

Supplementary Information

Rapid Automated Total Arsenic and Arsenic Speciation by Inductively Coupled Plasma Mass Spectrometry

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Table S1. Comparison of results from the total arsenic measurements to reference values. Reference values provided by NYDOH (UE) and CTQ (QM and PC). n = 3.

Proficiency Testing Sample ID	Reference Value ($\mu\text{g L}^{-1}$ As)	Measured Value ($\mu\text{g L}^{-1}$ As)
UE19-10	188 \pm 38	207 \pm 13
UE19-11	3.7 \pm 6	4.0 \pm 0.2
UE20-06	61 \pm 12	57 \pm 1
UE20-08	21 \pm 6	20 \pm 1
UE20-10	101 \pm 20	109 \pm 7
QM-U-Q2004	93.3 \pm 1.1	89.0 \pm 0.8
QM-U-Q2005	49.9 \pm 0.5	51.4 \pm 3.8
QM-U-Q2006	32.4 \pm 0.4	32.8 \pm 2.1
QM-U-Q2013	42.3 \pm 0.5	44.1 \pm 2.4
QM-U-Q2014	378 \pm 4	362 \pm 14
QM-U-Q2015	86 \pm 1	85 \pm 4
PC-U-S1907	128 \pm 20	131 \pm 7
PC-U-S1908	172 \pm 27	173 \pm 6
PC-U-S1912	631 \pm 95	633 \pm 18
PC-U-S1913	26.2 \pm 5.6	26.5 \pm 1.6
PC-U-S2008	378 \pm 52	375 \pm 9

Table S2. Comparison of results from the one-column arsenic speciation measurements to reference values. Reference values provided by NYDOH (UE) and CTQ (QM and PC). n = 3.

	Total As Target (Ref. Range)	iAs Target (Ref. Range)	One-Column Method ($\mu\text{g L}^{-1}$ As)						Sum	iAs
			As III	DMA	AsC	MMA	As V	AsB		
PC-U-S1907	128 (108-148)	2.44 (0.475-4.41)	0.909 ± 0.036	1.84 ± 0.19	0	0	0.395 ± 0.042	129 ± 4	132	1.30
PC-U-S1908	172 (145-199)	153 (122-184)	0	1.69 ± 0.11	0	0.471 ± 0.011	149 ± 12	10.4 ± 1.1	162	149
PC-U-S1912	631 (535-726)	2.08 (0.123-4.03)	2.45 ± 0.21	2.01 ± 0.11	0	0	0	647 ± 22	651	2.45
PC-U-S1913	26.2 (20.6-31.8)	23.9 (17.5-30.3)	18.3 ± 1.0	4.28 ± 0.04	0	0	1.70 ± 0.15	0	24.3	20.0
PC-U-S2008	378 (326-430)	2.73 (1.08-4.38)	0.635 ± 0.011	4.80 ± 0.02	0	0.172 ± 0.005	1.69 ± 0.08	366 ± 28	373	2.33
QM-U-Q2004	93.3 (92.2-94.4)	80.4	72.0 ± 3.5	3.04 ± 0.11	0	0	6.17 ± 0.49	6.84 ± 0.11	88.0	78.2
QM-U-Q2005	49.9 (49.4-50.4)	40.2	0	1.72 ± 0.08	0	2.64 ± 0.23	40.9 ± 1.7	3.02 ± 0.16	48.3	40.9
QM-U-Q2006	32.4 (32.0-32.8)	28.7	27.8 ± 2.2	1.73 ± 0.06	0	0	1.98 ± 0.24	1.67 ± 0.01	33.2	29.8
QM-U-Q2013	42.3 (41.8-42.8)	6.12	6.90 ± 0.11	20.1 ± 0.9	0	4.44 ± 0.24	2.56 ± 0.19	6.15 ± 0.09	40.2	9.46
QM-U-Q2014	378 (374-382)	0	0	2.18 ± 0.11	0	0	0	383 ± 22	385	0
QM-U-Q2015	86.0 (85.0-87.0)	0	0	74.1 ± 2.8	0	0	0	8.89 ± 0.38	83.0	0
UE19-10	188 (150-226)	-	120 ± 4	1.76 ± 0.18	0.373 ± 0.050	0	60.5 ± 2.4	7.39 ± 0.16	190	181
UE19-11	3.70 (0.0-9.7)	-	1.45 ± 0.05	0.560 ± 0.020	1.71 ± 0.02	0	1.33 ± 0.18	3.10 ± 0.08	8.15	2.78
UE20-06	61.0 (49-73)	-	21.9 ± 1.6	9.22 ± 0.45	7.72 ± 0.15	3.95 ± 0.10	7.84 ± 0.42	26.1 ± 1.9	76.7	29.7
UE20-08	21.0 (15-27)	-	19.8 ± 0.2	0.538 ± 0.036	2.26 ± 0.09	0	2.06 ± 0.09	2.71 ± 0.03	27.4	21.9
UE20-10	101 (81-121)	-	54.9 ± 3.1	10.7 ± 0.5	6.52 ± 0.23	0	16.5 ± 0.3	24.5 ± 1.5	113	71.4
Urine Spike 1	60	20	10.5 ± 0.4	9.78 ± 0.43	10.4 ± 0.4	10.5 ± 0.6	9.23 ± 0.75	9.54 ± 0.34	60.0	19.7
Urine Spike 2	60	20	10.2 ± 0.4	9.3 ± 0.5	10.7 ± 0.4	9.67 ± 0.41	10.7 ± 0.6	10.2 ± 0.6	60.8	20.9

Table S3. One and two-column arsenic speciation method results compared to the CTQ QM reference values. Samples are sorted by arsenic species. n = 3.

	Target Value ($\mu\text{g L}^{-1}$)	One-Column Method Measured Value ($\mu\text{g L}^{-1}$)	Two-Column Method Measured Value ($\mu\text{g L}^{-1}$)
	As III	As III	As III
QM-U-Q2004	77.3 \pm 6.7	72.0 \pm 3.5	82.7 \pm 4.9
QM-U-Q2006	26.8 \pm 2.2	27.8 \pm 2.2	27.8 \pm 2.4
QM-U-Q2013	6.12 \pm 0.06	6.90 \pm 0.11	5.37 \pm 0.25
	As V	As V	As V
QM-U-Q2004	3.1 \pm 0.2	6.17 \pm 0.49	5.15 \pm 0.61
QM-U-Q2005	40.2 \pm 1.8	40.9 \pm 1.7	46.1 \pm 6.0
QM-U-Q2006	1.92 \pm 0.73	1.98 \pm 0.24	1.89 \pm 0.21
QM-U-Q2013	-	2.56 \pm 0.19	2.91 \pm 0.31
	AsB	AsB	AsB
QM-U-Q2004	6.65 \pm 0.25	6.84 \pm 0.11	6.87 \pm 0.52
QM-U-Q2005	3.05 \pm 0.28	3.02 \pm 0.16	3.20 \pm 0.19
QM-U-Q2006	1.24 \pm 0.38	1.67 \pm 0.01	1.49 \pm 0.08
QM-U-Q2013	5.66 \pm 0.12	6.15 \pm 0.09	5.71 \pm 0.34
QM-U-Q2014	378 \pm 24	383 \pm 22	374 \pm 21
QM-U-Q2015	8.68 \pm 0.68	8.89 \pm 0.38	9.88 \pm 0.74
	DMA	DMA	DMA
QM-U-Q2004	1.9 \pm 0.1	3.04 \pm 0.11	2.39 \pm 0.19
QM-U-Q2005	1.79 \pm 0.19	1.72 \pm 0.08	1.78 \pm 0.07
QM-U-Q2006	1.8 \pm 0.1	1.73 \pm 0.06	1.89 \pm 0.03
QM-U-Q2013	22.5 \pm 0.3	20.1 \pm 0.9	22.0 \pm 2.9
QM-U-Q2014	3.85 \pm 1.4	2.18 \pm 0.11	2.95 \pm 0.21
QM-U-Q2015	72.1 \pm 3.2	74.1 \pm 2.8	73.5 \pm 5.1
	MMA	MMA	MMA
QM-U-Q2005	-	2.64 \pm 0.23	1.17 \pm 0.09
QM-U-Q2013	3.89 \pm 0.12	4.44 \pm 0.24	3.8 \pm 0.4

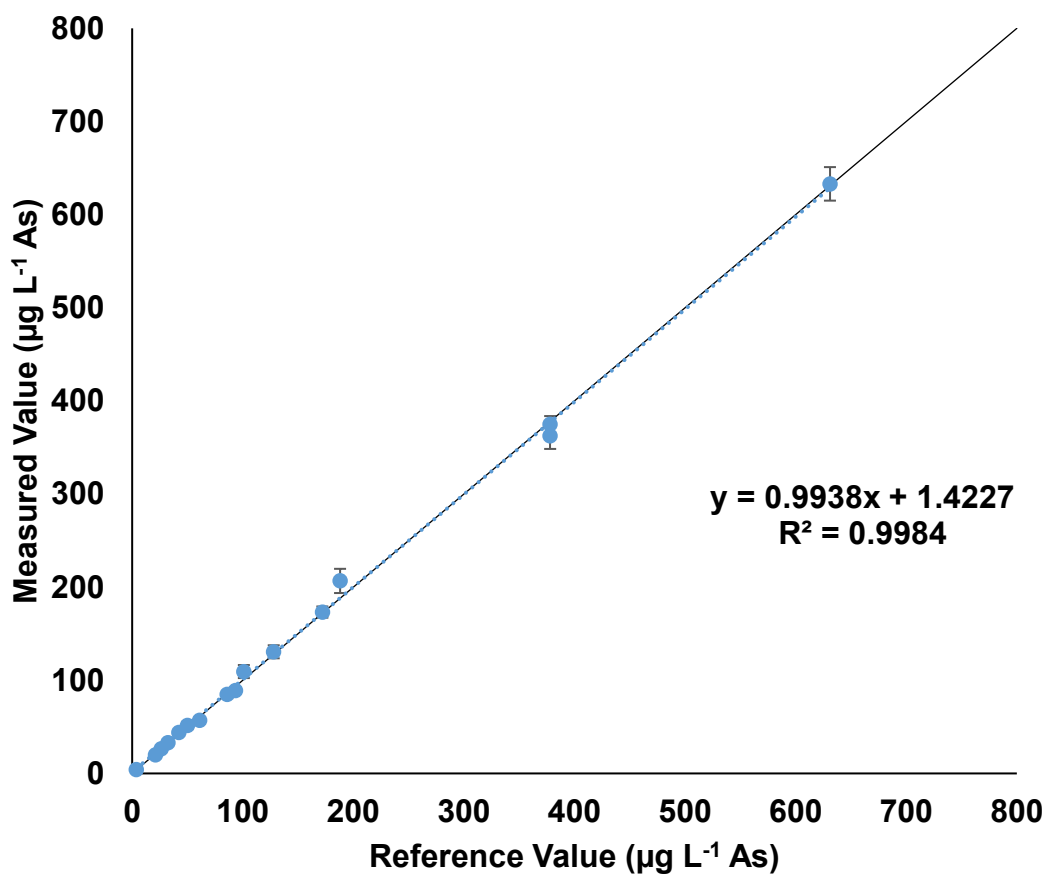


Figure S1. Linear regressions comparing the measured values for the total arsenic measurements to the target values (n=3).

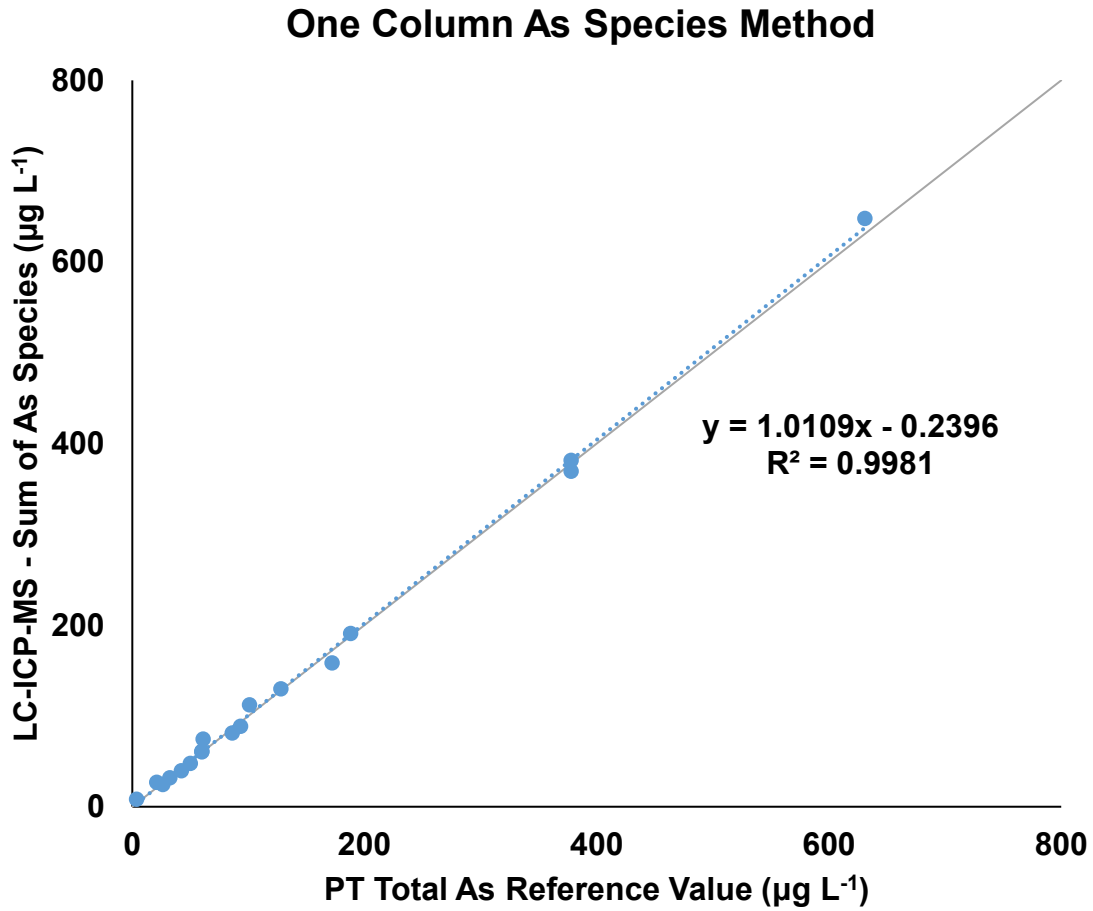


Figure S2. Linear regressions comparing the measured values from the one-column method to the target values for the sum of the arsenic species.

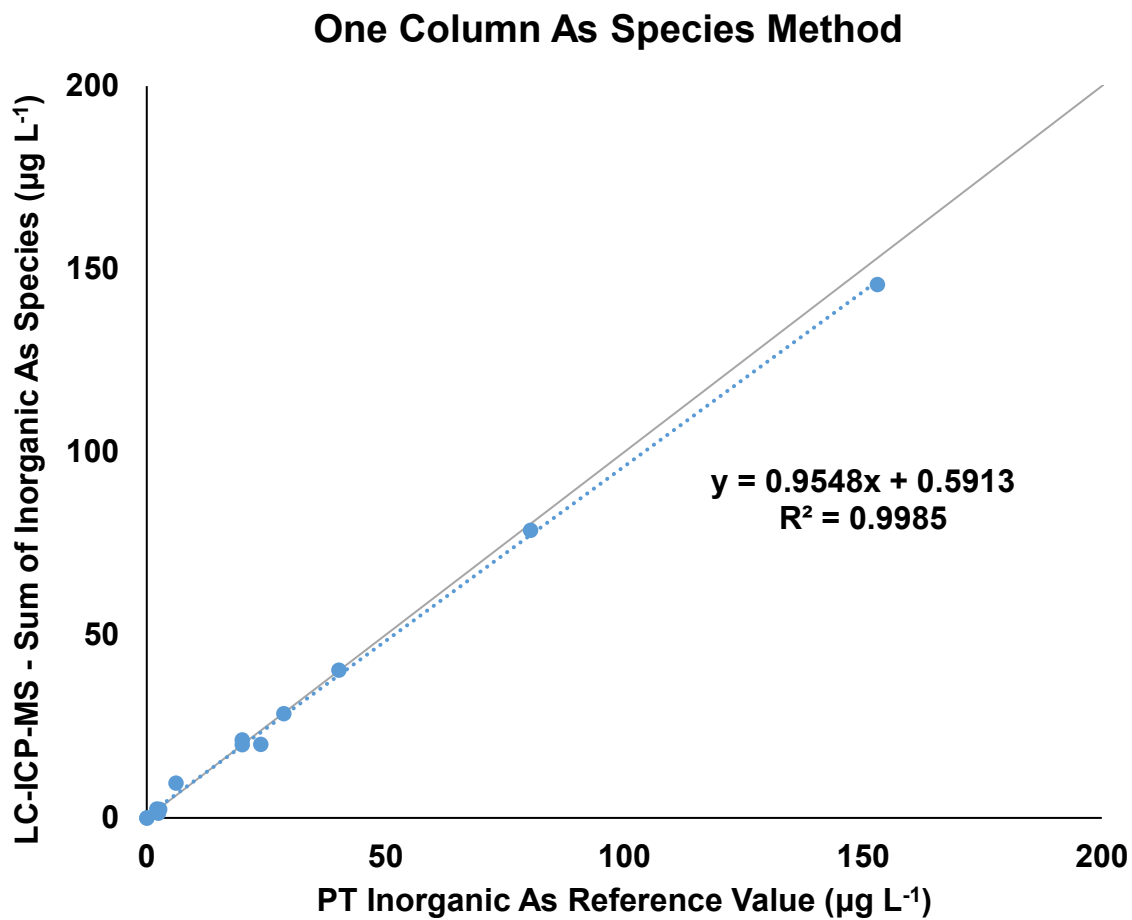


Figure S3. Linear regressions comparing the measured values from the one-column method to the target values for the inorganic arsenic species.

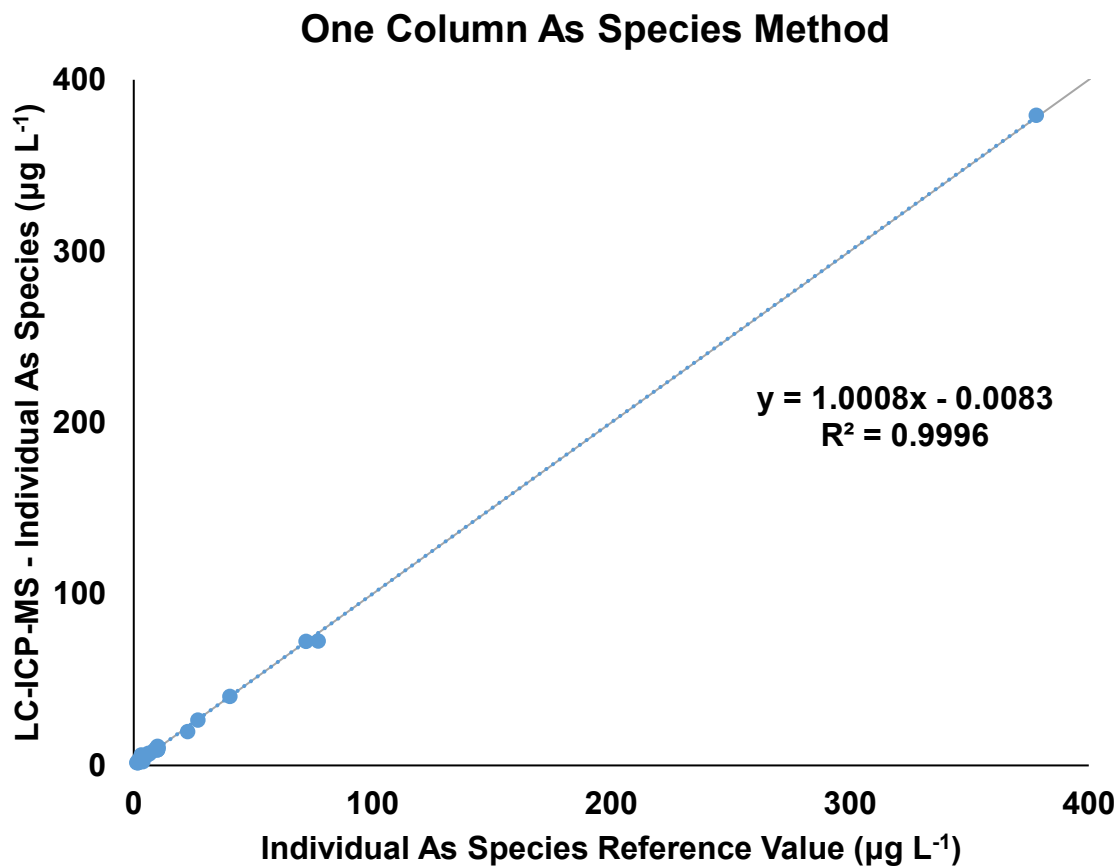


Figure S4. Linear regressions comparing the measured values from the one-column method to the target values for the individual arsenic species.

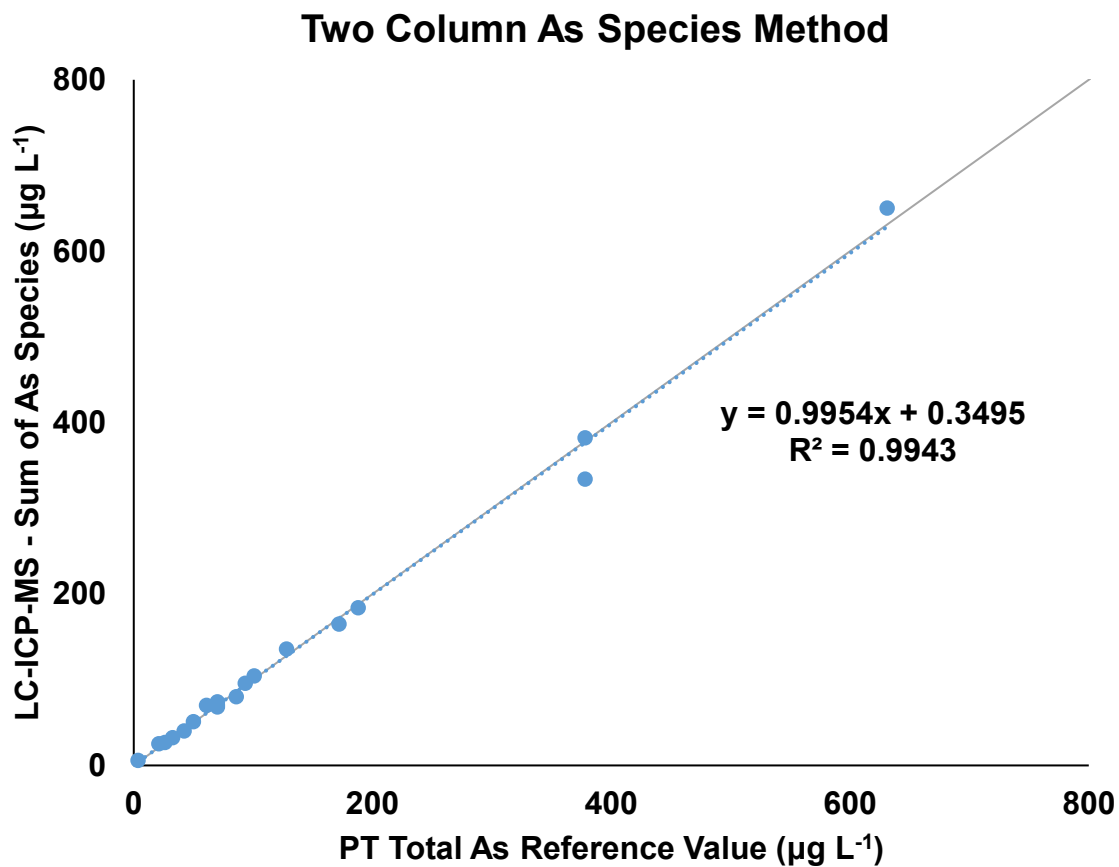


Figure S5. Linear regressions comparing the measured values from the two-column method to the target values for the sum of the arsenic species.

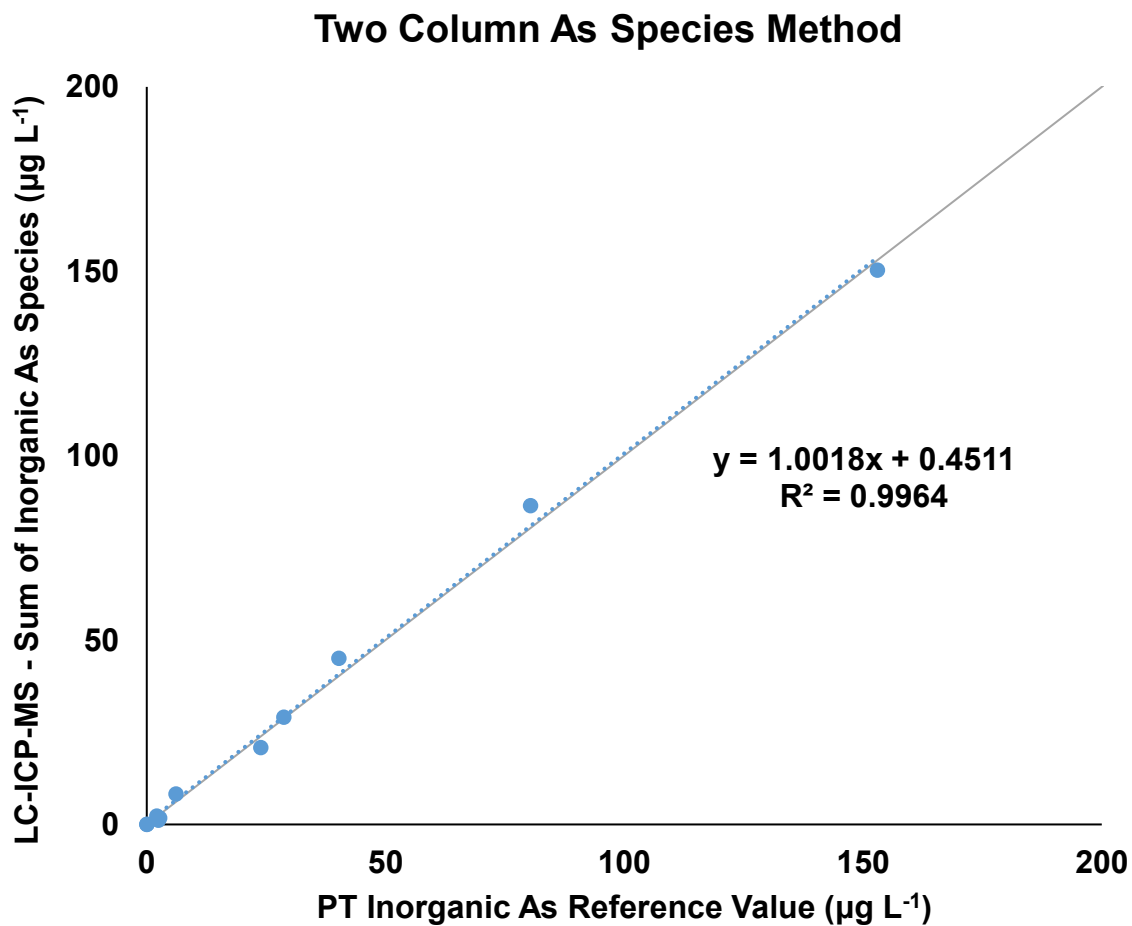


Figure S6. Linear regressions comparing the measured values from the two-column method to the target values for the inorganic arsenic species.

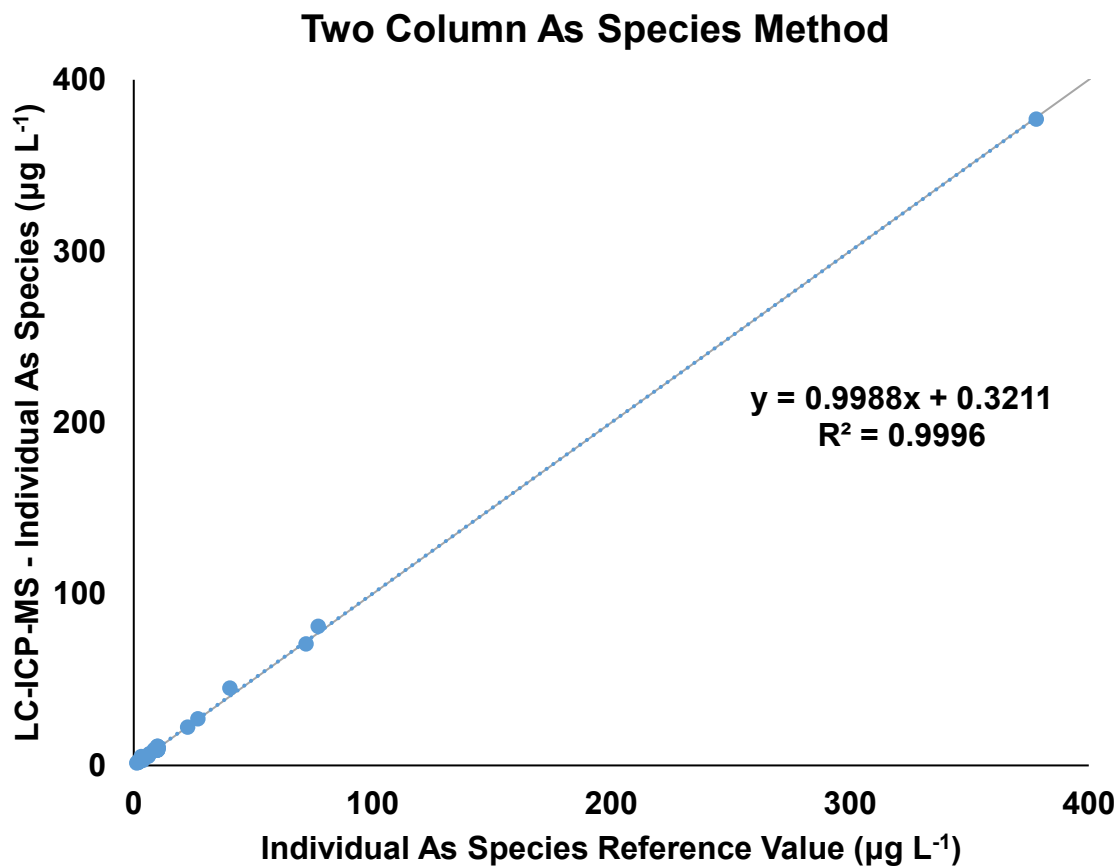


Figure S7. Linear regressions comparing the measured values from the two-column method to the target values for the individual arsenic species.