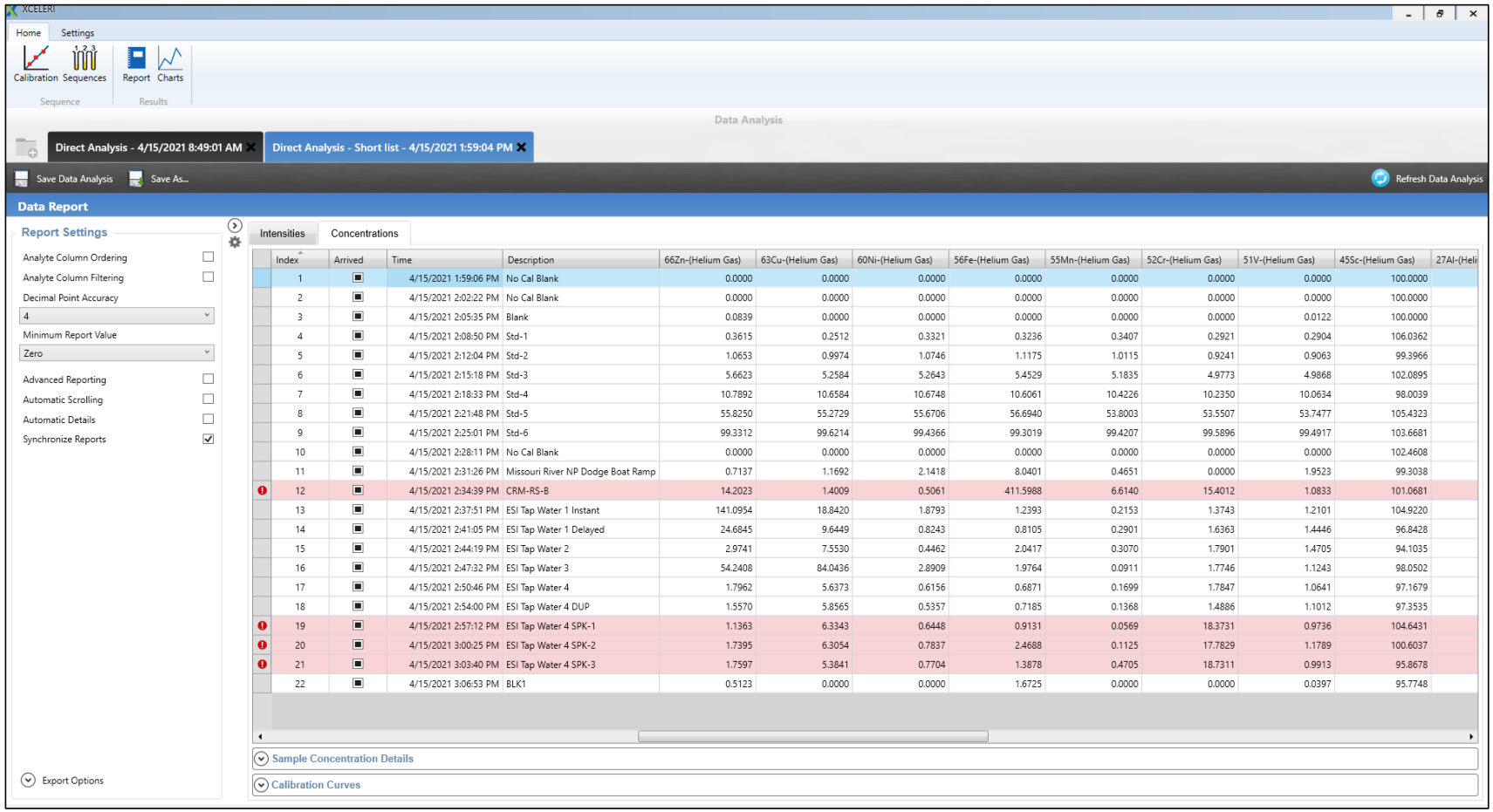
Apply

	Analyte	Line Fit	Forcing	Internal Standard	Unit	Blank	Std-1	Std-2	Std-3	Std-4	Std-5	Std-6
12	27Al (Helium Gas)	Linear + I.S.	ThroughBlank	45Sc (Helium Gas)	ppb	0	0.5	1	5	10	50	100
13	45Sc (Helium Gas)	Linear + I.S.	ThroughZero		ppb	5	5	5	5	5	5	5
14	51V (Helium Gas)	Linear + I.S.	ThroughZero	45Sc (Helium Gas)	ppb	0	0.5	1	5	10	50	100
15	52Cr (Helium Gas)	Linear + I.S.	ThroughBlank	45Sc (Helium Gas)	ppb	0	0.5	1	5	10	50	100
16	55Mn (Helium Gas)	Linear + I.S.	ThroughBlank	45Sc (Helium Gas)	ppb	0	0.5	1	5	10	50	100
17	56Fe (Helium Gas)	Linear + I.S.	ThroughBlank	89Y (Helium Gas)	ppb	0	0.5	1	5	10	50	100
18	59Co (No Gas)	Linear + I.S.	ThroughBlank	89Y (Helium Gas)	ppb	0	0.5	1	5	10	50	100
19	60Ni (Helium Gas)	Linear + I.S.	ThroughBlank	89Y (Helium Gas)	ppb	0	0.5	1	5	10	50	100
20	63Cu (Helium Gas)	Linear + I.S.	ThroughBlank	89Y (Helium Gas)	ppb	0	0.5	1	5	10	50	100
21	66Zn (Helium Gas)	Linear + I.S.	ThroughZero	89Y (Helium Gas)	ppb	0	0.5	1	5	10	50	100
22	72Ge (Helium Gas)	Linear + I.S.	ThroughZero		ppb	5	5	5	5	5	5	5
23	75As (Helium Gas)	Linear + I.S.	ThroughZero	72Ge (Helium Gas)	ppb	0	0.5	1	5	10	50	100
24	78Se (Helium Gas)	Linear + I.S.	ThroughBlank	72Ge (Helium Gas)	ppb	0	0.5	1	5	10	50	100
25	7Li (No Gas)	Linear + I.S.	ThroughZero		ppb	5	5	5	5	5	5	5
26	89Y (Helium Gas)	Linear + I.S.	ThroughZero		ppb	5	5	5	5	5	5	5
27	89Y (No Gas)	Linear + I.S.	ThroughZero		ppb	5	5	5	5	5	5	5
28	95Mo (Helium Gas)	Linear + I.S.	ThroughZero	115In (Helium Gas)	ppb	0	0.5	1	5	10	50	100

Xceleri - Total Metals Calibration



Xceleri - Total Metals Drinking Water Results



Index	Arrived	Time	Description	66Zn-(Helium Gas)	63Cu-(Helium Gas)	60Ni-(Helium Gas)	56Fe-(Helium Gas)	55Mn-(Helium Gas)	52Cr-(Helium Gas)	51V-(Helium Gas)	45Sc-(Helium Gas)	27Al-(Heli
1		4/15/2021 1:59:06 PM	No Cal Blank	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	100.0000	
2		4/15/2021 2:02:22 PM	No Cal Blank	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	100.0000	
3		4/15/2021 2:05:35 PM	Blank	0.0839	0.0000	0.0000	0.0000	0.0000	0.0000	0.0122	100.0000	
4		4/15/2021 2:08:50 PM	Std-1	0.3615	0.2512	0.3321	0.3236	0.3407	0.2921	0.2904	106.0362	
5		4/15/2021 2:12:04 PM	Std-2	1.0653	0.9974	1.0746	1.1175	1.0115	0.9241	0.9063	99.3966	
6		4/15/2021 2:15:18 PM	Std-3	5.6623	5.2584	5.2643	5.4529	5.1835	4.9773	4.9868	102.0895	
7		4/15/2021 2:18:33 PM	Std-4	10.7892	10.6584	10.6748	10.6061	10.4226	10.2350	10.0634	98.0039	
8		4/15/2021 2:21:48 PM	Std-5	55.8250	55.2729	55.6706	56.6940	53.8003	53.5507	53.7477	105.4323	
9		4/15/2021 2:25:01 PM	Std-6	99.3312	99.6214	99.4366	99.3019	99.4207	99.5896	99.4917	103.6681	
10		4/15/2021 2:28:11 PM	No Cal Blank	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	102.4608	
11		4/15/2021 2:31:26 PM	Missouri River NP Dodge Boat Ramp	0.7137	1.1692	2.1418	8.0401	0.4651	0.0000	1.9523	99.3038	
12		4/15/2021 2:34:39 PM	CRM-RS-B	14.2023	1.4009	0.5061	411.5988	6.6140	15.4012	1.0833	101.0681	
13		4/15/2021 2:37:51 PM	ESI Tap Water 1 Instant	141.0954	18.8420	1.8793	1.2393	0.2153	1.3743	1.2101	104.9220	
14		4/15/2021 2:41:05 PM	ESI Tap Water 1 Delayed	24.6845	9.6449	0.8243	0.8105	0.2901	1.6363	1.4446	96.8428	
15		4/15/2021 2:44:19 PM	ESI Tap Water 2	2.9741	7.5530	0.4462	2.0417	0.3070	1.7901	1.4705	94.1035	
16		4/15/2021 2:47:32 PM	ESI Tap Water 3	54.2408	84.0436	2.8909	1.9764	0.0911	1.7746	1.1243	98.0502	
17		4/15/2021 2:50:46 PM	ESI Tap Water 4	1.7962	5.6373	0.6156	0.6871	0.1699	1.7847	1.0641	97.1679	
18		4/15/2021 2:54:00 PM	ESI Tap Water 4 DUP	1.5570	5.8565	0.5357	0.7185	0.1368	1.4886	1.1012	97.3535	
19		4/15/2021 2:57:12 PM	ESI Tap Water 4 SPK-1	1.1363	6.3343	0.6448	0.9131	0.0569	18.3731	0.9736	104.6431	
20		4/15/2021 3:00:25 PM	ESI Tap Water 4 SPK-2	1.7395	6.3054	0.7837	2.4688	0.1125	17.7829	1.1789	100.6037	
21		4/15/2021 3:03:40 PM	ESI Tap Water 4 SPK-3	1.7597	5.3841	0.7704	1.3878	0.4705	18.7311	0.9913	95.8678	
22		4/15/2021 3:06:53 PM	BLK1	0.5123	0.0000	0.0000	1.6725	0.0000	0.0000	0.0397	95.7748	

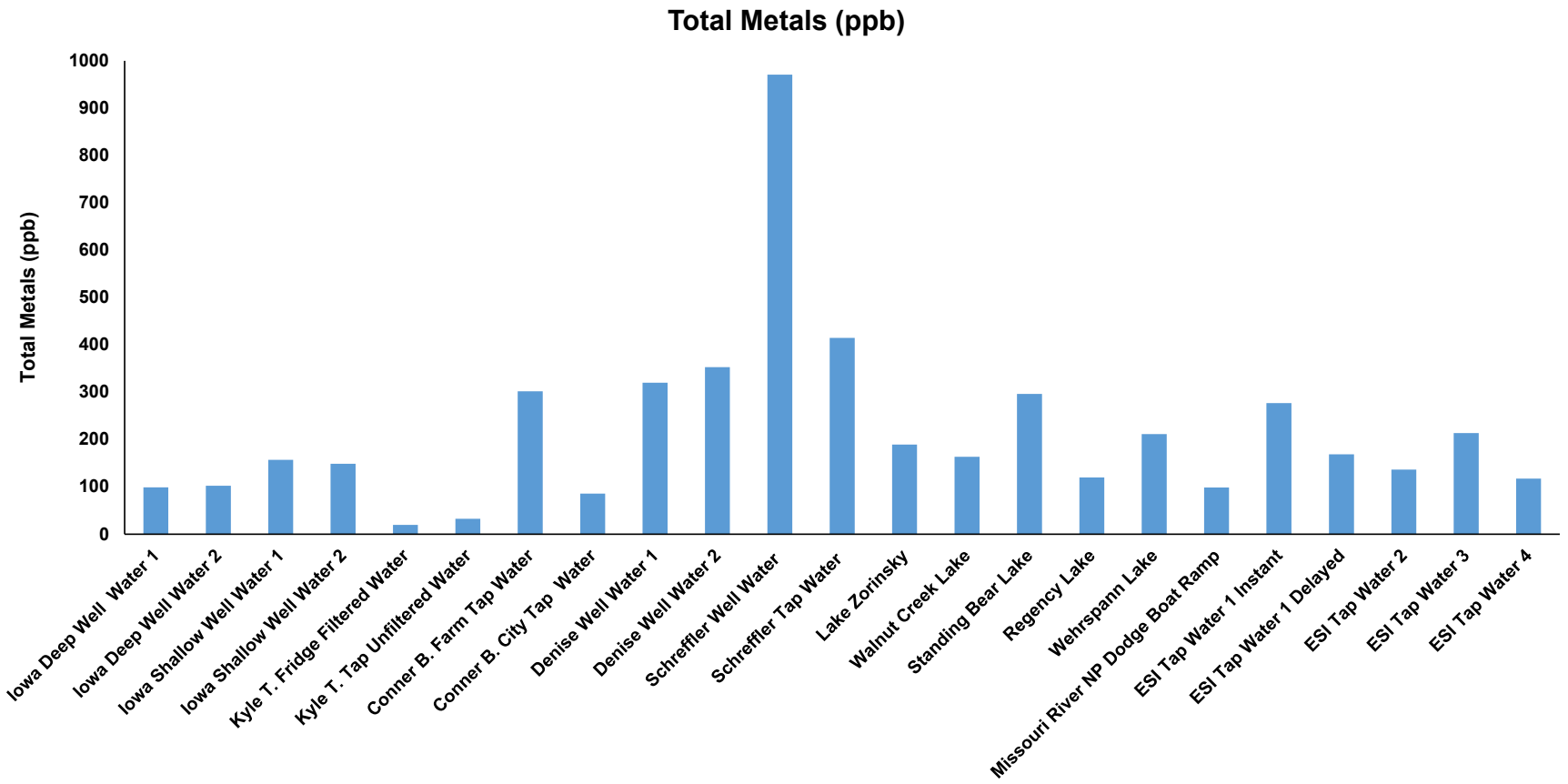
Drinking Water Results Overview

	137Ba	121Sb	111Cd	95Mo	78Se	75As	66Zn	63Cu	60Ni	56Fe	55Mn	52Cr	51V	27Al	238U	232Th	208Pb	205Tl	107Ag	59Co	9Be
Iowa Deep Well Water 1	58	0.057	0.00	1.3	5.8	0.8	13	1.2	0.0	4.1	0.4	0.9	6.7	0.0	4.8	1.89	0.043	0.022	0.013	0.042	0.000
Iowa Deep Well Water 2	57	0.068	0.00	1.3	3.2	0.6	24	1.6	0.0	0.0	0.0	1.6	6.1	0.4	4.7	0.68	0.062	0.007	0.000	0.032	0.000
Iowa Shallow Well Water 1	68	0.239	0.09	2.2	0.0	3.7	58	6.4	0.9	0.7	1.1	0.5	1.0	13.5	1.0	0.27	0.156	0.017	0.000	0.093	0.000
Iowa Shallow Well Water 2	67	0.230	0.05	1.7	0.0	4.4	57	6.4	0.9	2.0	0.4	0.5	1.5	5.6	0.9	0.12	0.100	0.013	0.000	0.067	0.000
Kyle T. Fridge Filtered Water	0	0.172	0.00	3.3	1.5	3.6	0.9	1.3	0.2	0.0	0.0	0.9	2.0	4.4	0.8	0.06	0.007	0.003	0.017	0.012	0.021
Kyle T. Tap Unfiltered Water	0	0.171	0.05	3.4	5.7	3.7	0.3	8.3	0.5	0.0	0.1	0.6	5.2	1.3	2.4	0.07	0.006	0.005	0.297	0.095	0.011
Conner B. Farm Tap Water	196	0.153	0.00	3.3	1.3	2.6	1.2	82	0.2	0.0	0.2	3.0	5.3	0.5	5.5	0.11	0.091	0.002	0.000	0.157	0.000
Conner B. City Tap Water	61	0.210	0.05	3.0	0.0	2.9	0.1	0.9	1.0	0.0	0.4	0.6	5.1	7.9	2.5	0.07	0.033	0.004	0.097	0.100	0.000
Denise Well Water 1	292	0.055	0.00	0.5	0.5	0.4	13	3.9	0.4	2.7	0.6	1.4	0.4	0.0	3.9	0.08	0.078	0.004	0.000	0.075	0.000
Denise Well Water 2	306	0.085	0.01	0.6	6.2	0.3	24	5.7	0.6	4.4	0.5	1.8	0.4	0.0	3.0	0.04	0.050	0.004	0.000	0.084	0.011
Schreffler Well Water	0	0.000	0.00	0.0	0.0	0.0	463	503	0.7	1.6	0.0	0.8	0.0	0.6	0.0	0.01	0.666	0.002	0.000	0.000	0.031
Schreffler Tap Water	44	0.211	0.07	2.7	0.0	0.7	290	5.9	4.0	1.3	0.2	2.0	1.1	61.2	0.8	0.03	0.097	0.008	0.000	0.081	0.000
Lake Zorinsky	147	0.382	0.00	3.5	0.0	2.2	0.1	0.9	2.6	9.5	1.8	1.0	1.2	15.1	4.0	0.03	0.022	0.015	0.000	0.134	0.011
Walnut Creek Lake	128	0.138	0.01	3.4	1.3	1.5	0.1	0.5	1.5	6.6	5.8	0.6	0.4	10.3	3.2	0.02	0.008	0.006	0.000	0.114	0.000
Standing Bear Lake	127	0.185	0.00	2.1	0.0	1.1	0.8	0.8	1.4	73	6.8	0.9	0.8	80.4	1.2	0.05	0.071	0.009	0.000	0.123	0.000
Regency Lake	105	0.210	0.00	0.9	0.8	3.2	0.4	0.7	0.3	3.5	1.8	0.9	0.5	0.6	0.9	0.02	0.014	0.013	0.000	0.094	0.000
Wehrspann Lake	163	0.430	0.02	7.7	6.7	1.2	0.5	1.0	1.2	9.5	8.1	0.4	0.7	7.3	3.2	0.04	0.032	0.009	0.000	0.107	0.022
Missouri River NP Dodge Boat Ramp	65	0.457	0.02	3.5	4.8	2.2	0.6	1.3	2.3	5.5	0.4	1.0	1.9	4.7	4.4	0.03	0.018	0.019	0.000	0.102	0.011
ESI Tap Water 1 Instant	30	0.315	0.00	2.6	6.8	0.4	132	18	2.2	1.2	0.2	2.7	1.2	79.1	0.6	0.02	0.019	0.011	0.101	0.134	0.011
ESI Tap Water 1 Delayed	27	0.229	0.00	3.0	0.0	0.3	25	10	0.7	3.9	0.4	2.5	1.1	94.3	0.6	0.02	0.010	0.015	0.027	0.150	0.011
ESI Tap Water 2	28	0.374	0.00	2.5	0.0	0.4	2.4	6.8	0.4	3.4	0.2	3.0	1.2	87.1	0.6	0.02	0.018	0.014	0.000	0.137	0.022
ESI Tap Water 3	27	0.245	0.09	2.8	7.3	0.5	53	83	3.1	0.6	0.0	2.5	1.0	32.2	0.5	0.01	0.036	0.009	0.000	0.088	0.000
ESI Tap Water 4	28	0.274	0.00	2.8	0.0	0.7	1.6	5.4	0.6	2.5	0.2	3.0	0.9	71.1	0.6	0.02	0.008	0.015	0.000	0.113	0.045

Drinking Water Results Overview

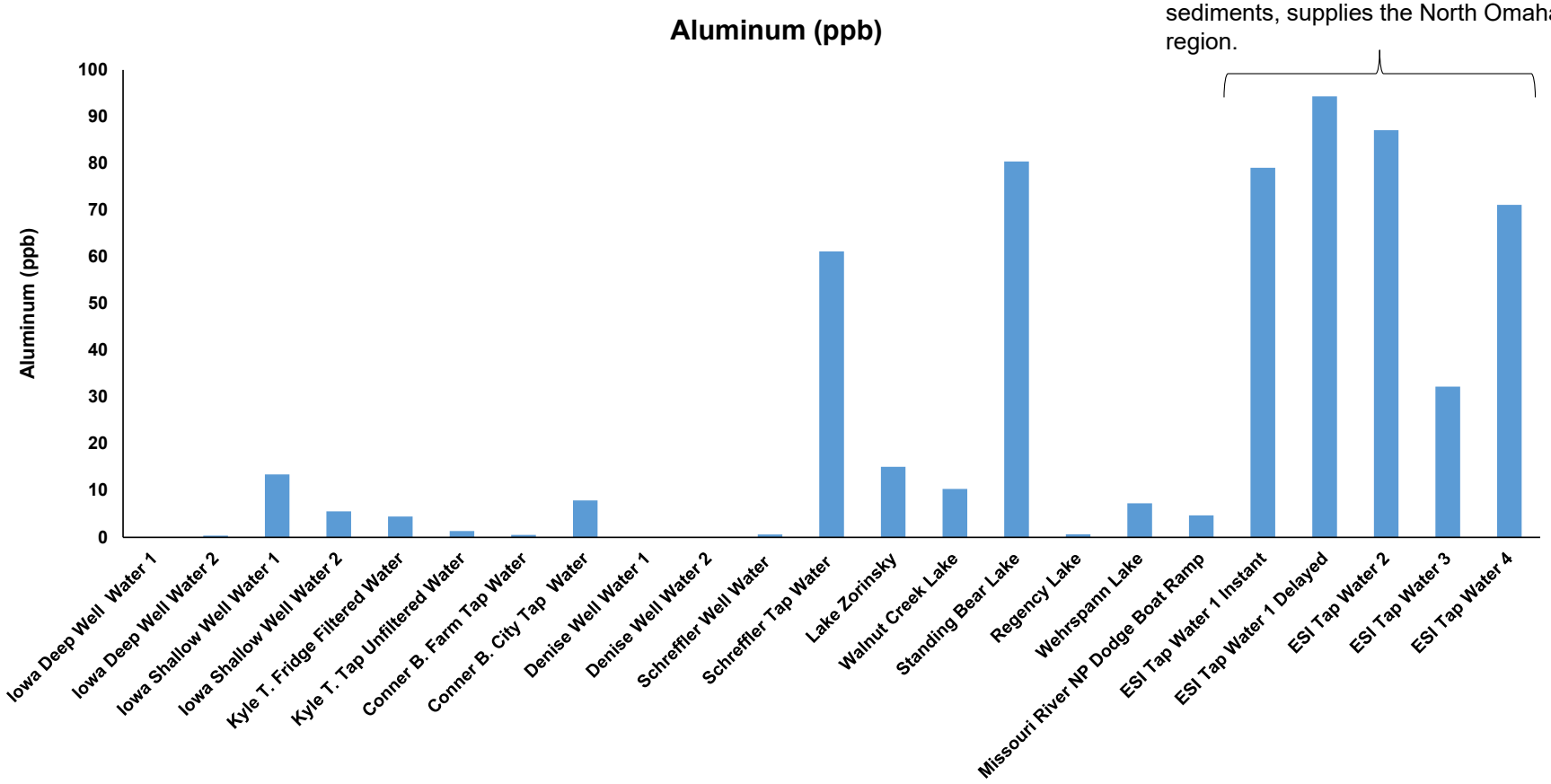
	137Ba	121Sb	111Cd	95Mo	78Se	75As	66Zn	63Cu	60Ni	56Fe	55Mn	52Cr	51V	27Al
Iowa Deep Well Water 1	58	0.057	0.00	1.3	5.8	0.8	13	1.2	0.0	4.1	0.4	0.9	6.7	0.0
Iowa Deep Well Water 2	57	0.068	0.00	1.3	3.2	0.6	24	1.6	0.0	0.0	0.0	1.6	6.1	0.4
Iowa Shallow Well Water 1	68	0.239	0.09	2.2	0.0	3.7	58	6.4	0.9	0.7	1.1	0.5	1.0	13.5
Iowa Shallow Well Water 2	67	0.230	0.05	1.7	0.0	4.4	57	6.4	0.9	2.0	0.4	0.5	1.5	5.6
Kyle T. Fridge Filtered Water	0	0.172	0.00	3.3	1.5	3.6	0.9	1.3	0.2	0.0	0.0	0.9	2.0	4.4
Kyle T. Tap Unfiltered Water	0	0.171	0.05	3.4	5.7	3.7	0.3	8.3	0.5	0.0	0.1	0.6	5.2	1.3
Conner B. Farm Tap Water	196	0.153	0.00	3.3	1.3	2.6	1.2	82	0.2	0.0	0.2	3.0	5.3	0.5
Conner B. City Tap Water	61	0.210	0.05	3.0	0.0	2.9	0.1	0.9	1.0	0.0	0.4	0.6	5.1	7.9
Denise Well Water 1	292	0.055	0.00	0.5	0.5	0.4	13	3.9	0.4	2.7	0.6	1.4	0.4	0.0
Denise Well Water 2	306	0.085	0.01	0.6	6.2	0.3	24	5.7	0.6	4.4	0.5	1.8	0.4	0.0
Schreffler Well Water	0	0.000	0.00	0.0	0.0	0.0	463	503	0.7	1.6	0.0	0.8	0.0	0.6
Schreffler Tap Water	44	0.211	0.07	2.7	0.0	0.7	290	5.9	4.0	1.3	0.2	2.0	1.1	61.2
Lake Zorinsky	147	0.382	0.00	3.5	0.0	2.2	0.1	0.9	2.6	9.5	1.8	1.0	1.2	15.1
Walnut Creek Lake	128	0.138	0.01	3.4	1.3	1.5	0.1	0.5	1.5	6.6	5.8	0.6	0.4	10.3
Standing Bear Lake	127	0.185	0.00	2.1	0.0	1.1	0.8	0.8	1.4	73	6.8	0.9	0.8	80.4
Regency Lake	105	0.210	0.00	0.9	0.8	3.2	0.4	0.7	0.3	3.5	1.8	0.9	0.5	0.6
Wehrspann Lake	163	0.430	0.02	7.7	6.7	1.2	0.5	1.0	1.2	9.5	8.1	0.4	0.7	7.3
Missouri River NP Dodge Boat Ramp	65	0.457	0.02	3.5	4.8	2.2	0.6	1.3	2.3	5.5	0.4	1.0	1.9	4.7
ESI Tap Water 1 Instant	30	0.315	0.00	2.6	6.8	0.4	132	18	2.2	1.2	0.2	2.7	1.2	79.1
ESI Tap Water 1 Delayed	27	0.229	0.00	3.0	0.0	0.3	25	10	0.7	3.9	0.4	2.5	1.1	94.3
ESI Tap Water 2	28	0.374	0.00	2.5	0.0	0.4	2.4	6.8	0.4	3.4	0.2	3.0	1.2	87.1
ESI Tap Water 3	27	0.245	0.09	2.8	7.3	0.5	53	83	3.1	0.6	0.0	2.5	1.0	32.2
ESI Tap Water 4	28	0.274	0.00	2.8	0.0	0.7	1.6	5.4	0.6	2.5	0.2	3.0	0.9	71.1

Drinking Water Results Overview

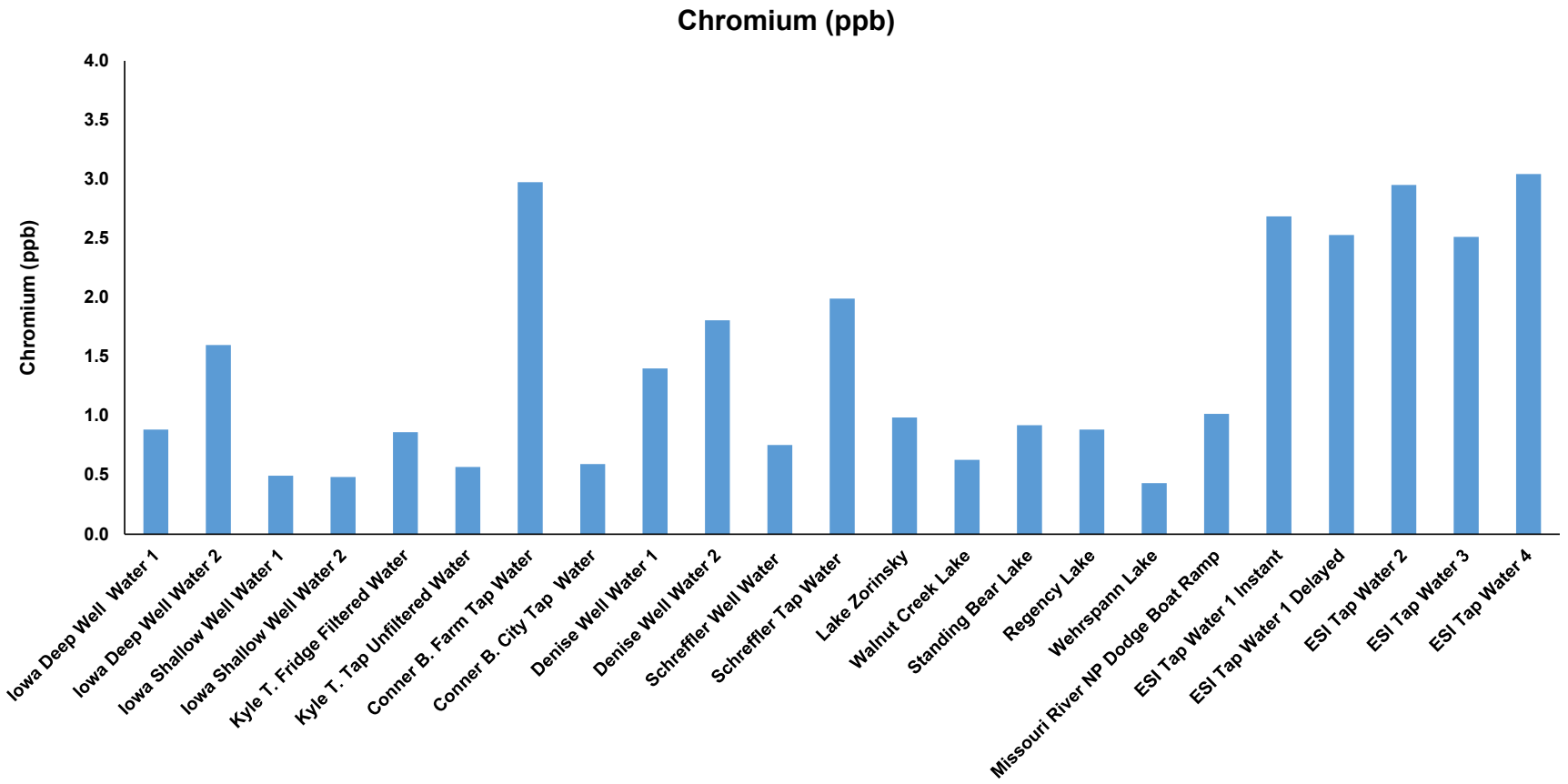


Drinking Water Results - Al

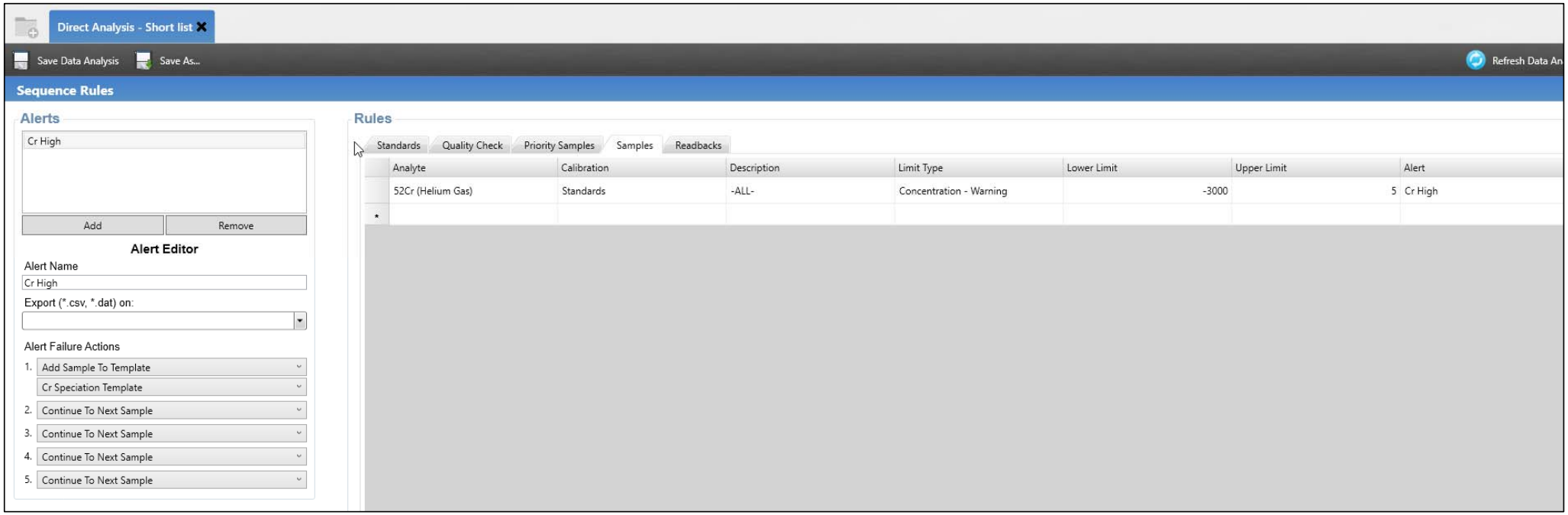
Florence water treatment plant uses an Al-based flocculant to remove river sediments, supplies the North Omaha region.



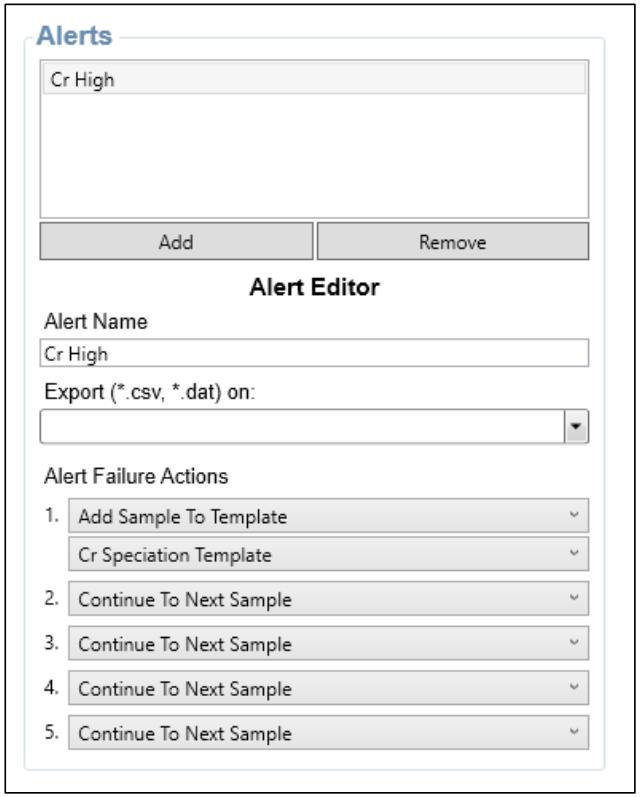
Drinking Water Results - Total Cr



Xceleri - Total Metals Drinking Water Results



Xceleri - Total Metals Drinking Water Results



Xceleri - Total Metals Drinking Water Results

Rules

Standards | Quality Check | Priority Samples | Samples | Readbacks

Analyte	Calibration	Description	Limit Type	Lower Limit	Upper Limit	Alert
52Cr (Helium Gas)	Standards	-ALL-	Concentration - Warning	-3000	5	Cr High
*						

Xceleri - Automated Cr Speciation Analysis

Intensities | Concentrations

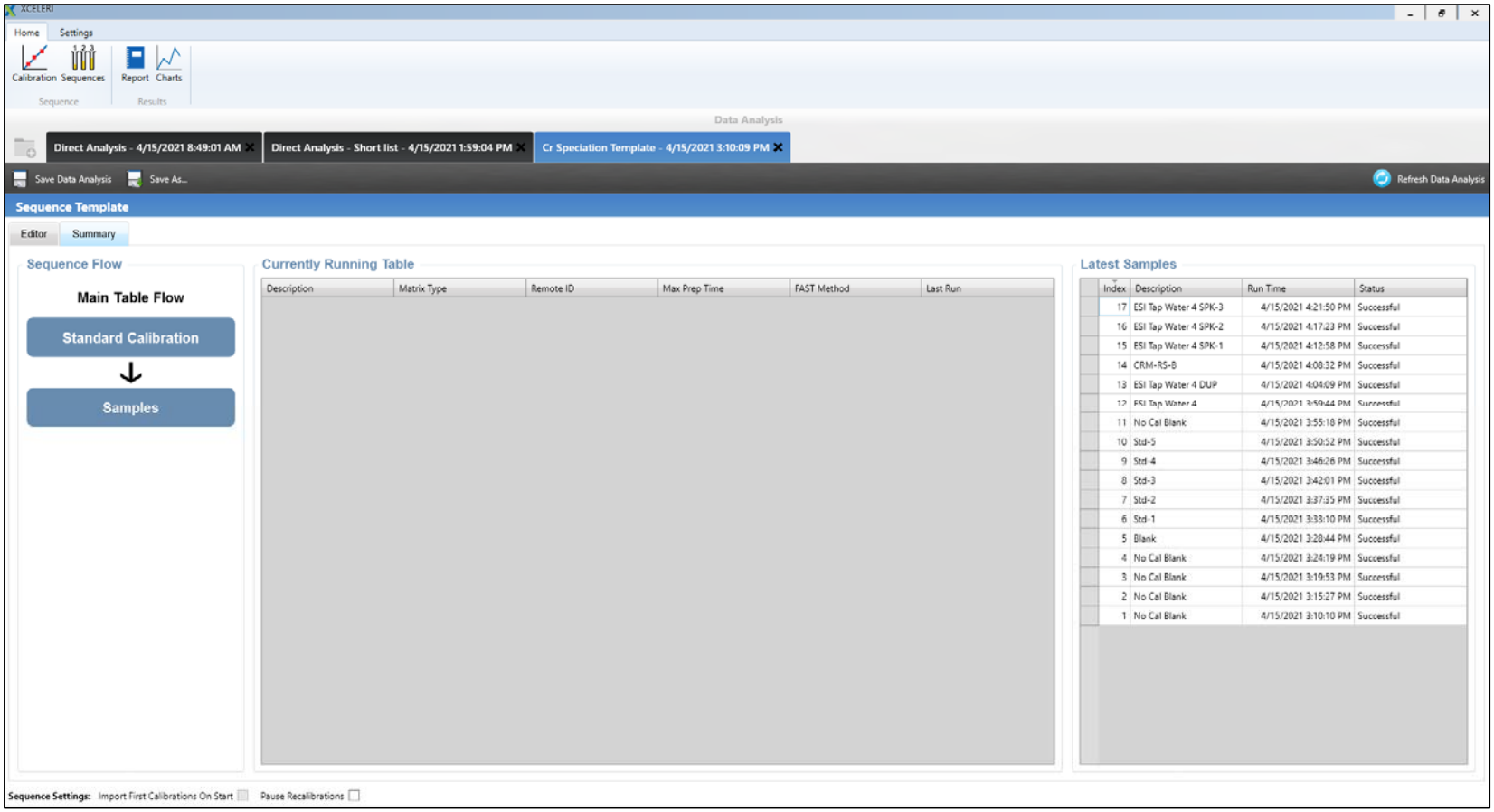
	Index	Arrived	Time	Description	52Cr-(Helium Gas)	51V-(Helium Gas)
	23	■	4/15/2021 9:59:51 AM	Lake Zorinsky	1.0	1.2
	24	■	4/15/2021 10:03:04 AM	Walnut Creek Lake	0.6	0.4
	25	■	4/15/2021 10:06:16 AM	Standing Bear Lake	0.9	0.8
	26	■	4/15/2021 10:09:28 AM	Regency Lake	0.9	0.5
	27	■	4/15/2021 10:12:40 AM	Wehrspann Lake	0.4	0.7
	28	■	4/15/2021 10:15:54 AM	Missouri River NP Dodge Boat Ramp	1.0	1.9
!	29	■	4/15/2021 10:19:07 AM	CRM-RS-B	15.6	1.0
	30	■	4/15/2021 10:22:19 AM	ESI Tap Water 1 Instant	2.7	1.2
	31	■	4/15/2021 10:25:31 AM	ESI Tap Water 1 Delayed	2.5	1.1
	32	■	4/15/2021 10:28:44 AM	ESI Tap Water 2	3.0	1.2
	33	■	4/15/2021 10:31:59 AM	ESI Tap Water 3	2.5	1.0
	34	■	4/15/2021 10:35:11 AM	ESI Tap Water 4	3.0	0.9
	35	■	4/15/2021 10:38:23 AM	ESI Tap Water 4 DUP	2.9	1.0
!	36	■	4/15/2021 10:41:37 AM	ESI Tap Water 4 SPK-1	19.3	1.1
!	37	■	4/15/2021 10:44:50 AM	ESI Tap Water 4 SPK-2	18.6	0.8
!	38	■	4/15/2021 10:48:02 AM	ESI Tap Water 4 SPK-3	18.9	0.9

Analytes detected by rules:
52Cr-(Helium Gas)

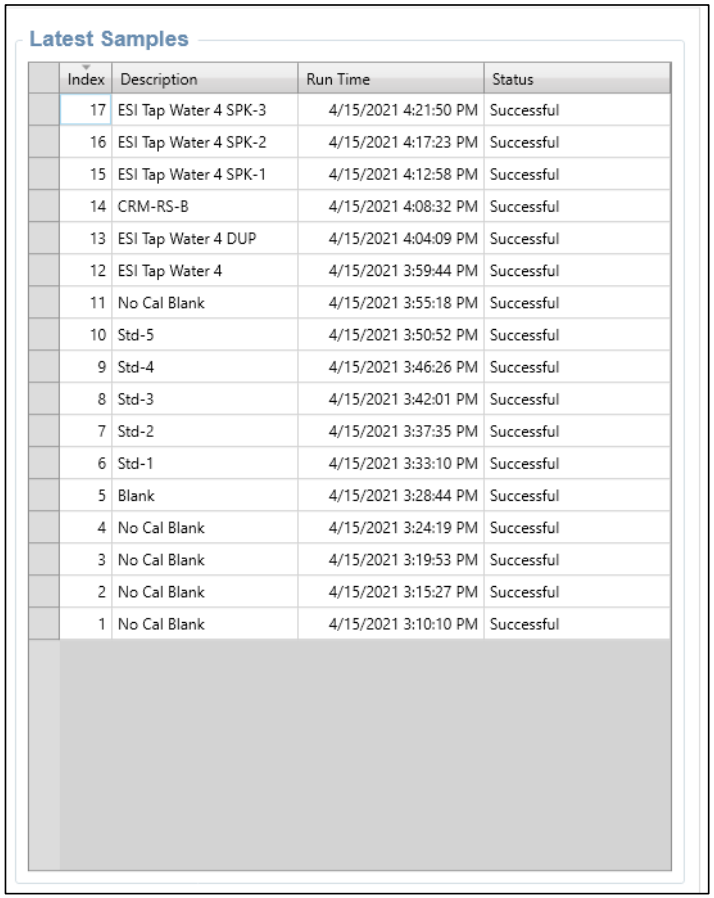
Priority action for: 52Cr (Helium Gas)
Failure number: 1
Limit Type: Concentration - Warning
Alert to run: Cr High

Executing: Add CRM-RS-B To Next Template

Xceleri - Automated Cr Speciation Analysis



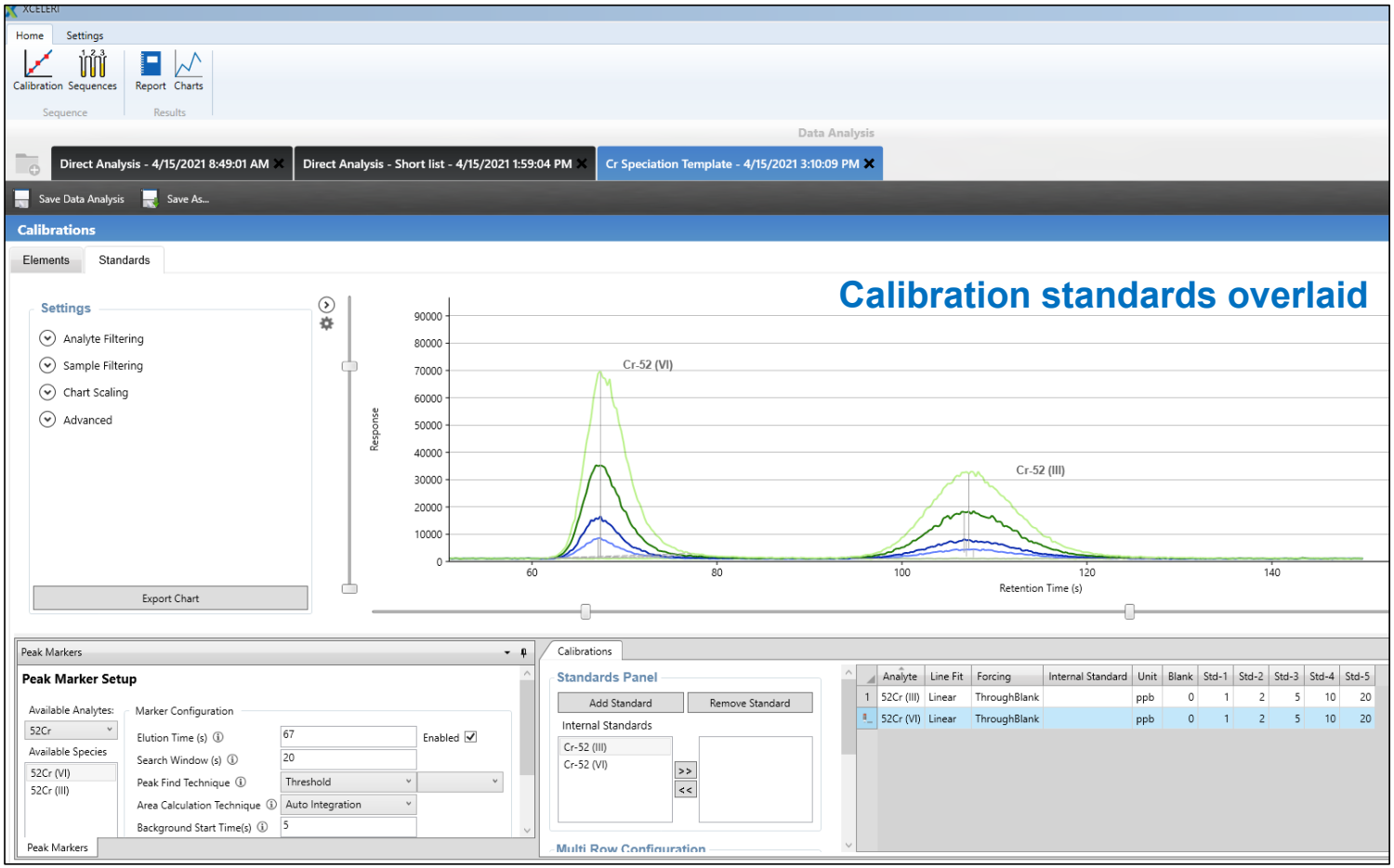
Xceleri - Automated Cr Speciation Analysis



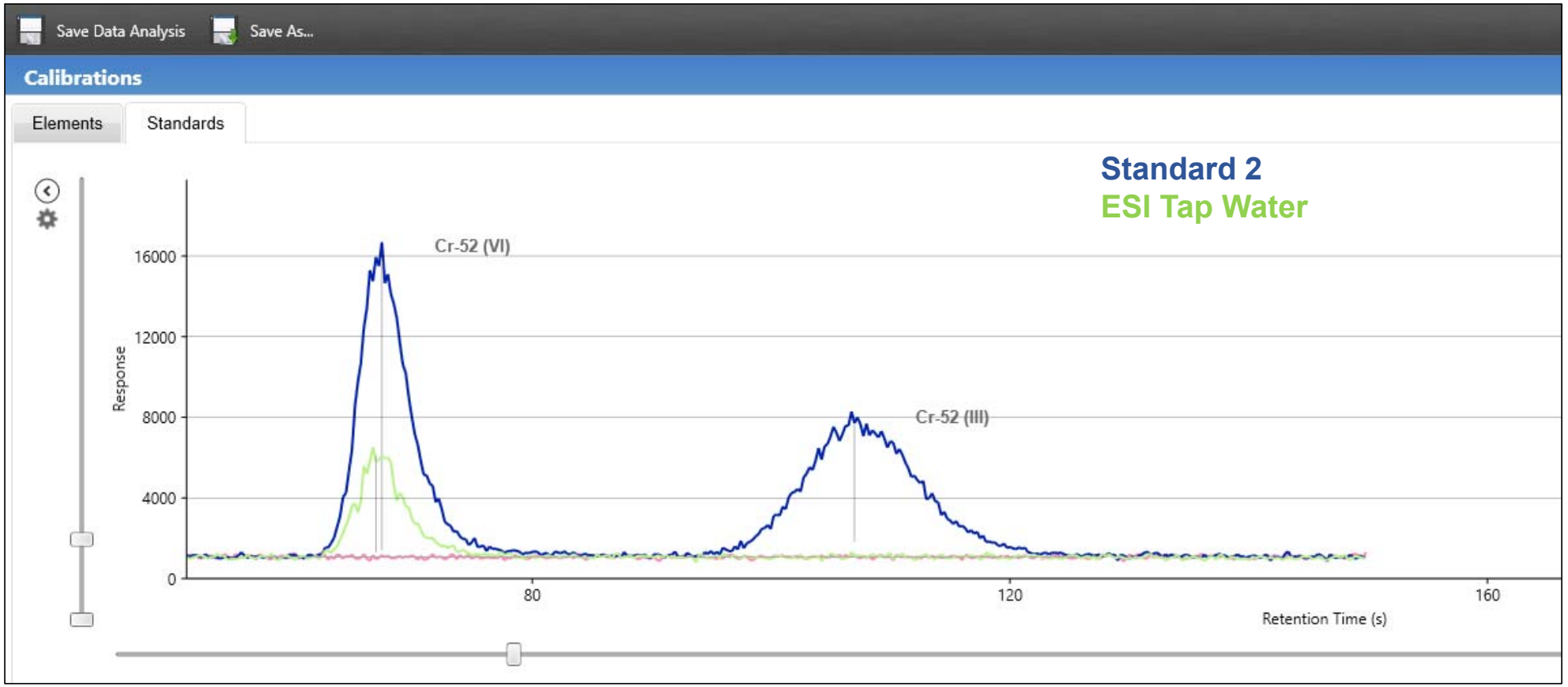
Latest Samples

Index	Description	Run Time	Status
17	ESI Tap Water 4 SPK-3	4/15/2021 4:21:50 PM	Successful
16	ESI Tap Water 4 SPK-2	4/15/2021 4:17:23 PM	Successful
15	ESI Tap Water 4 SPK-1	4/15/2021 4:12:58 PM	Successful
14	CRM-RS-B	4/15/2021 4:08:32 PM	Successful
13	ESI Tap Water 4 DUP	4/15/2021 4:04:09 PM	Successful
12	ESI Tap Water 4	4/15/2021 3:59:44 PM	Successful
11	No Cal Blank	4/15/2021 3:55:18 PM	Successful
10	Std-5	4/15/2021 3:50:52 PM	Successful
9	Std-4	4/15/2021 3:46:26 PM	Successful
8	Std-3	4/15/2021 3:42:01 PM	Successful
7	Std-2	4/15/2021 3:37:35 PM	Successful
6	Std-1	4/15/2021 3:33:10 PM	Successful
5	Blank	4/15/2021 3:28:44 PM	Successful
4	No Cal Blank	4/15/2021 3:24:19 PM	Successful
3	No Cal Blank	4/15/2021 3:19:53 PM	Successful
2	No Cal Blank	4/15/2021 3:15:27 PM	Successful
1	No Cal Blank	4/15/2021 3:10:10 PM	Successful

Xceleri - Automated Cr Speciation Analysis



Xceleri - Automated Cr Speciation Analysis



Xceleri - Automated Cr Speciation Analysis

Chromatograms | Intensities | Concentrations

Index	Arrived	Time	Description	Cr-52 (VI)	Cr-52 (III)
1	■	4/15/2021 3:10:10 PM	No Cal Blank	0.0	0.0
2	■	4/15/2021 3:15:27 PM	No Cal Blank	0.0	0.0
3	■	4/15/2021 3:19:53 PM	No Cal Blank	0.0	0.0
4	■	4/15/2021 3:24:19 PM	No Cal Blank	0.0	0.0
5	■	4/15/2021 3:28:44 PM	Blank	0.0	0.0
6	■	4/15/2021 3:33:10 PM	Std-1	1.1	0.8
7	■	4/15/2021 3:37:35 PM	Std-2	2.3	2.0
8	■	4/15/2021 3:42:01 PM	Std-3	5.4	5.5
9	■	4/15/2021 3:46:26 PM	Std-4	10.8	10.3
10	■	4/15/2021 3:50:52 PM	Std-5	19.5	19.8
11	■	4/15/2021 3:55:18 PM	No Cal Blank	0.0	0.0
12	■	4/15/2021 3:59:44 PM	ESI Tap Water 4	3.0	0.0
13	■	4/15/2021 4:04:09 PM	ESI Tap Water 4 DUP	3.0	0.0
14	■	4/15/2021 4:08:32 PM	CRM-RS-B	0.0	19.0
15	■	4/15/2021 4:12:58 PM	ESI Tap Water 4 SPK-1	19.8	0.0
16	■	4/15/2021 4:17:23 PM	ESI Tap Water 4 SPK-2	19.5	0.0
17	■	4/15/2021 4:21:50 PM	ESI Tap Water 4 SPK-3	19.8	0.1

Summary

- Demonstrated a method for the determination of Total Metals in water with automated Cr Speciation of samples that were over the set 5 ppb threshold (user setting in the software).
- Analyzed water samples from around the Omaha, NE, USA area. None of these samples exceeded ~ 3.0 ppb Cr.
- Water samples from Elemental Scientific HQs showed higher levels of Al, which is most likely a result of the aluminum-based flocculant used in the water treatment process.
- Demonstrated good spike recoveries for Cr VI species.