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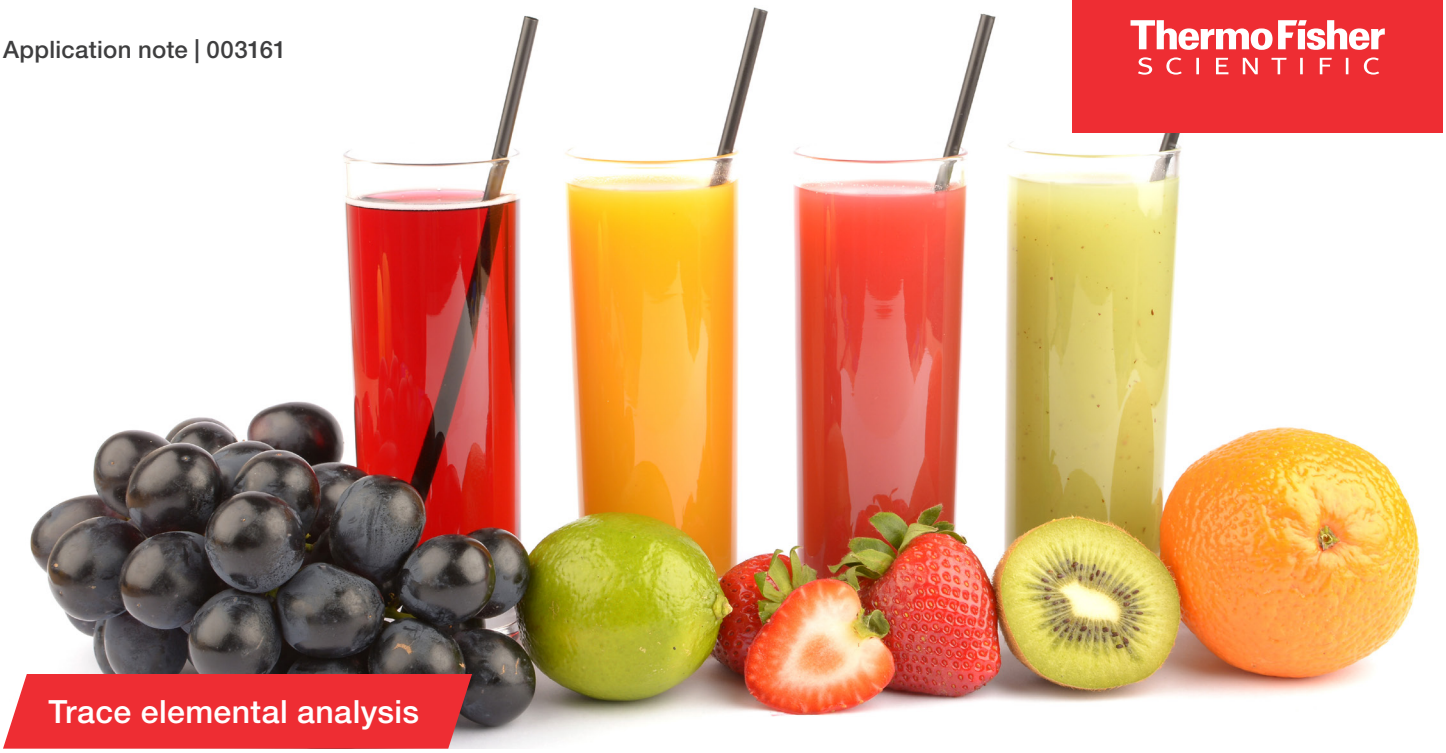

Trace elemental analysis

A comprehensive workflow for beverage analysis using inductively coupled plasma mass spectrometry (ICP-MS)

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Keywords

Beverage, Argon Gas Dilution (AGD), inductively coupled plasma mass spectrometry (ICP-MS), essential nutrients, heavy metals, interference removal

Goal

This application note will highlight a complete and comprehensive workflow for the analysis of nutrients and toxic trace elements in different types of beverages. Samples were digested using a microwave system prior to analysis using triple quadrupole ICP-MS for analysis.

Introduction

Trace metals analysis in beverages plays a crucial role in ensuring the safety, quality, and compliance of these products, helping to protect consumer health and maintain the reputation of beverage manufacturers.

Trace metals can enter beverages through various sources, starting from their natural occurrence in the ingredients, water used in production, or through processing equipment, packaging materials, etc. The presence of these metals in excessive amounts can pose potential health risks to consumers, making it necessary to monitor and control their levels. Typical analytes include, but are not limited to, arsenic, cadmium, lead, mercury, and copper. The analysis is essential to ensure the safety and quality of beverages consumed by humans.

Regulatory bodies, such as the World Health Organization (WHO) and the Food and Drug Administration (FDA), have established guidelines and maximum allowable limits for trace metals in beverages to ensure consumer safety. Manufacturers and regulatory authorities rely on the analysis to verify compliance with these regulations and to maintain the quality and integrity of beverages in the market.

It is important to note that concentration limits can vary depending on the specific beverage type and the intended consumer population (e.g., infants, children, adults). Furthermore, applicable regulations and guidelines are regularly updated, so it is crucial for beverage manufacturers to stay informed about the latest requirements in their respective markets to ensure compliance.

On the other hand, there are several essential inorganic elements that are vital for various physiological processes in the body. Nutrients such as calcium, phosphorous, sodium, potassium, magnesium, iron, and zinc serve essential roles in various physiological processes within the human body and provide the building blocks for growth, development, and maintenance of tissues and organs. These elements therefore play crucial roles in maintaining overall health and supporting various bodily functions.

This application note demonstrates a workflow for highly reproducible sample preparation combined with sensitive and robust analysis for a wide variety of beverages. The proposed workflow allowed accurate determination of both essential nutrients and potentially toxic trace metals without any compromise and can be implemented, for example, in analytical testing laboratories performing the analysis on behalf of manufacturers or regulatory authorities.

Experimental

A Thermo Scientific™ iCAP™ MTX ICP-MS and a Thermo Scientific™ iSC-65 Autosampler were used for analysis. The triple quadrupole ICP-MS was operated using the configuration and parameters highlighted in Table 1. To analyze the beverage samples, the instrument was operated using argon gas dilution (AGD). The calibration standards and the sample were automatically diluted 5 times to ensure sensitivity and robustness for all soft beverage samples in a high productivity laboratory environment. The iCAP MTX ICP-MS was operated in SQ-KED and TQ-O_2 modes to remove the polyatomic and isobaric interferences and to reach the best quantification limits for the critical elements.

Sample and standard preparation

A total of 13 different beverages, including a variety of fruit juices and soft drinks, described in Table 2, were purchased in a local supermarket. Among the selected beverages, both natural fruit juices as well as industrially processed drinks (peach tea, cola soda, etc.) were included to analyze different kinds of matrix and to determine the elemental composition in the samples.

Table 1. Instrument parameters for the iCAP MTX ICP-MS

Parameter	Value
Nebulizer	iCAP MX Series Nebulizer
Interface cones	Ni – tipped sample and skimmer
Spray chamber	Cyclonic quartz
Injector	Quartz, 1.5 mm ID
Torch	PLUS torch
Auxiliary flow (L·min^{-1})	0.8
Cool Gas flow (L·min^{-1})	14
AGD dilution level	Level-5
AGD humidifier	ON
Nebulizer flow (L·min^{-1})	0.45
Argon gas dilution flow (L·min^{-1})	0.50
QCell KED flow (mL·min^{-1})	4.91
QCell O_2 Flow (mL·min^{-1})	0.31
RF power (W)	1,550
Number of replicates	3
Spray chamber temp. (°C)	2.7

Table 2. List of beverage samples

Label	Fruit content	Origin	Comment
Apple juice 1	100%	France	
Orange juice	100%	Brazil	
Cranberry	30%	N/A	
Prune juice	Not specified	France	
Grape juice	100%	EU	Bio
Peach Tea	Not specified	N/A	
Coconut water	100%	N/A	
Multifruits	Not specified	EU	
Apple juice 2	Not specified	N/A	
Muscat grape juice		N/A	
Sweet orange	Not applicable	N/A	
Cola soda	Not applicable	N/A	
Refreshing drink	Not applicable	N/A	

Given that these samples are vastly different in their physical properties (i.e., viscosity), microwave assisted acid digestion was chosen as the most suitable and universal approach for sample preparation. Even though some of the samples may be analyzed directly after dilution, all samples were prepared using a single preparation mode for comparability.

An UltraWAVE microwave system (Milestone Srl., Sorisole, Bergamo, Italy) was used for the sample preparation. Due to the capacity of the UltraWAVE to digest high sample amounts and the ability of the iCAP MTX ICP-MS to be tolerant to high dissolved solid samples, 5 g of each beverage was weighted in the Quartz UltraWAVE tubes. The UltraWAVE parameters and program are described in Tables 3 and 4.

To improve the reproducibility and the productivity of the workflow, an EasyFILL acid dispenser (Milestone Srl., Sorisole, Bergamo, Italy) was used to automatically add 2 mL of HNO_3 and 0.5 mL of HCl in all UltraWAVE tubes. The EasyFILL utilization allowed completion of the workflow with minimal operator interaction.

During analysis, an internal standard solution was added online (500 µg·L^{-1} Sc and Ge; 20 µg·L^{-1} Rh and Ir) before nebulization to compensate for matrix effects in the plasma.

Calibration curves were prepared with a multi-element stock solution containing 34 elements. Mercury was also analyzed, however at a 50 times lower concentration. A low QC (0.2 µg·L^{-1}) and a high QC (25 µg·L^{-1}) were independently prepared to verify the validity of the calibration curve throughout the run and to check the instrument´s stability (see Table 5 for details). For the analysis of common nutrients, a second calibration block was prepared. A dedicated QC solution (at a concentration level of 1 mg·L^{-1}) was also prepared and periodically analyzed.

Tables 6 and 7 summarize the analytical figures of merit for all analytes, including correlation coefficients, blank equivalent concentrations (BEC), and limits of detection and quantification of the method. Whereas the instrumental detection limit (LOD) only considers what can be detected by the instrument, the method quantification limit (MQL) also accounts for the complete sample preparation (i.e., the sample weight and the dilution factor).

Table 3. UltraWAVE parameters

Parameter	Value
Pre-loaded pressure (N_2) (bar)	40
Cooling temperature (liquid chiller) (°C)	8
Vessel cooling activation (°C)	40
Pressure release (°C)	80
Pressure release rate (bar/min)	8

Table 4. UltraWAVE program

Step	Time	Temp (T1)	Temp (T2)	P	Power
1	00:20:00	220 °C	60 °C	110 bar	1,500 W
2	00:10:00	220 °C	60 °C	110 bar	1,500 W

Table 5. Calibration standard and QC for all analytes

Trace elements	STD 1	STD 2	STD 3	STD 4	STD 5	STD 6	QC 0.2 ppb	QC 25 ppb
Multielement solution	0.1 µg·L^{-1}	0.5 µg·L^{-1}	1 µg·L^{-1}	10 µg·L^{-1}	20 µg·L^{-1}	50 µg·L^{-1}	0.2 µg·L^{-1}	25 µg·L^{-1}
Hg	0.002 µg·L^{-1}	0.01 µg·L^{-1}	0.02 µg·L^{-1}	0.2 µg·L^{-1}	0.4 µg·L^{-1}	1 µg·L^{-1}	0.004 µg·L^{-1}	0.5 µg·L^{-1}
Na, Mg, Si, P, S, K, Ca	0.02 mg·L^{-1}	0.1 mg·L^{-1}	0.5 mg·L^{-1}	2 mg·L^{-1}	10 mg·L^{-1}	50 mg·L^{-1}	1 mg·L^{-1}	-
Al, Fe, Zn	1 µg·L^{-1}	5 µg·L^{-1}	25 µg·L^{-1}	100 µg·L^{-1}	500 µg·L^{-1}	2500 µg·L^{-1}	50 µg·L^{-1}	-

Table 6. Analytes' correlation coefficients (R^2), background equivalent concentration (BEC), detection limits, and quantification limits obtained for trace elements

	R^2	BEC (µg·L^{-1})	LOD (µg·L^{-1})	MQL (µg/kg)
^{7}Li (M-Level 5-KED-SQ)	0.9992	0.226	0.526	15.79
^{9}Be (M-Level 5-KED-SQ)	0.9993	0.039	0.203	6.102
^{27}Al (M-Level 5-KED-SQ)	>0.9999	0.691	1.347	40.40
^{48}Ti | ^{48}Ti.^{16}O (M-Level 5-O_2-TQ)	0.9999	0.020	0.007	0.200
^{51}V | ^{51}V.^{16}O (M-Level 5-O_2-TQ)	0.9999	0.069	0.017	0.515
^{52}Cr | ^{52}Cr.^{16}O (M-Level 5-O_2-TQ)	0.9999	0.083	0.022	0.652
^{55}Mn | ^{55}Mn (M-Level 5-O_2-TQ)	0.9999	0.013	0.008	0.251
^{56}Fe (M-Level 5-KED-SQ)	0.9999	0.186	0.023	0.702
^{59}Co (M-Level 5-KED-SQ)	0.9999	0.001	0.001	0.042
^{60}Ni (M-Level 5-KED-SQ)	0.9999	0.073	0.035	1.060
^{63}Cu (M-Level 5-KED-SQ)	0.9998	0.018	0.005	0.138
^{66}Zn (M-Level 5-KED-SQ)	0.9999	2.340	0.195	5.838
^{75}As | ^{75}As.^{16}O (M-Level 5-O_2-TQ)	0.9999	0.031	0.040	1.211
^{80}Se | ^{80}Se.^{16}O (M-Level 5-O_2-TQ)	0.9996	0.035	0.068	2.053
^{85}Rb (M-Level 5-KED-SQ)	0.9999	0.003	0.00003	0.001
^{88}Sr | ^{88}Sr.^{16}O (M-Level 5-O_2-TQ)	0.9998	0.009	0.009	0.265
^{98}Mo | ^{98}Mo.^{16}O (M-Level 5-O_2-TQ)	0.9997	0.008	0.043	1.301
^{107}Ag (M-Level 5-KED-SQ)	0.9999	0.034	0.016	0.493
^{111}Cd (M-Level 5-KED-SQ)	0.9998	0.001	0.003	0.102
^{118}Sn (M-Level 5-KED-SQ)	0.9999	0.015	0.008	0.238
^{121}Sb (M-Level 5-KED-SQ)	0.9995	0.021	0.010	0.308
^{125}Te (M-Level 5-KED-SQ)	0.9999	0.045	0.234	7.033
^{137}Ba (M-Level 5-KED-SQ)	0.9999	0.003	0.009	0.265
^{139}La (M-Level 5-KED-SQ)	0.9999	0.0003	0.001	0.025
^{140}Ce | ^{140}Ce.^{16}O (M-Level 5-O_2-TQ)	0.9999	0.0004	0.00001	0.0002
^{202}Hg (M-Level 5-KED-SQ)	0.9996	0.004	0.001	0.031
^{205}Tl (M-Level 5-KED-SQ)	0.9999	0.002	0.0004	0.012
^{208}Pb (M-Level 5-KED-SQ)	0.9999	0.002	0.001	0.023
^{209}Bi (M-Level 5-KED-SQ)	0.9999	0.004	0.003	0.083
^{238}U (M-Level 5-KED-SQ)	0.9999	0.002	0.001	0.016

Table 7. Analytes' correlation coefficients (R2), background equivalent concentration (BEC), detection limits, and quantification limits obtained for major elements

	R^2	BEC (mg·L^{-1})	LOD (mg·L^{-1})	MQL (mg/kg)
^{11}B (M-Level 5-KED-SQ)	0.9762	0.0128	0.0132	0.396
^{23}Na (M-Level 5-KED-SQ)	0.9999	0.0068	0.0004	0.011
^{24}Mg (M-Level 5-KED-SQ)	0.9999	0.0002	0.0005	0.015
^{28}Si | ^{28}Si.^{16}O (M-Level 5-O_2-TQ)	0.9997	0.0246	0.0026	0.078
^{31}P | ^{31}P.^{16}O (M-Level 5-O_2-TQ)	0.9999	0.0014	0.0006	0.017
^{32}S | ^{32}S.^{16}O (M-Level 5-O_2-TQ)	0.9999	0.0383	0.0023	0.070
^{39}K (M-Level 5-KED-SQ)	0.9999	0.0835	0.0080	0.239
^{44}Ca (M-Level 5-KED-SQ)	0.9998	0.0398	0.0221	0.662

Robustness

The workflow was designed to analyze a wide variety of beverages using a single method. Due to the variability of the nutrient content across different sample types, the instrument´s robustness to run all the different samples in one sequence was investigated thoroughly. This was accomplished by analyzing the different samples periodically and checking the internal standard response during more than 8 hours of analysis, carried out on two different days. Thanks to the automatic 5-times dilution delivered by the iCAP MTX ICP-MS, the four internal standards (Sc, Ge, Rh, and Ir) could be read out with similar response (between 75% and 125%) compared to the first sample in both modes utilized (KED and TQ-O_2). The data is summarized in Figure 1.

Stability

Three QC standards, prepared independently from the calibration standards, were analyzed every 2 hours as part of the sequence (details summarized in Table 5).

Figure 2 presents an overview of the average recovery for all QC checks (0.2 µg·L^{-1}, 25 µg·L^{-1}, and 1 mg·L^{-1}) across all replicates (N=5), with target values in the range 80–120% for all elements.

It must be highlighted that even for the low QC of 0.2 µg·L^{-1}, excellent QC recovery was obtained. This shows that the iCAP MTX ICP-MS instrument offers the robustness to analyze beverage samples without any additional dilution before the analysis, thanks to the 5-fold dilution using argon gas, yet maintains the required sensitivity to detect potential contaminants at relevant levels. This is specifically important for toxic elements such as arsenic, cadmium, mercury, and lead.

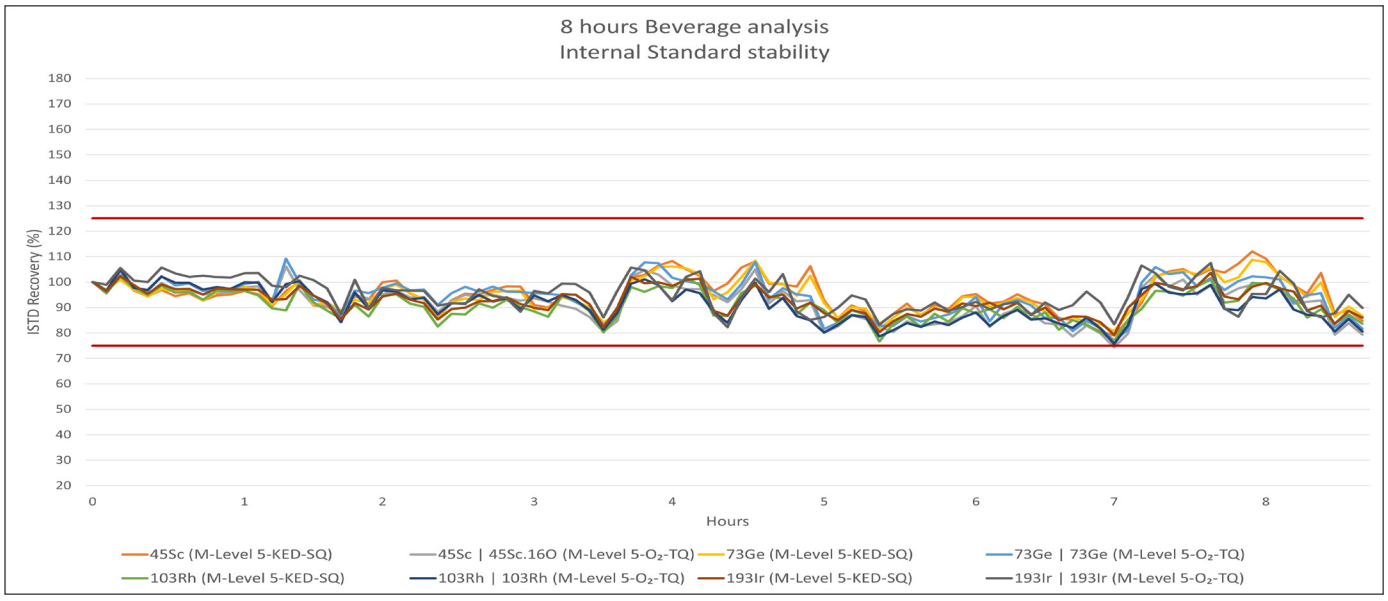
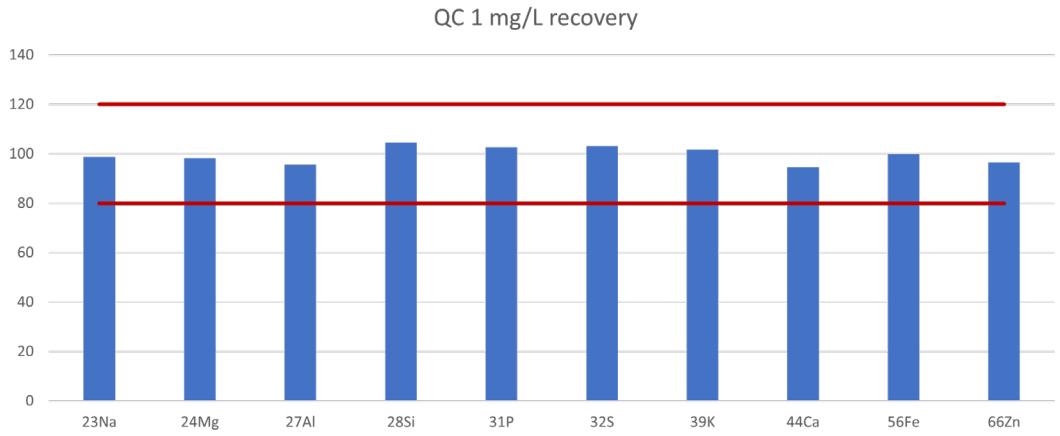
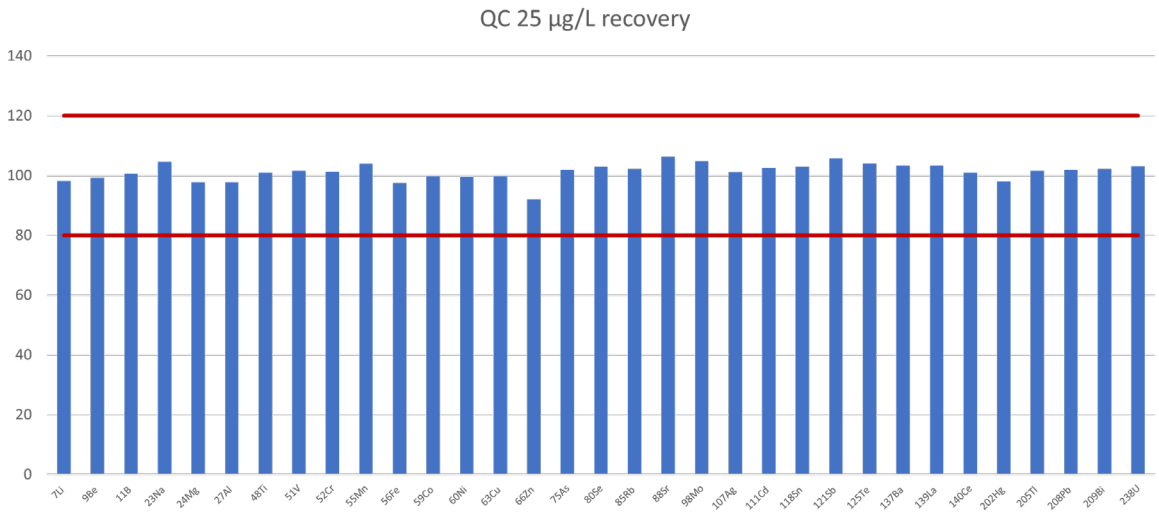


Figure 1. Internal standard stability (Sc, Ge, Rh, Ir) for 8 hours of analysis of beverage samples





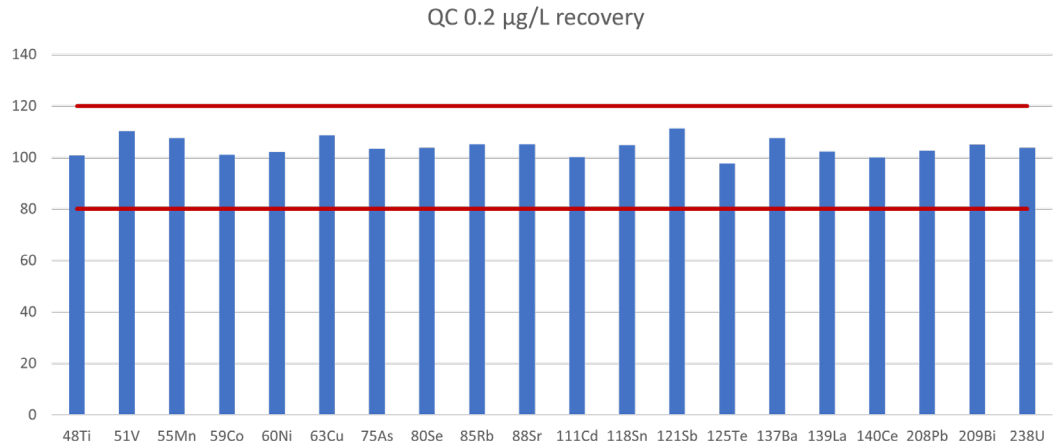


Figure 2. Average recovery of analytes in the QC checks, periodically analyzed during the entire sequence (N=5)

Accuracy

To test the workflow accuracy, two Standard Reference Material (SRM) were prepared and analyzed in the same way as all unknown samples. NIST SRM 3282 Low Calorie Cranberry is certified for a wide range of abundant nutrients and was also microwave digested. LGC6027 Soft Drinking Water was analyzed directly without any sample preparation. All results are given in Table 8.

The majority of elements certified for one or both of the two SRM showed excellent recovery between 85% and 115% and allowed validation of the accuracy of the workflow for both nutrients present in high concentrations (hundreds of mg/kg) as well as toxic elements at very low concentration (below 1 µg/kg).

To additionally verify the accuracy for all elements present in the method and to check the sample preparation efficiency, all samples were spiked before the microwave digestion with a target concentration of 10 µg/L for the trace elements and 10 mg/L for the nutrients. Except for boron and manganese, for which the spike concentration of 10 µg/L was not sufficient in respect to concentrations present in the samples, the spike recoveries for trace and major elements were found to be between 80% and 120%, again demonstrating the excellent accuracy of the workflow from the sample preparation to the acquisition.

Results and discussion

The thirteen samples analyzed in this study were found to contain variable levels of nutrient elements and generally very low levels of potentially toxic elements (Table 9) and found to be below regulated exposure limits in all cases. Only the two grape juices revealed arsenic and lead concentrations above 5 µg/kg.

Table 8. Certified values, concentration measured, and percentage recoveries of SRM samples (high concentrations in mg/kg or mg/L are highlighted in blue)

	NIST 3282 - low-calorie cranberry (µg/kg; mg/kg in blue)			LGC6027 – soft drinking water (µg/L; mg/L in blue)		
	Certified value	Concentration measured	Recovery (%)	Certified value	Concentration measured	Recovery (%)
^{7}Li				10.4 ± 0.6	9.08 ± 1.01	87
^{9}Be				5.09 ± 0.22	4.75 ± 0.47	93
^{11}B				1006 ± 49	912 ± 53	91
^{23}Na	201 ± 20	189 ± 1	94	4.36 ± 0.29	3.97 ± 0.10	91
^{24}Mg	13.0 ± 0.8	11.5 ± 0.3	88	1.03 ± 0.04	0.89 ± 0.02	87
^{27}Al				196 ± 7	182 ± 3	93
^{31}P	8.68 ± 0.60	8.98 ± 0.20	103			
^{39}K	247 ± 12	219 ± 3	89	0.37 ± 0.02	0.35 ± 0.01	95
^{44}Ca	26.3 ± 1.6	28.4 ± 2.0	108	8.53 ± 0.16	9.83 ± 0.17	115
^{51}V				4.93 ± 0.21	4.48 ± 0.22	91
^{52}Cr				49.9 ± 1.1	45.8 ± 1.9	92
^{55}Mn	493 ± 16	467 ± 17	95	49.9 ± 1.1	45.0 ± 1.8	90
^{56}Fe	540 ± 14	531 ± 22	98	200 ± 3	185 ± 6	93
^{59}Co				4.87 ± 0.17	4.30 ± 0.21	88
^{60}Ni				20.0 ± 0.5	17.5 ± 0.6	87
^{63}Cu	154 ± 61	197 ± 3	85	1995 ± 66	1564 ± 68	78
^{66}Zn				613 ± 19	593 ± 21	97
^{75}As				10.0 ± 0.4	8.82 ± 0.24	88
^{80}Se				10.2 ± 0.4	9.24 ± 0.55	90
^{88}Sr				496 ± 24	454 ± 21	92
^{98}Mo				4.62 ± 0.40	4.44 ± 0.34	96
^{111}Cd				5.09 ± 0.24	4.78 ± 0.10	94
^{121}Sb				5.21 ± 0.24	5.14 ± 0.09	99
^{137}Ba				116 ± 4	113 ± 2	98
^{205}Tl				4.88 ± 0.32	4.66 ± 0.06	96
^{208}Pb				10.2 ± 0.2	9.30 ± 0.14	92
^{238}U				4.95 ± 0.26	4.89 ± 0.11	99

Table 9. Multielement composition of 13 beverage samples (high concentrations in mg/kg are highlighted in blue)

	Label	Apple juice 1	Orange juice	Cranberry juice	Prune juice	Grape juice	Peach tea	Coconut water	Multifruit	Apple juice 2	Muscat grape juice	Sweet orange	Cola soda	Refreshing drink
	Amount (g)	5.211	5.141	5.235	5.242	5.254	5.111	5.108	5.169	5.207	5.267	5.842	4.996	5.091
^{7}Li	µg/kg	<LOD	<LOD	2.98	<LOD	3.48	4.65	<LOD	3.27	0.61	7.70	<LOD	0.71	1.88
^{9}Be	µg/kg	1.27	0.70	0.38	<LOD	<LOD	0.37	0.82	1.05	0.67	<LOD	0.24	0.71	0.74
^{11}B	µg/kg	1697	1084	146.5	2296	4115	469.9	830.8	2199	1147	3763	1233	143.2	87.39
^{23}Na	mg/kg	7.77	2.06	6.29	6.84	29.35	153.3	217.5	13.13	8.56	16.01	3.10	14.35	16.68
^{24}Mg	mg/kg	28.60	86.95	14.29	85.96	53.43	6.64	116.7	54.44	24.27	60.96	90.03	0.12	3.96
^{27}Al	µg/kg	43.89	140.3	76.97	218.5	608.7	1656	14.13	440.1	69.65	1630	83.52	69.33	53.56
^{28}Si	mg/kg	5.09	7.41	6.28	9.10	14.31	7.15	65.78	12.83	4.94	14.44	4.80	8.36	7.94
^{31}P	mg/kg	80.93	189.1	13.06	221.6	102.1	4.68	67.54	94.60	58.14	126.5	185.2	0.17	1.88
^{32}S	mg/kg	13.86	44.67	17.61	28.46	45.75	17.00	55.55	25.85	14.43	83.61	55.65	54.42	8.57
^{39}K	mg/kg	861.6	1371	185.5	1853	813.0	46.08	1648	1101	828.7	1048	1651	0.84	37.40
^{44}Ca	mg/kg	24.48	70.01	31.71	95.42	88.97	21.38	182.9	63.70	17.05	116.2	86.30	1.20	20.49
^{48}Ti	µg/kg	<LOD	16.20	3.34	18.37	25.14	2.17	3.95	18.26	4.13	131.2	13.04	5.72	2.96
^{51}V	µg/kg	<LOD	0.34	0.59	0.50	45.71	0.35	0.36	3.69	0.30	325.5	0.67	0.57	0.52
^{52}Cr	µg/kg	2.19	1.90	3.34	11.61	13.17	1.78	0.83	10.32	1.61	35.37	3.35	3.20	0.79
^{55}Mn	µg/kg	191.0	337.6	627.4	612.6	646.1	722.1	3515	636.1	118.4	613.3	287.7	1.74	9.74
^{56}Fe	µg/kg	96.49	573.3	248.52	3231	1086	35.86	86.17	742.8	55.88	2789	695.9	15.28	35.90
^{59}Co	µg/kg	1.59	3.13	0.41	1.82	1.07	0.33	1.19	1.61	0.56	2.46	2.63	0.03	0.10
^{60}Ni	µg/kg	4.39	10.33	17.77	39.86	10.83	7.66	531.0	18.38	2.02	13.26	9.24	1.87	1.03
^{63}Cu	µg/kg	161.2	263.5	42.43	432.7	2724	11.24	81.89	136.4	192.8	519.9	361.6	1.60	3.52
^{66}Zn	µg/kg	350.7	317.6	184.9	958.7	217.5	95.07	166.6	522.4	258.1	829.1	387.7	339.0	871.6
^{75}As	µg/kg	0.92	0.30	0.56	1.09	5.74	0.54	0.21	1.70	0.47	12.95	<LOD	<LOD	0.29
^{80}Se	µg/kg	<LOD	0.09	<LOD	0.48	0.37	0.14	1.86	2.17	<LOD	0.39	<LOD	0.07	<LOD
^{85}Rb	µg/kg	420.0	1328	128.1	1346	828.5	108.0	5166	885.9	339.1	1246	1451	0.42	24.06
^{88}Sr	µg/kg	19.75	340.5	175.0	203.9	481.3	161.2	161.6	184.8	16.72	460.6	415.9	2.65	58.46
^{98}Mo	µg/kg	2.97	5.12	1.68	6.29	12.11	0.67	2.00	5.73	3.03	43.51	5.83	0.62	0.36
^{107}Ag	µg/kg	<LOD	0.03	<LOD	0.47	0.07	0.06	0.13	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
^{111}Cd	µg/kg	0.06	<LOD	0.71	0.16	0.39	<LOD	0.34	0.60	0.07	0.19	0.02	0.02	0.06
^{118}Sn	µg/kg	2.10	4.65	5.02	11.02	4.15	7.67	0.85	1.74	1.27	1.43	0.45	0.82	0.43
^{121}Sb	µg/kg	0.07	<LOD	<LOD	0.13	0.79	0.11	<LOD	0.57	0.14	0.50	<LOD	0.34	0.32
^{125}Te	µg/kg	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.21	0.21	<LOD	<LOD	<LOD	<LOD
^{138}Ba	µg/kg	14.40	212.8	140.5	118.3	74.49	13.34	18.73	113.2	45.33	88.67	234.4	2.33	10.13
^{139}La	µg/kg	0.10	3.11	0.03	0.41	1.15	0.09	0.08	0.35	0.15	5.01	4.75	0.01	0.01
^{140}Ce	µg/kg	0.15	1.25	0.06	0.55	2.36	0.10	0.09	0.62	0.22	9.12	1.93	0.01	0.04
^{202}Hg	µg/kg	0.13	0.06	0.07	0.12	0.06	0.08	0.08	0.09	0.07	0.08	0.03	0.09	0.08
^{205}Tl	µg/kg	0.31	1.03	0.79	0.98	1.80	1.38	2.57	0.43	0.82	1.10	1.28	1.12	1.28
^{208}Pb	µg/kg	0.49	0.18	0.21	2.95	18.96	0.30	0.06	1.61	0.61	6.52	0.07	0.25	0.16
^{209}Bi	µg/kg	0.04	<LOD	0.03	0.07	0.33	0.05	0.02	0.08	0.04	0.06	0.06	0.02	0.04
^{238}U	µg/kg	0.01	0.02	0.10	0.10	0.83	0.14	0.01	0.30	0.05	1.12	0.01	0.01	0.04

For all beverages, the matrix composition can be displayed as the sum of the major components. As displayed in Figure 3, the total nutrient concentration and the composition is similar between each of the two juice samples from the same fruit type (apple, orange and grape).

Whereas all other juice types showed a similar matrix load (between 1,000 and 2,500 mg·L^{-1}) and composition (major component potassium, making up for typically 70–80% of the sample matrix), other sample types such as the processed beverages showed a completely different composition. For these beverages, including peach tea, cola soda, and a refreshing drink, the sum of the nutrient elements is significantly lower (79 to 256 mg·L^{-1}), as is the composition. This is highlighted in Figure 4. For peach tea, sodium accounts for roughly 60% of the nutrient elements, whereas in the refreshing drink potassium makes up about 40%, with calcium and sodium accounting for a similar amount together. The presence of sulfur in the soda can be explained by the adjunction of gases to make the soda fizzy.

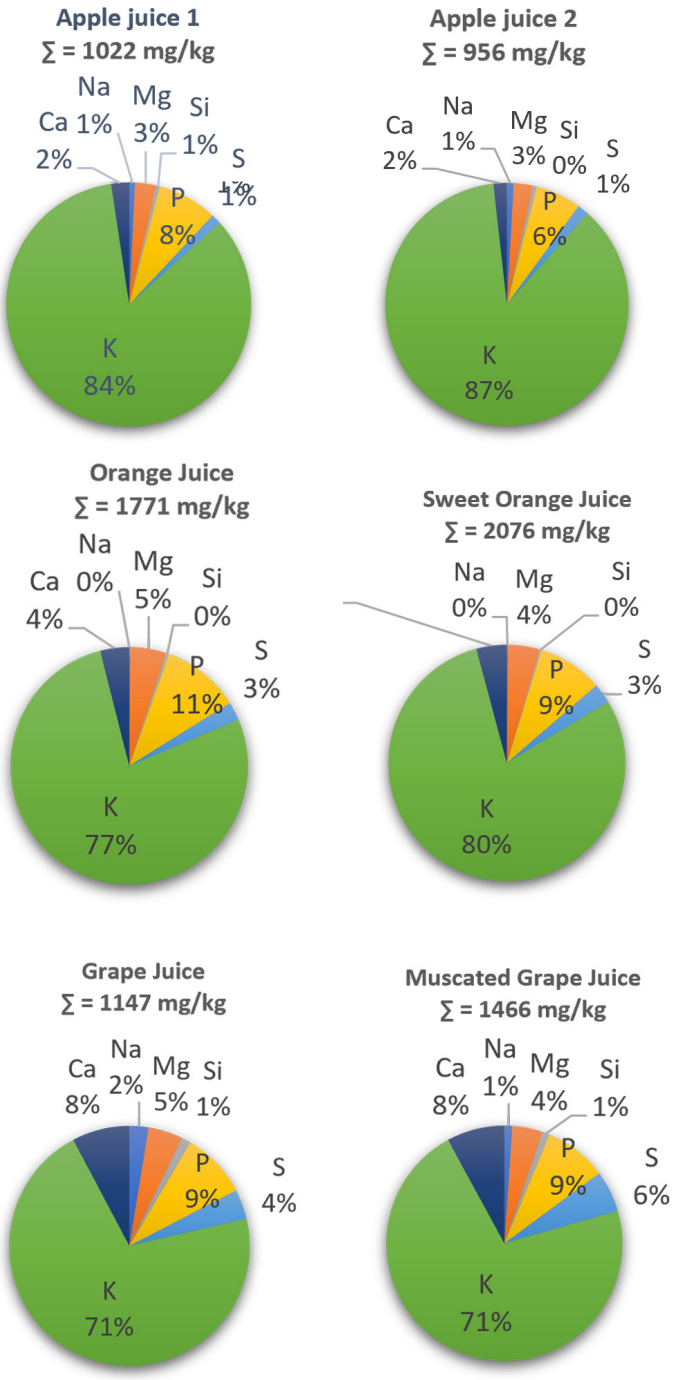


Figure 3. Nutrient composition of each fruit juice where two different samples were analyzed

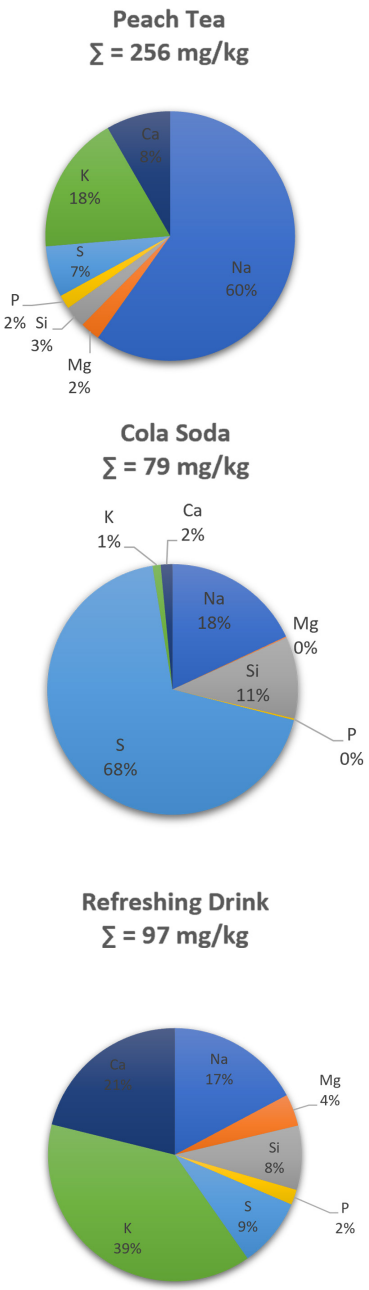


Figure 4. Nutrient composition of processed beverages

Conclusion

This workflow, combining sample preparation using microwave assisted digestion and analysis using the iCAP MTX ICP-MS, allows the determination of nutrient composition of fruit juices and processed beverages as required by the food labeling regulations and detection of any contaminants such as toxic elements present in the beverages.

The analytical method was proven to provide accurate and precise results and can provide reliable performance over long analysis sequences, ensuring productivity in an applied testing laboratory. Based on the automatic and constant 5-times dilution of all samples, there are no matrix effects that would lead to unwanted interruptions of the analysis due to QC failures. Samples can be placed on the autosampler after completing preparation; no additional dilution is required. All types of interferences (polyatomic as well as isobaric interference, including doubly charged ions) are effectively suppressed with either helium collision gas or by using oxygen as a reactive gas in triple quadrupole mode. The instrument method could be easily set up thanks to the Reaction Finder method development assistant for Qtegra ISDS Software.

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