Electronic Supplementary Material (ESI) for Journal of Analytical Atomic Spectrometry

SUPPLEMENTAL INFORMATION

Analytical method for total chromium and nickel in urine using an inductively coupled plasma-universal cell technology-mass spectrometer (ICP-UCT-MS) in kinetic energy discrimination (KED) mode

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Table S1. List of potential interferences for analyzing ^{52}Cr in urine. Masses determined using ThermoFinnigan Element2 ICP-MS Interference Workshop software.

^{52}Cr (m/z)	Potential Interference (AB)	Isotopic Abundance A %	Expected Concentration of A in Urine (µg L^{-1})	Isotopic Abundance B %	Expected Concentration of B in Urine (µg L^{-1})
51.4528	$^{103}Rh^{++}$	100	0.001 - 0.039	-	-
51.9520	$^{104}Pd^{++}$	11.1	0.07 - 0.64	-	-
51.9527	$^{104}Ru^{++}$	18.7	Expected to be low	-	-
51.9620	$^{36}S^{16}O^{+}$	0.02	High	99.8	atmosphere
51.9624	$^{12}C^{40}Ar^{+}$	98.9	High	99.6	ICP gas
51.9625	$^{36}Ar^{16}O^{+}$	0.3	ICP gas	99.8	atmosphere
51.9658	$^{14}N^{38}Ar^{+}$	99.6	atmosphere	0.06	ICP gas
51.9680	$^{35}Cl^{17}O^{+}$	75.8	≤ 5,900,000	0.04	atmosphere
52.4530	$^{105}Pd^{++}$	22.3	0.07 - 0.64	-	-
51.9518	$^{51}V^{1}H^{+}$	99.8	0.2 - 10	100	atmosphere
51.9626	$^{40}Ca^{12}C^{+}$	96.9	30,000 – 200,000	98.9	~ 5,000,000
51.9671	$^{39}K^{13}C^{+}$	93.3	542,000 - 9,770,000	1.1	~ 5,000,000
51.9660	$^{37}Cl^{15}N^{+}$	24.2	≤ 5,900,000	0.4	atmosphere
51.9768	$^{37}Cl^{14}N^{1}H^{+}$	24.2	≤ 5,900,000	99.6/100	atmosphere
51.9716	$^{35}Cl^{16}O^{1}H^{+}$	75.8	≤ 5,900,000	99.8/100	atmosphere
51.9699	$^{33}S^{19}F^{+}$	0.8	High	100	200 - 3,200
51.9676	$^{21}Ne^{31}P^{+}$	0.3	Expected to be low	100	220,000 - 2,600,000
51.9645	$^{20}Ne^{32}S^{+}$	90.5	Expected to be low	95.0	~ 5,000,000

Table S2. List of potential interferences for analyzing ^{60}Ni in urine. Masses determined using ThermoFinnigan Element2 ICP-MS Interference Workshop software.

^{60}Ni (m/z)	Potential Interference (AB)	Isotopic Abundance A %	Expected Concentration of A in Urine (µg L^{-1})	Isotopic Abundance B %	Expected Concentration of B in Urine (µg L^{-1})
59.4516	$^{119}Sn^{++}$	8.6	0.05 - 2.28	-	-
59.9504	$^{44}Ca^{16}O^{+}$	2.1	30,000 - 200,000	99.8	atmosphere
59.9511	$^{120}Sn^{++}$	32.6	0.05 - 2.28	-	-
59.9520	$^{120}Te^{++}$	0.1	Expected to be low	-	-
59.9526	$^{24}Mg^{36}Ar^{+}$	79	40,500 - 243,000	0.3	ICP gas
59.9541	$^{22}Ne^{38}Ar^{+}$	9.2	Expected to be low	0.06	ICP gas
59.9548	$^{20}Ne^{40}Ar^{+}$	90.5	Expected to be low	99.6	ICP gas
60.4519	$^{121}Sb^{++}$	57.3	0.12 - 10.0	-	-
59.9410	$^{59}Co^{1}H^{+}$	100	0.28 - 2.0	100	atmosphere
59.9495	$^{58}Ni^{2}H^{+}$	68.3	0.055 - 20.0	0.02	atmosphere
59.9480	$^{48}Ti^{12}C^{+}$	73.8	0.1 - 3.7	98.9	~ 5,000,000
59.9525	$^{48}Ca^{12}C^{+}$	0.2	30,000 - 200,000	98.9	~ 5,000,000
59.9551	$^{47}Ti^{13}C^{+}$	7.3	0.1 - 3.7	1.1	~ 5,000,000
59.9557	$^{46}Ti^{14}N^{+}$	8.0	0.1 - 3.7	99.6	atmosphere
59.9560	$^{45}Sc^{15}N^{+}$	100	-	0.4	atmosphere
59.9668	$^{45}Sc^{14}N^{1}H^{+}$	100	-	99.6/100	atmosphere
59.9615	$^{43}Ca^{16}O^{1}H^{+}$	0.1	30,000 - 200,000	99.8/100	atmosphere
59.9688	$^{41}K^{18}O^{1}H^{+}$	6.7	542,000 - 9,770,00	0.2/99.9	atmosphere
59.9602	$^{41}K^{19}F^{+}$	6.7	542,000 - 9,770,00	100	200 - 3,200
59.9503	$^{29}Si^{31}P^{+}$	4.7	100 - 51,600	100	220,000 - 2,600,000
59.9490	$^{28}Si^{32}S^{+}$	92.2	100 - 51,600	95.0	~ 5,000,000
59.9505	$^{26}Mg^{34}S^{+}$	11.0	40,500 - 243,000	4.2	~ 5,000,000
59.9521	$^{24}Mg^{36}S^{+}$	79.0	40,500 - 243,000	0.02	~ 5,000,000
59.9530	$^{27}Al^{33}S^{+}$	100	5 - 30	0.8	~ 5,000,000
59.9547	$^{25}Mg^{35}Cl^{+}$	10.0	40,500 - 243,000	75.8	~ 6,000,000
59.9557	$^{23}Na^{37}Cl^{+}$	100	281 - 10,110	24.2	~ 6,000,000

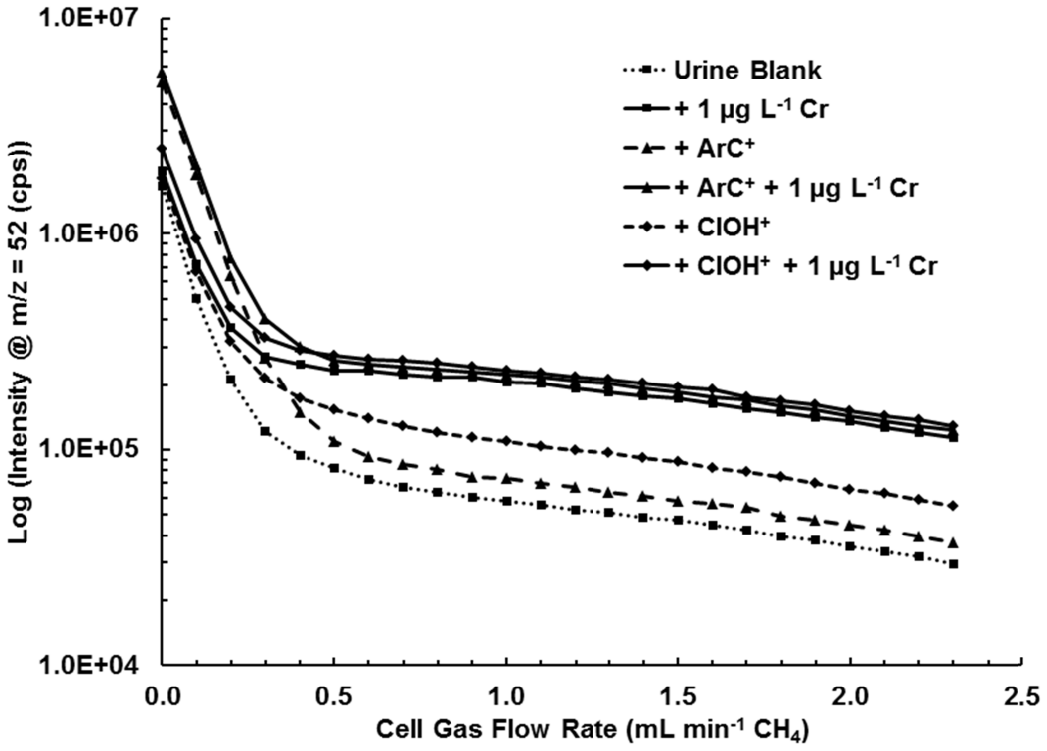


Figure S1a. The effects of cell gas flow rate on ion signal intensity at m/z 52 using methane gas on Cr analysis in urine samples spiked with 1 µg L^{-1} Cr, 1% ethanol ($^{40}Ar^{12}C^{+}$), and/or 1% HCl ($^{35}Cl^{16}O^{1}H^{+}$).

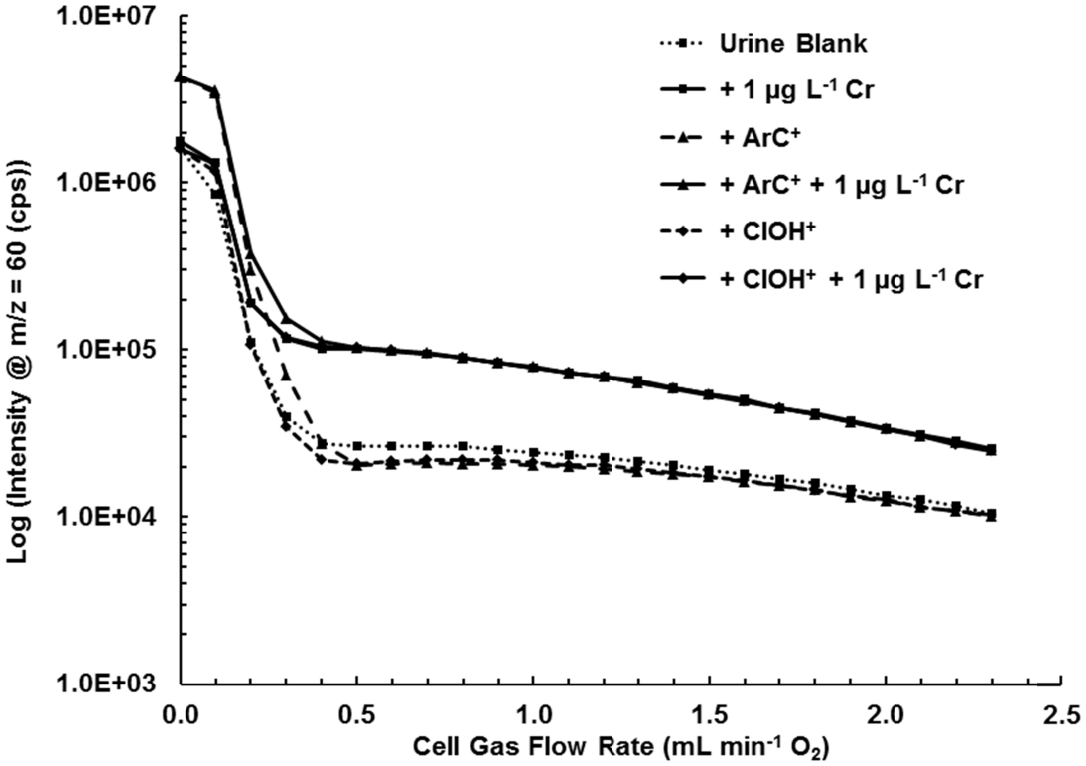


Figure S1b. The effects of cell gas flow rate on ion signal intensity at m/z 52 using oxygen gas on Cr analysis in urine samples spiked with 1 µg L^{-1} Cr, 1% ethanol ($^{40}Ar^{12}C^{+}$), and/or 1% HCl ($^{35}Cl^{16}O^{1}H^{+}$).

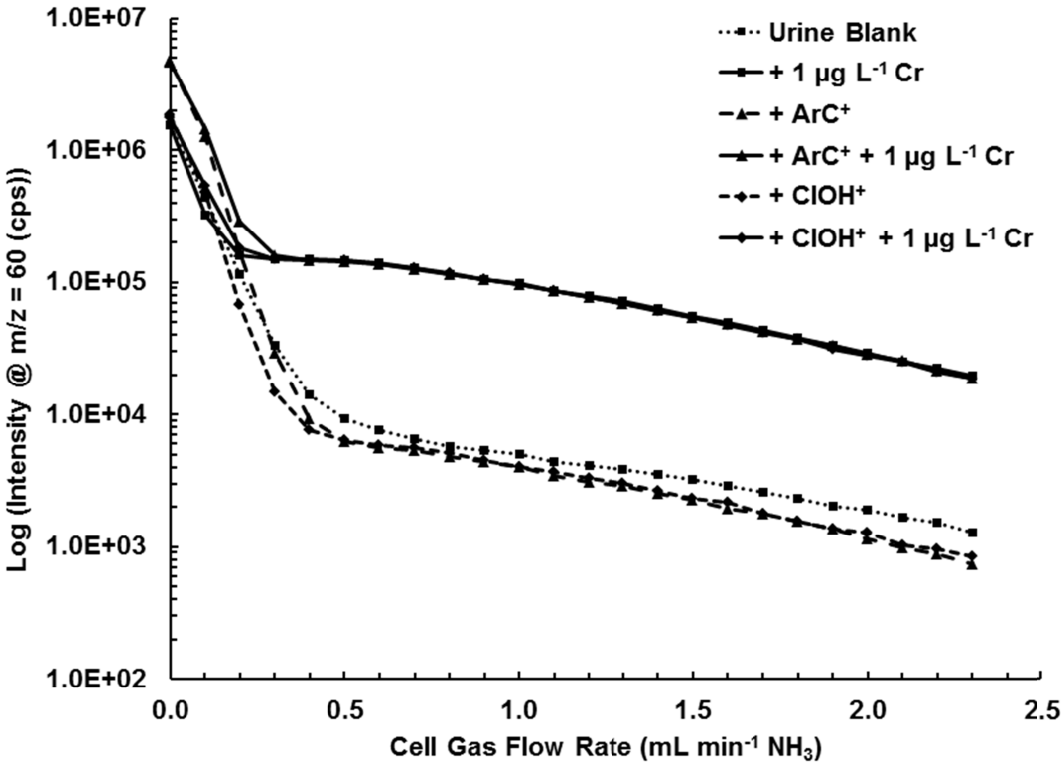
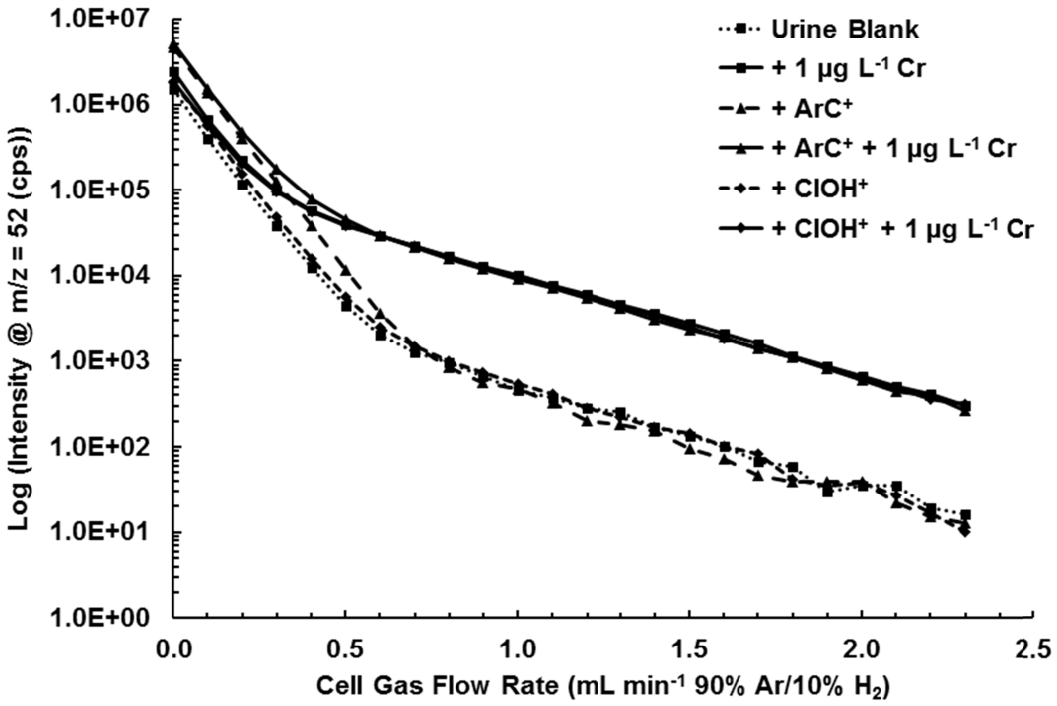


Figure S1c. The effects of cell gas flow rate on ion signal intensity at m/z 52 using ammonia gas on Cr analysis in urine samples spiked with 1 µg L^{-1} Cr, 1% ethanol ($^{40}Ar^{12}C^{+}$), and/or 1% HCl ($^{35}Cl^{16}O^{1}H^{+}$).



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43 **Figure S1d.** The effects of cell gas flow rate on ion signal intensity at m/z 52 using
44 argon/hydrogen gas on Cr analysis in urine samples spiked with 1 µg L^{-1} Cr, 1% ethanol
45 ($^{40}Ar^{12}C^{+}$), and/or 1% HCl ($^{35}Cl^{16}O^{1}H^{+}$).

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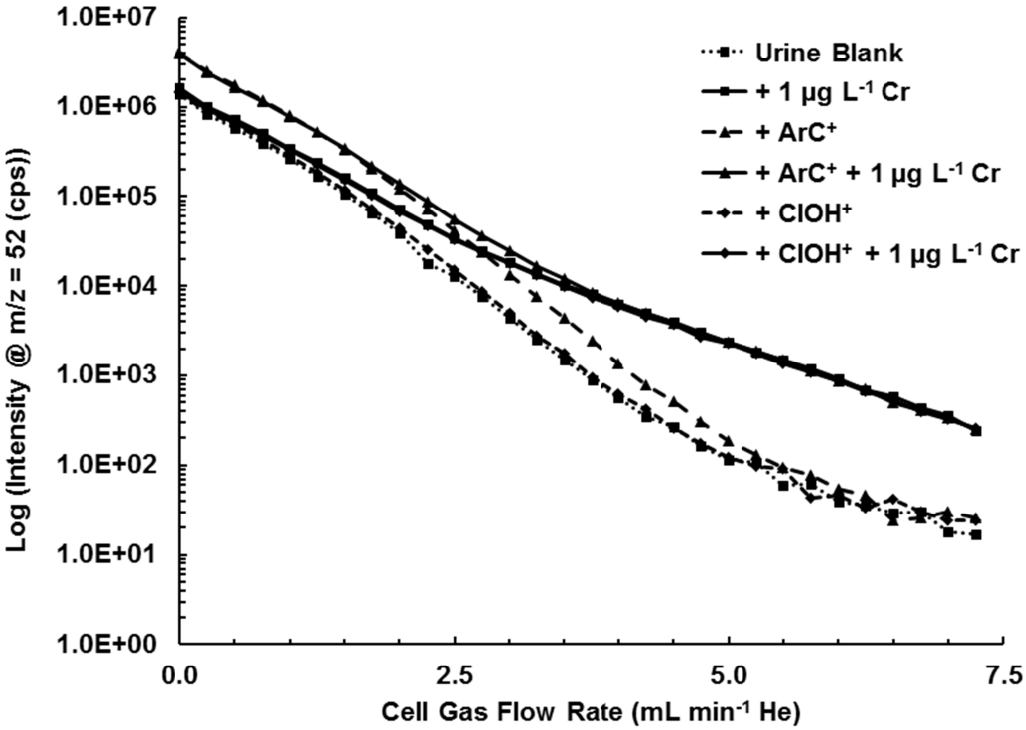


Figure S1e. The effects of cell gas flow rate on ion signal intensity at m/z 52 using helium gas on Cr analysis in urine samples spiked with 1 µg L^{-1} Cr, 1% ethanol ($^{40}Ar^{12}C^{+}$), and/or 1% HCl ($^{35}Cl^{16}O^{1}H^{+}$).

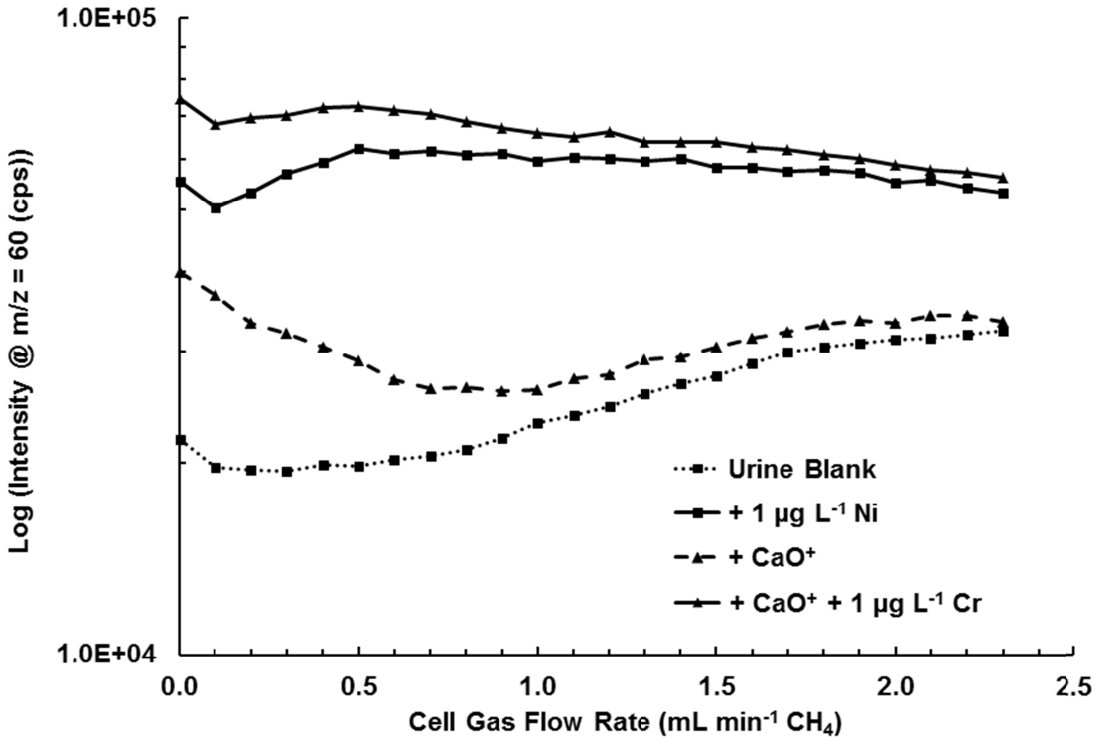


Figure S2a. The effects of cell gas flow rate on ion signal intensity at m/z 60 using methane gas on Ni analysis in urine samples spiked with 1 µg L^{-1} Ni and/or 1% ethanol + 20 mg L^{-1} Ca ($^{44}Ca^{16}O^{+}$).

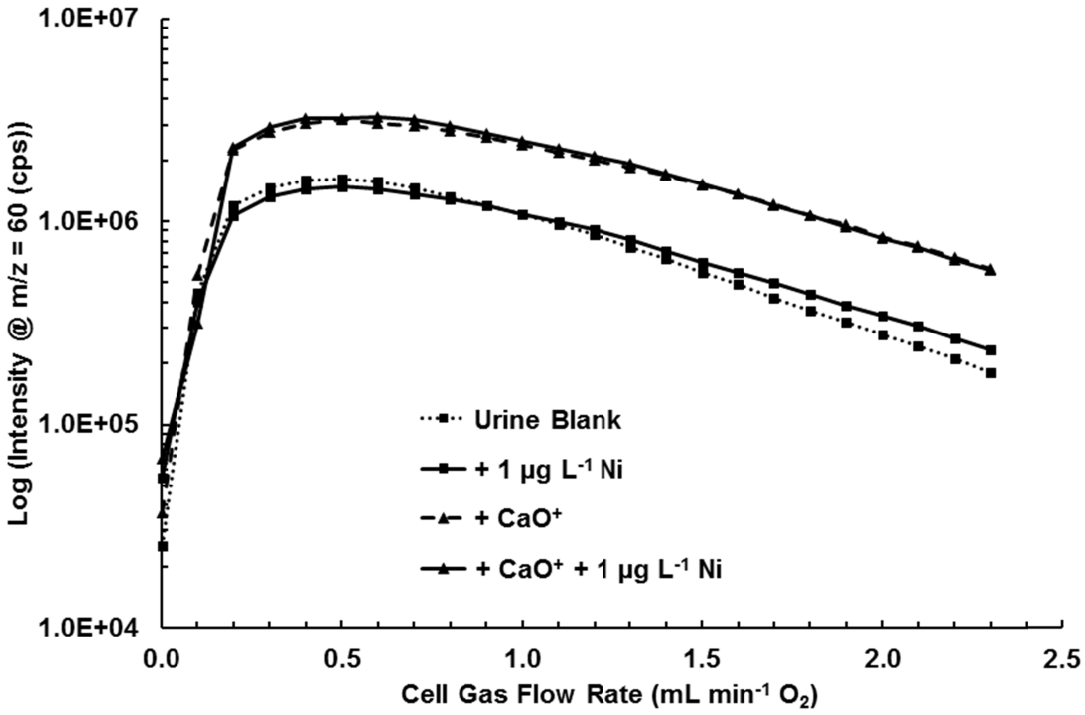
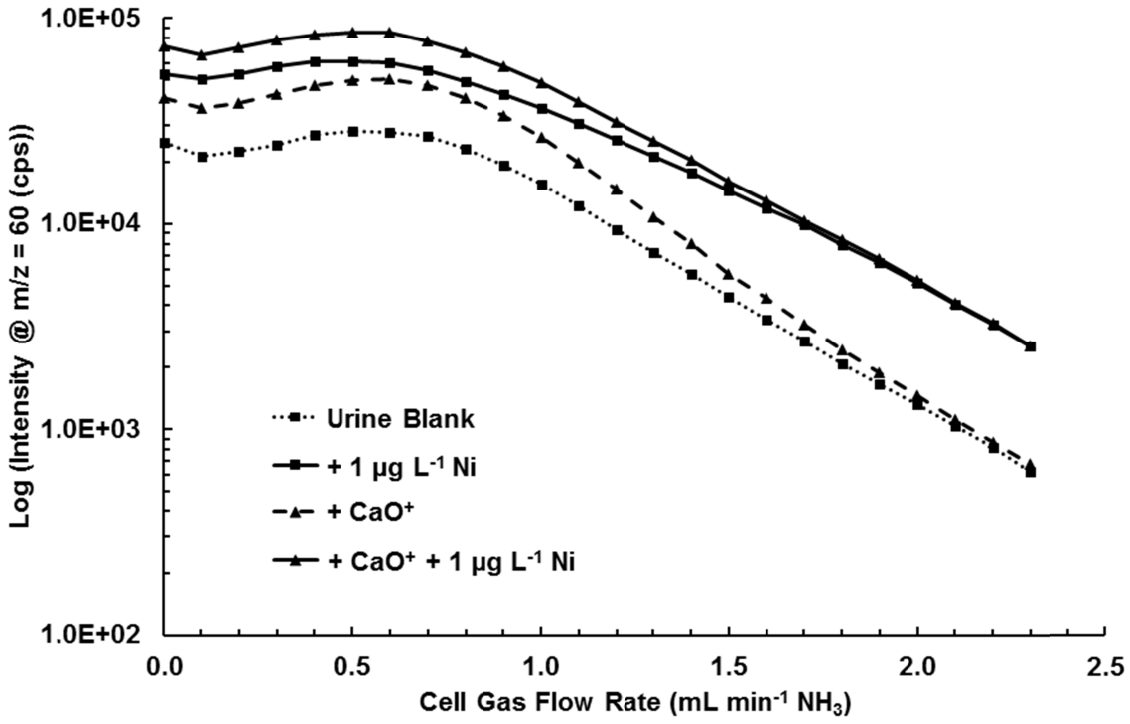


Figure S2b. The effects of cell gas flow rate on ion signal intensity at m/z 60 using oxygen gas on Ni analysis in urine samples spiked with 1 µg L^{-1} Ni and/or 1% ethanol + 20 mg L^{-1} Ca ($^{44}Ca^{16}O^{+}$).



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65 **Figure S2c.** The effects of cell gas flow rate on ion signal intensity at m/z 60 using
66 ammonia gas on Ni analysis in urine samples spiked with 1 µg L^{-1} Ni and/or 1% ethanol
67 + 20 mg L^{-1} Ca ($^{44}Ca^{16}O^{+}$).

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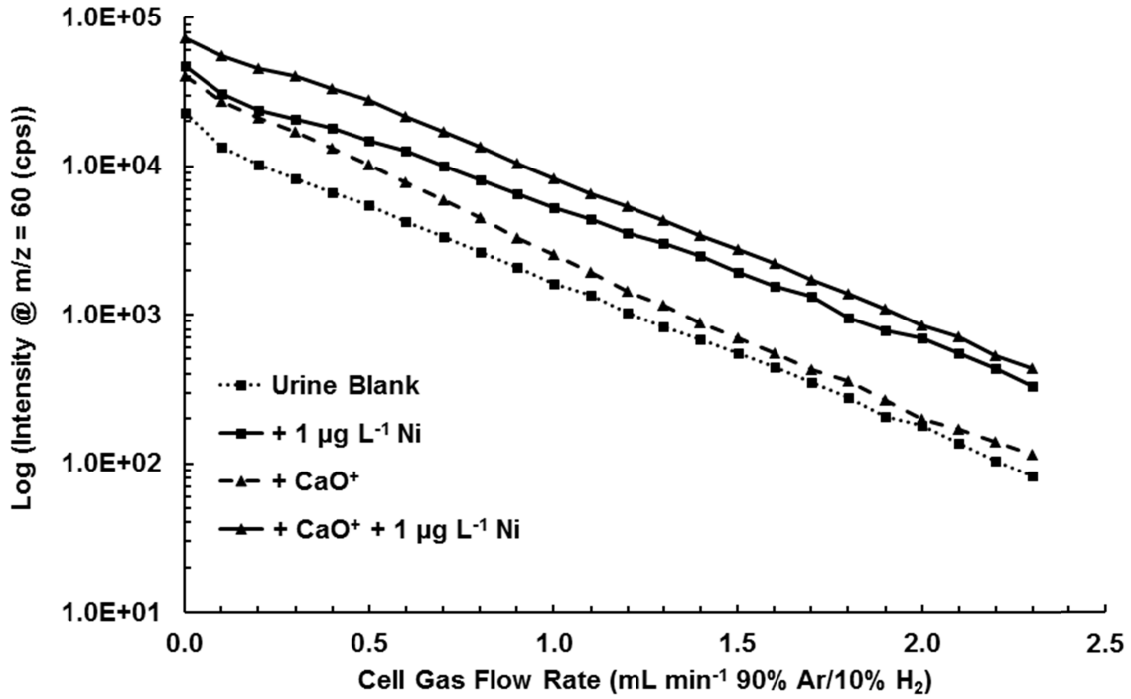

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70 **Figure S2d.** The effects of cell gas flow rate on ion signal intensity at m/z 60 using
71 argon/hydrogen gas on Ni analysis in urine samples spiked with 1 µg L^{-1} Ni and/or 1%
72 ethanol + 20 mg L^{-1} Ca ($^{44}Ca^{16}O^{+}$).

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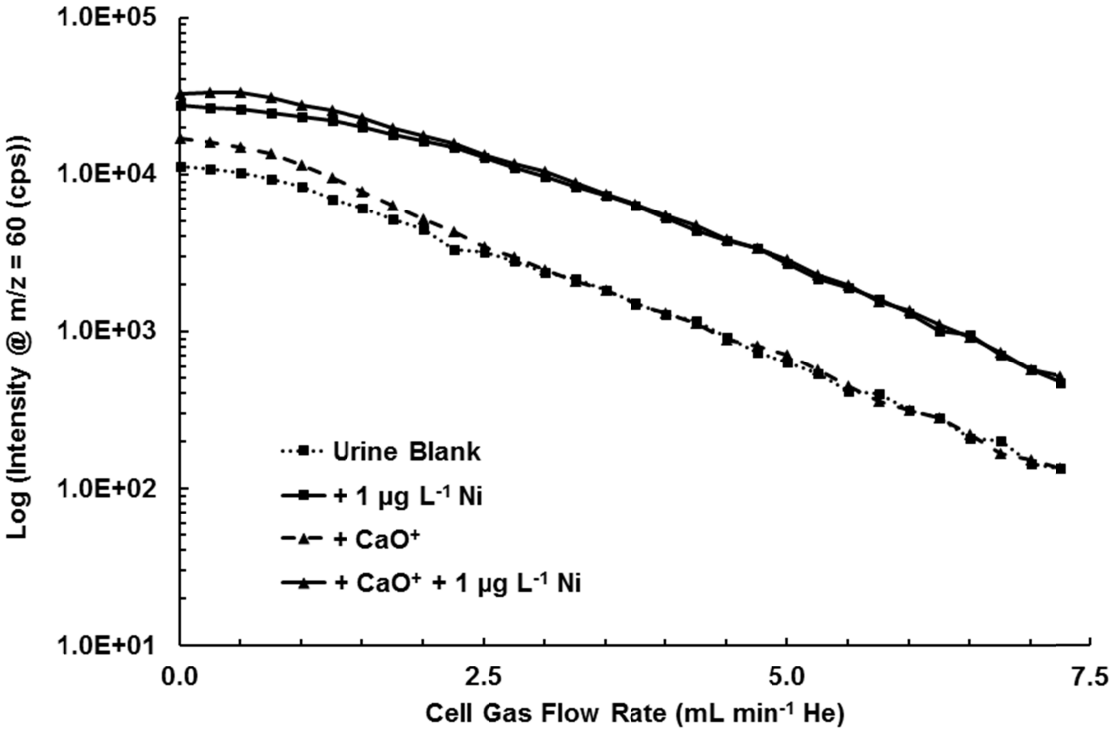

Figure S2e. The effects of cell gas flow rate on ion signal intensity at m/z 60 using helium gas on Ni analysis in urine samples spiked with 1 µg L^{-1} Ni and/or 1% ethanol + 20 mg L^{-1} Ca ($^{44}Ca^{16}O^{+}$).

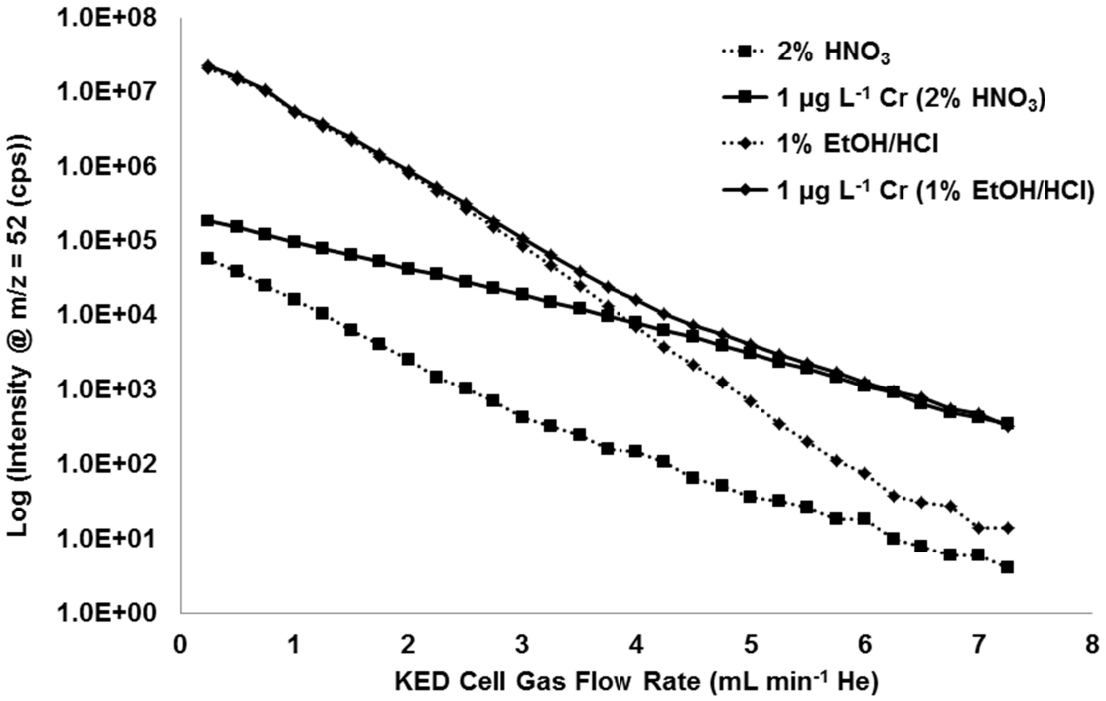

Figure S3. Displays the response at m/z 52 for 2% HNO_3, 1% EtOH, and/or 1 µg L^{-1} Cr under increasing helium cell gas flow rates in KED mode.

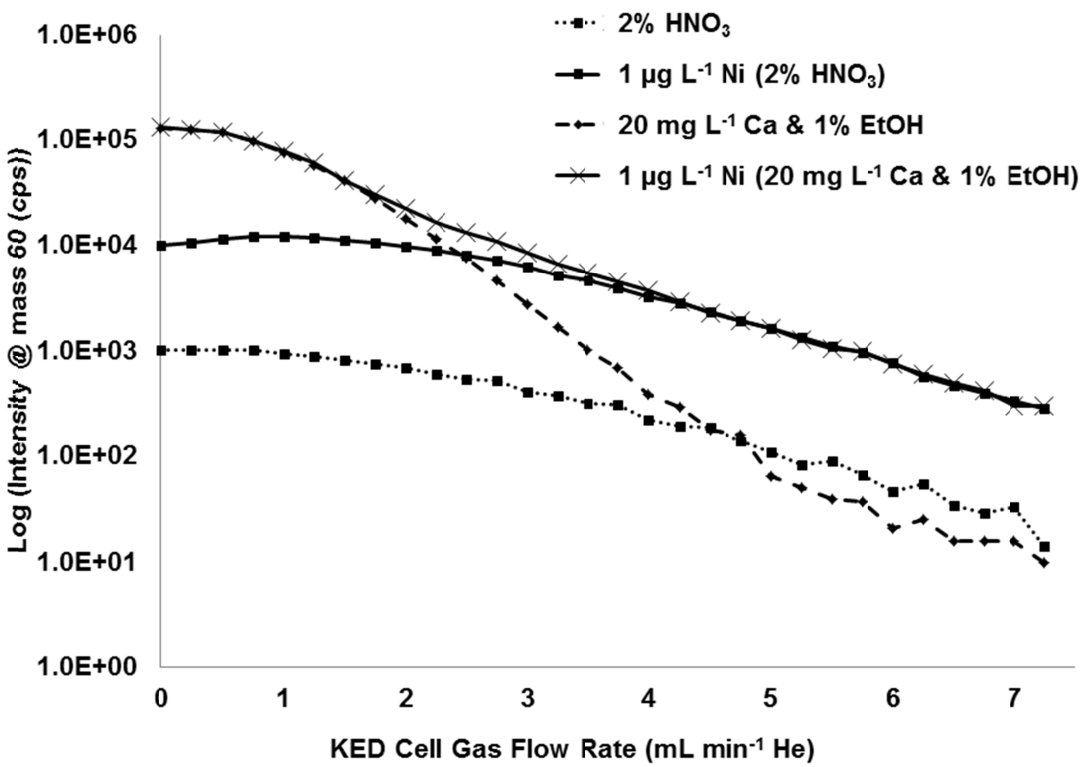

Figure S4. Displays the response at m/z 60 for 2% HNO_3, 1% EtOH and 20 mg L^{-1} Ca, and/or 1 µg L^{-1} Ni under increasing helium cell gas flow rates in KED mode.

Table S3. ESI FAST method control parameters that control the functions for the autosampler events during the NexION ICP-MS wash time.

Event	Action	Parameters	Parameter Units
On Probe Down	Vacuum1 On		
On Probe Down	Load1		
Probe In Sample	Timer A	4	seconds
Timer A Expires	Inject1		
Timer A Expires	Move Rinse		
Rinse Completed	Probe Up		
On Rinse	Vacuum1 On		
On Rinse	Load1		
On Rinse	Probe Down		
On Rinse	Timer B	2	seconds
Timer B Expires	Probe Up		
Timer B Expires	Timer C	2	seconds
Timer C Expires	Probe Down		
Timer C Expires	Timer D	2	seconds
Timer D Expires	Probe Up		
Timer D Expires	Timer E	2	seconds
Timer E Expires	Probe Down		
Timer E Expires	Timer F	2	seconds
Timer F Expires	Move Next		

Table S4. In house CDC quality control samples used to show % recovery of the method. N = 5.

	Cr		
Sample ID	**Target (µg L^{-1})**	**Average ± 1 SD (µg L^{-1})**	**% Recovery ± 1 SD**
Low QC	0.820	0.885 ± 0.128	
+ 1 µg L^{-1}	1.82	1.75 ± 0.13	96.3 ± 7.1
+ 3 µg L^{-1}	3.82	3.87 ± 0.53	101 ± 14
+ 10 µg L^{-1}	10.8	10.6 ± 0.2	98.4 ± 1.9
	Ni		
Sample ID	**Target (µg L^{-1})**	**Average ± 1 SD (µg L^{-1})**	**% Recovery ± 1 SD**
Low QC	1.36	1.59 ± 0.10	
+ 1 µg L^{-1}	2.36	2.44 ± 0.12	103 ± 5
+ 3 µg L^{-1}	4.36	4.38 ± 0.40	101 ± 9
+ 10 µg L^{-1}	11.4	11.1 ± 0.3	97.9 ± 2.6