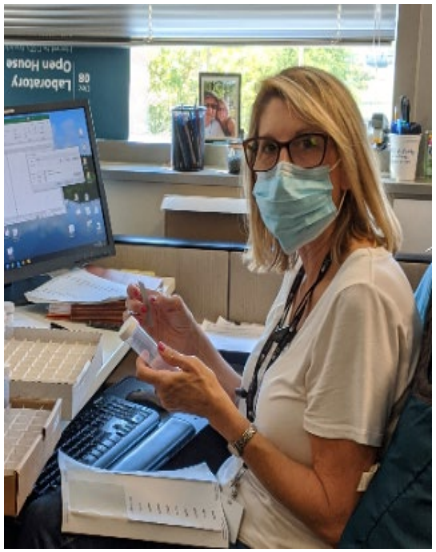
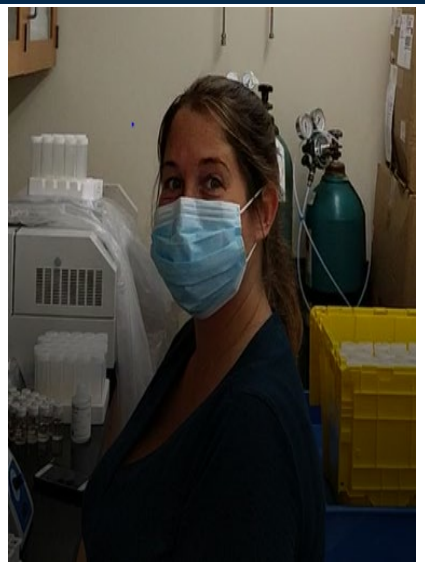
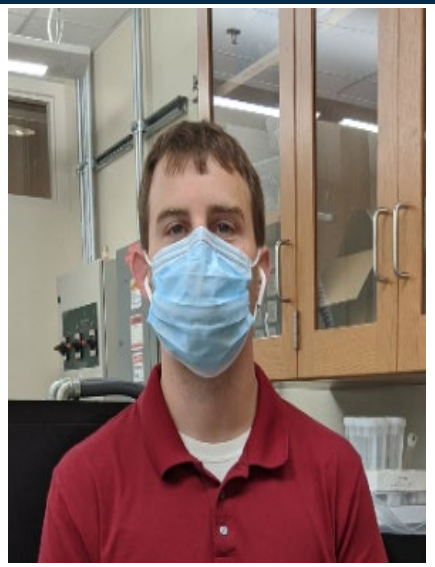
IMPROVE Steering Committee Meeting

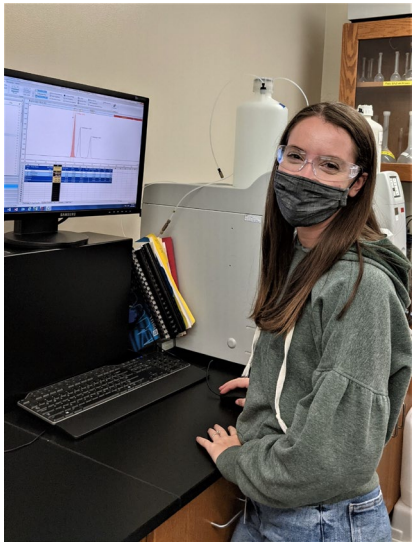
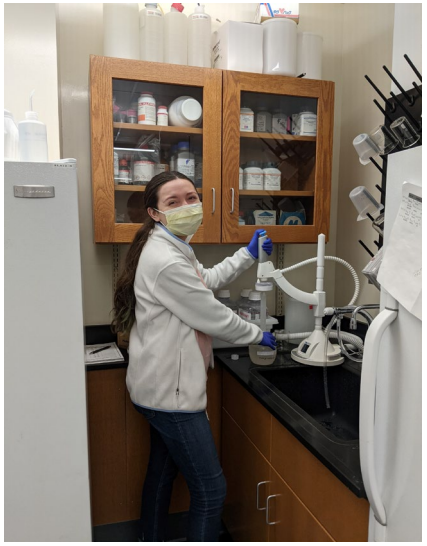
Virtual 2021

Tracy Dombek, Ions Report

RTI International



Minimum Detection Limits & Process

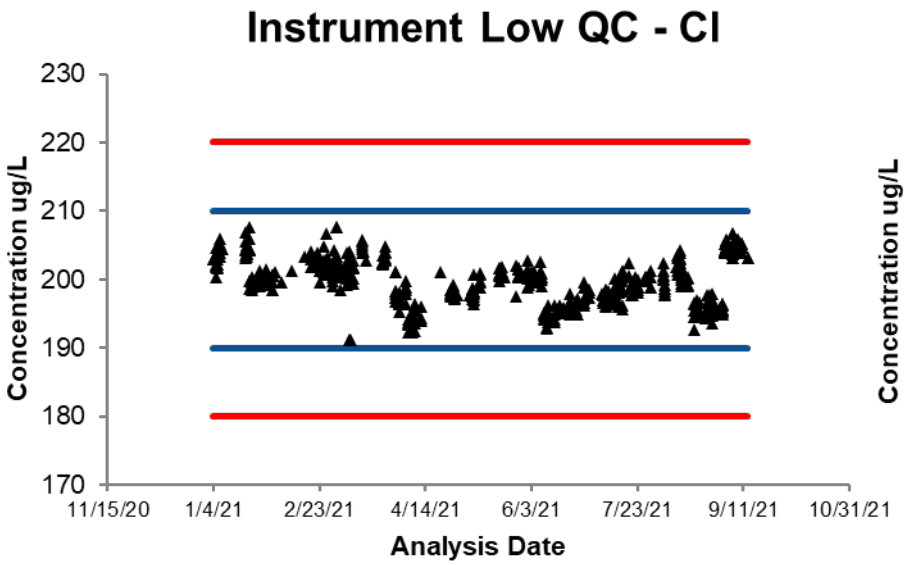
- Extract nylon filters in 20 mL of DI water.
- Calibrate systems daily using primary stock standards.
- Quality Controls using secondary source standards before and after every ten samples analyzed.
- Duplicates at a rate of 3 per batch of 50 samples.
- Perform matrix spikes at a rate of 2 per batch of 50 samples.
- Random reanalysis of 5% of the sample total.
- Re-extraction of filters to evaluate extraction efficiencies.

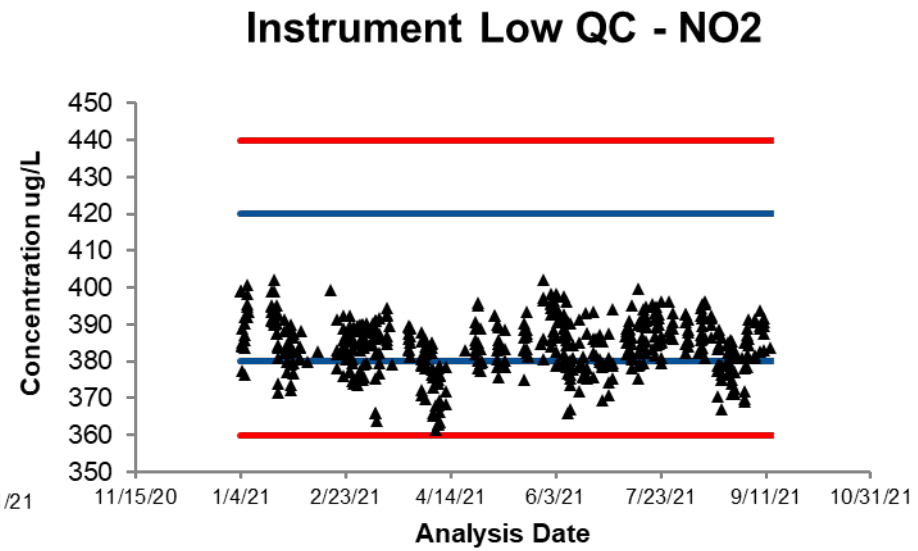
2021 MDL's	Chloride	Nitrite	Nitrate	Sulfate
µg/filter	0.100	0.200	0.160	0.220
mg/L	0.005	0.010	0.008	0.011

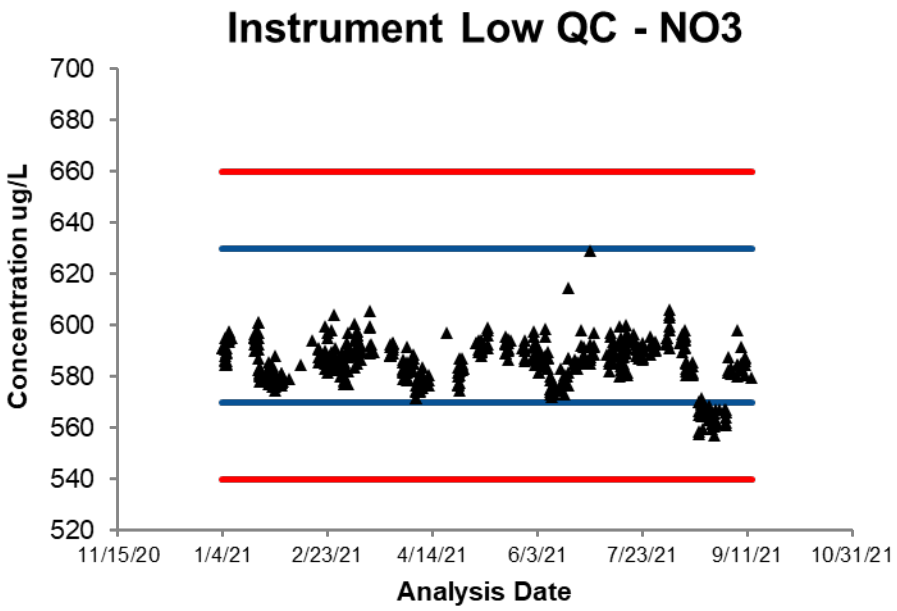
Quality Control Standards

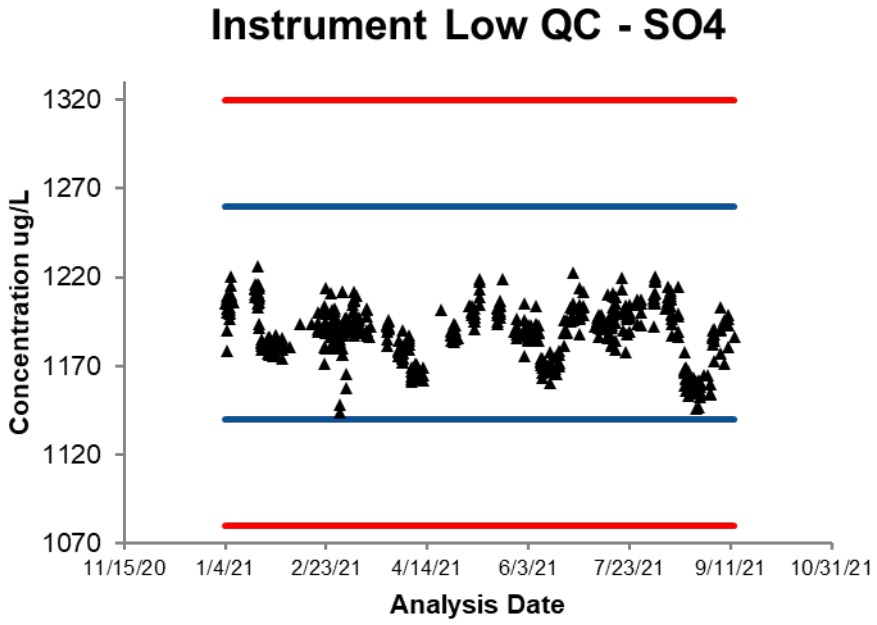
	Average Recovery Chloride	Average Recovery Nitrite	Average Recovery Nitrate	Average Recovery Sulfate
QC-Low n= 589	98.8%	95.2%	96.6%	98.1%
QC-Med n=1024	100%	98.4%	99.2%	99.8%
QC-Med-HI n=531	101%	101%	99.6%	101%
QC-High n-= 279	102%	103%	100%	102%

Instrument Control Charts

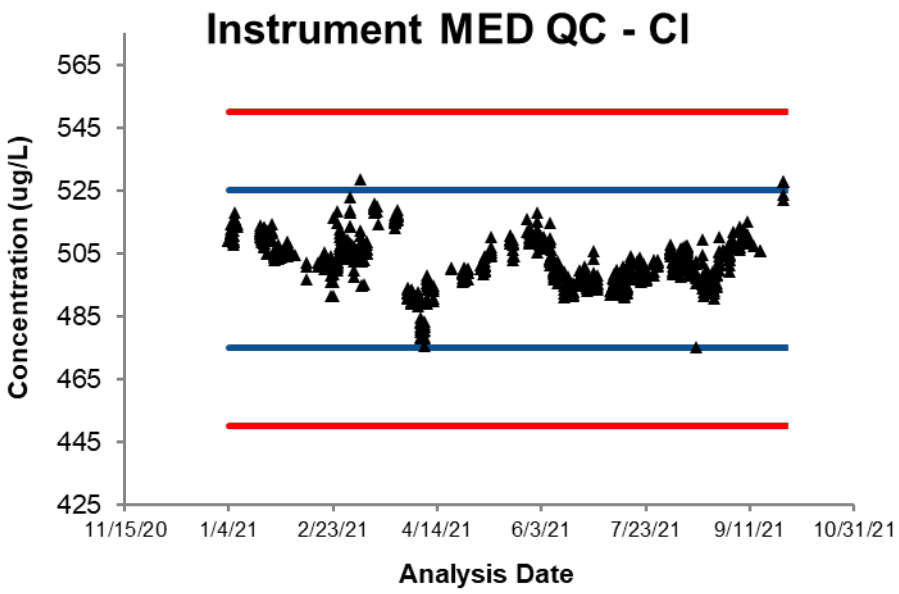


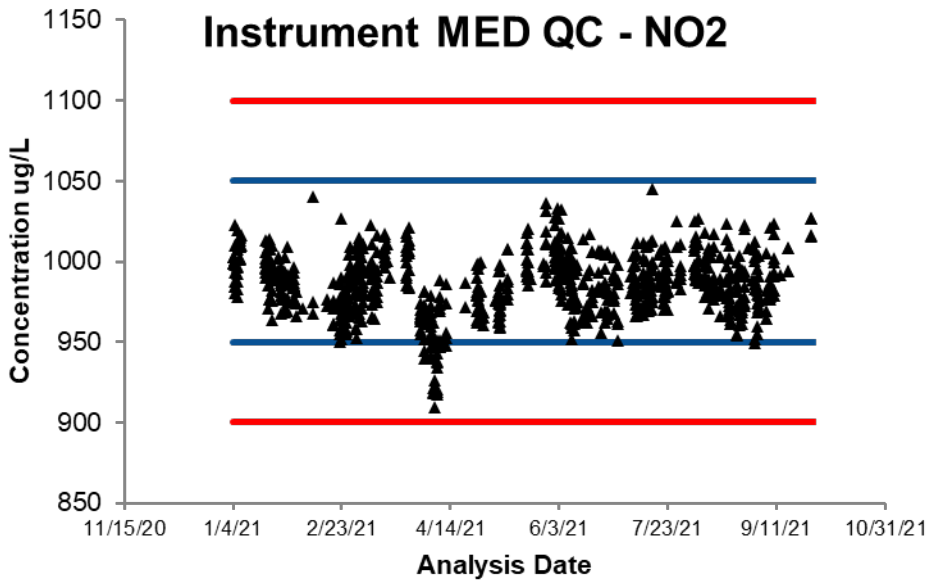


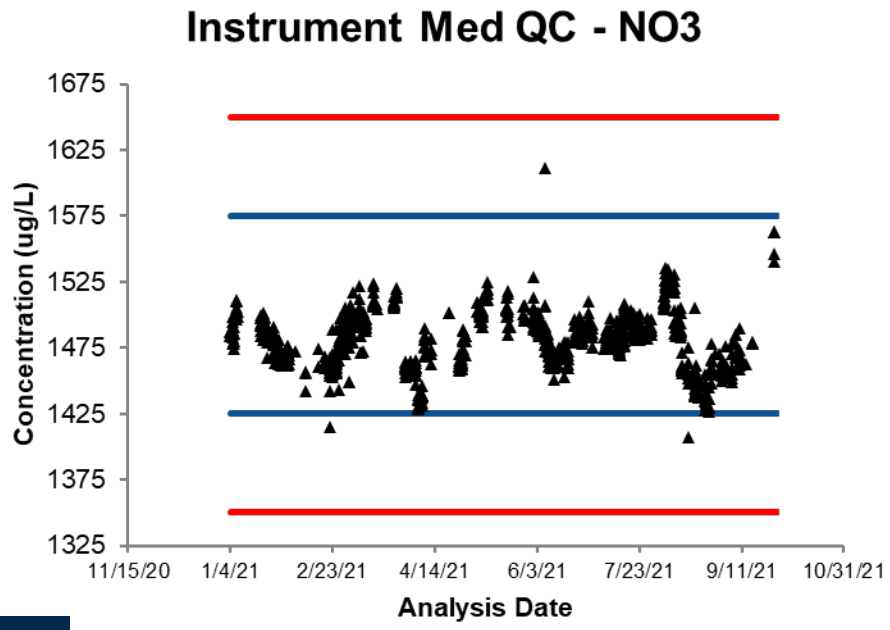


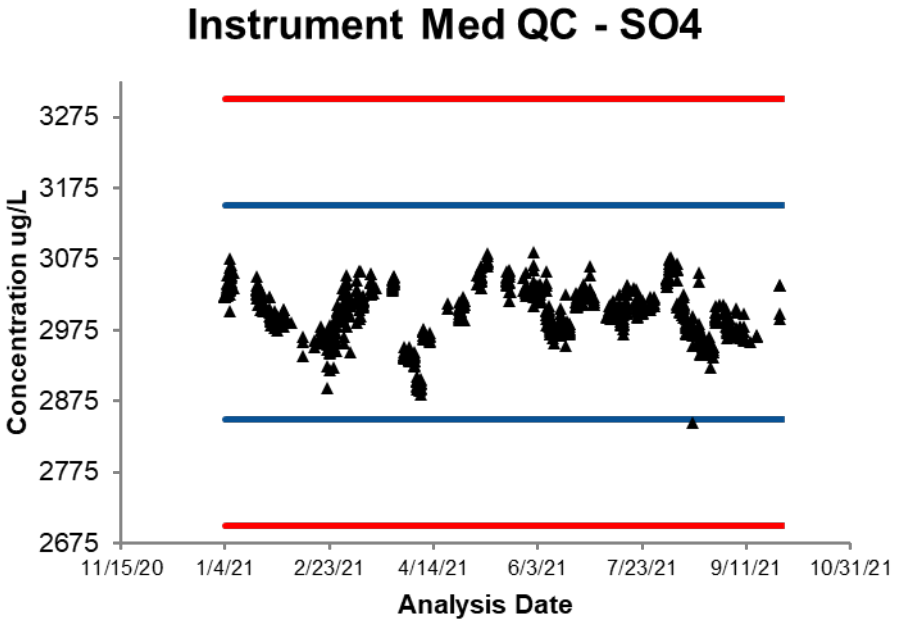


Instrument Control Charts

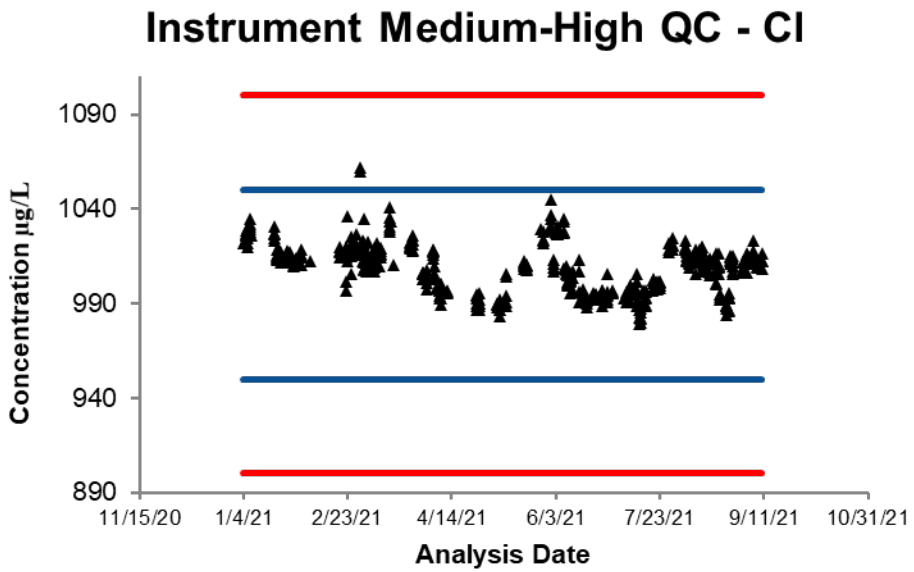


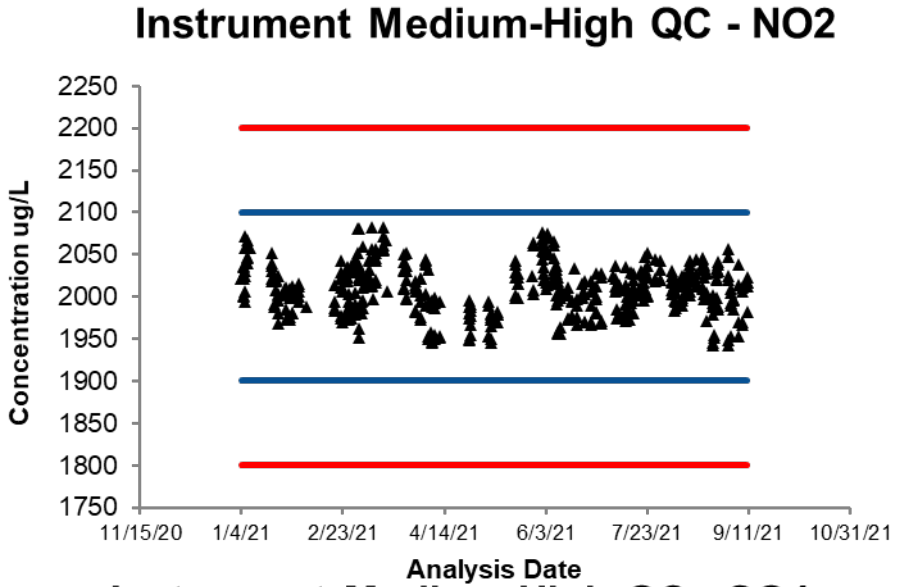


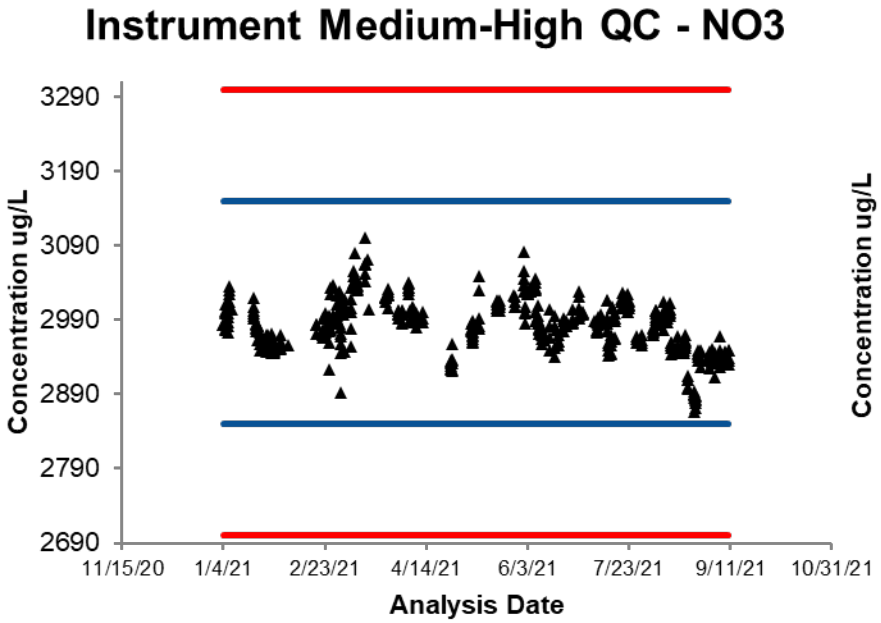


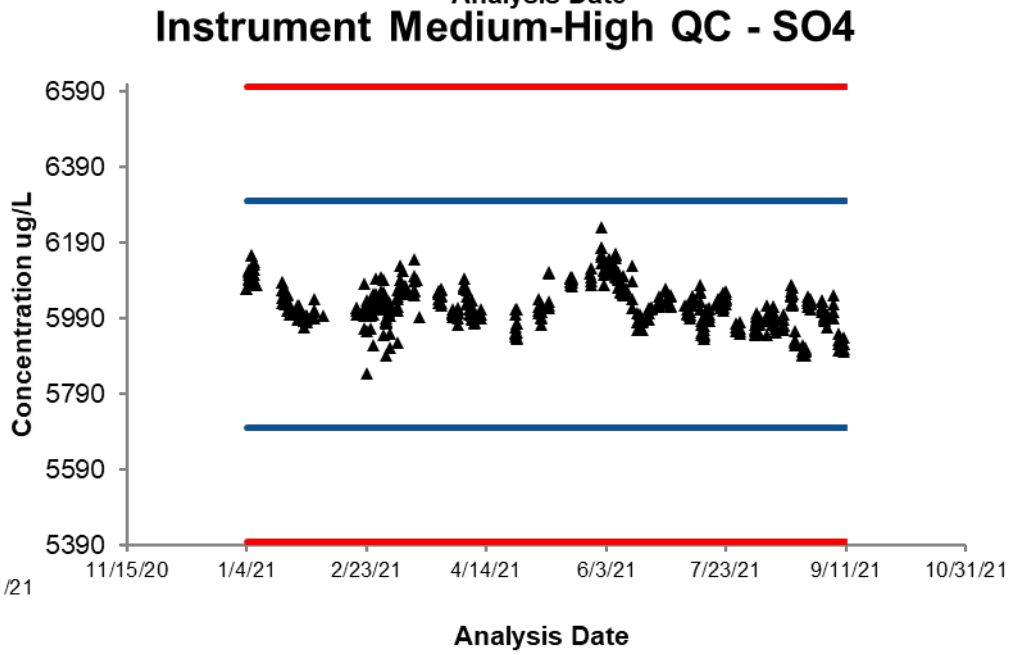


Instrument Control Charts

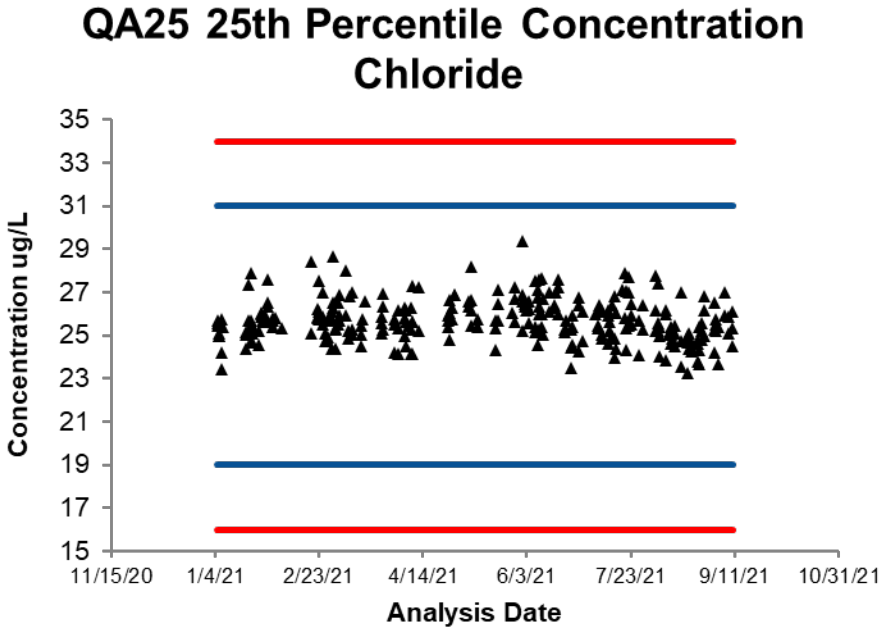


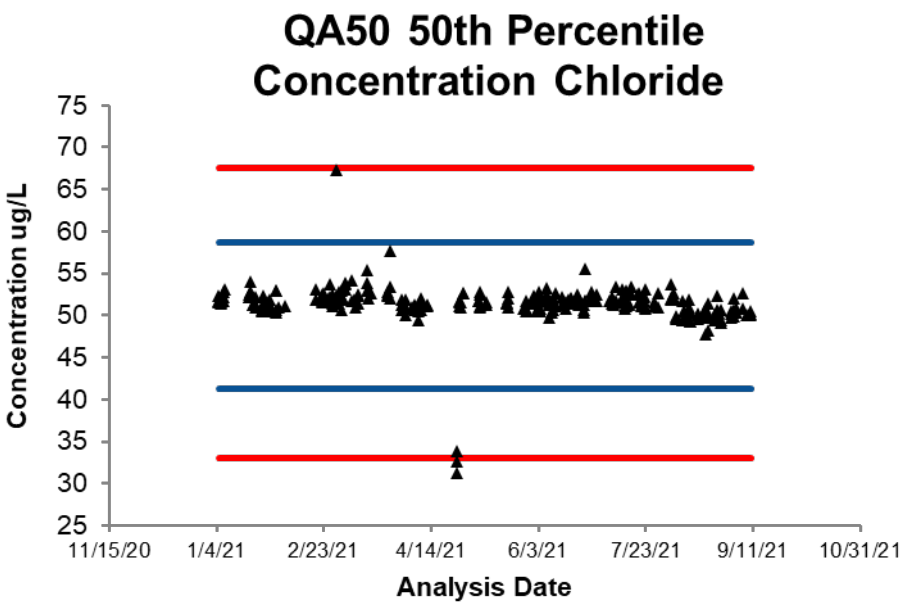






25th, 50th,& 75th Percentile Chloride



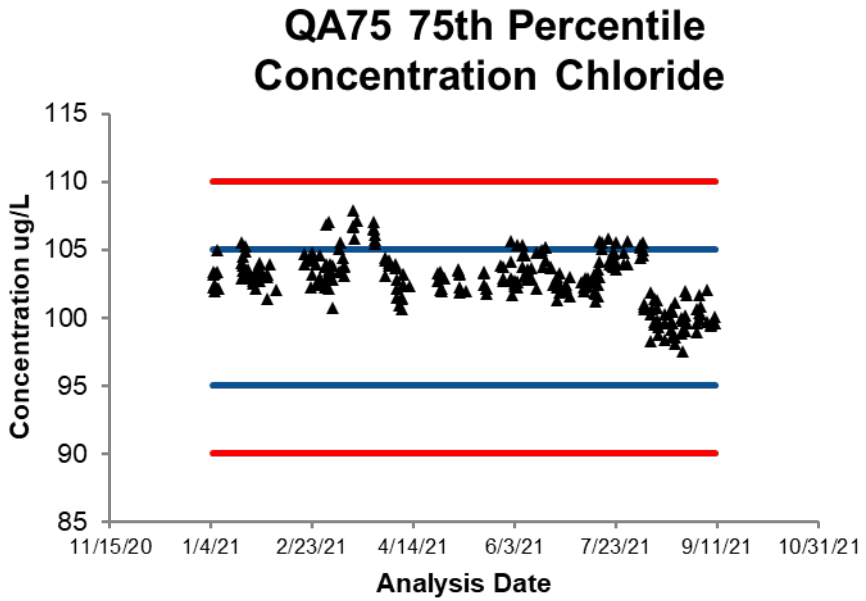


Approximate Air Concentrations

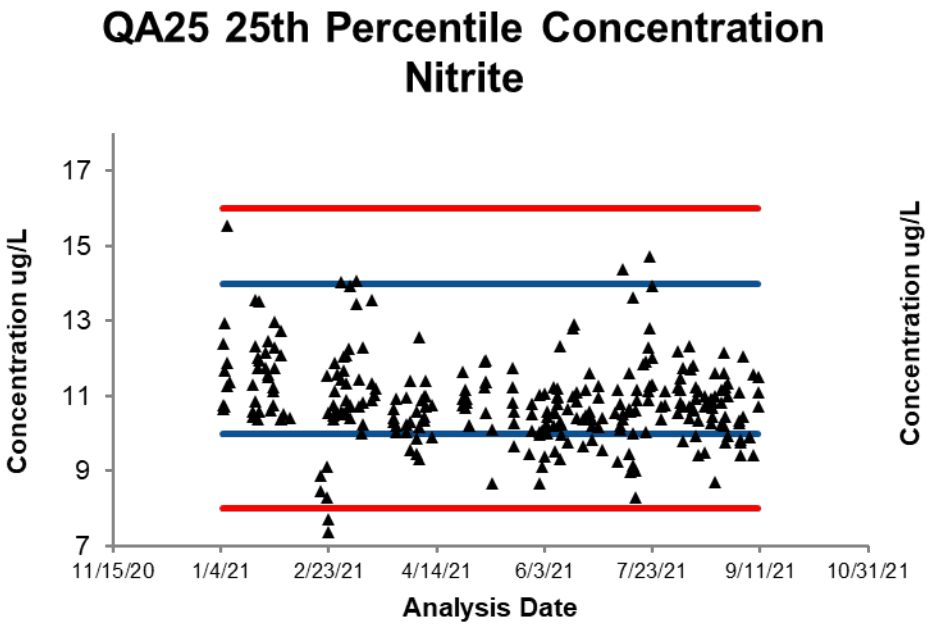
25th Chloride - 0.016 ug/m^3

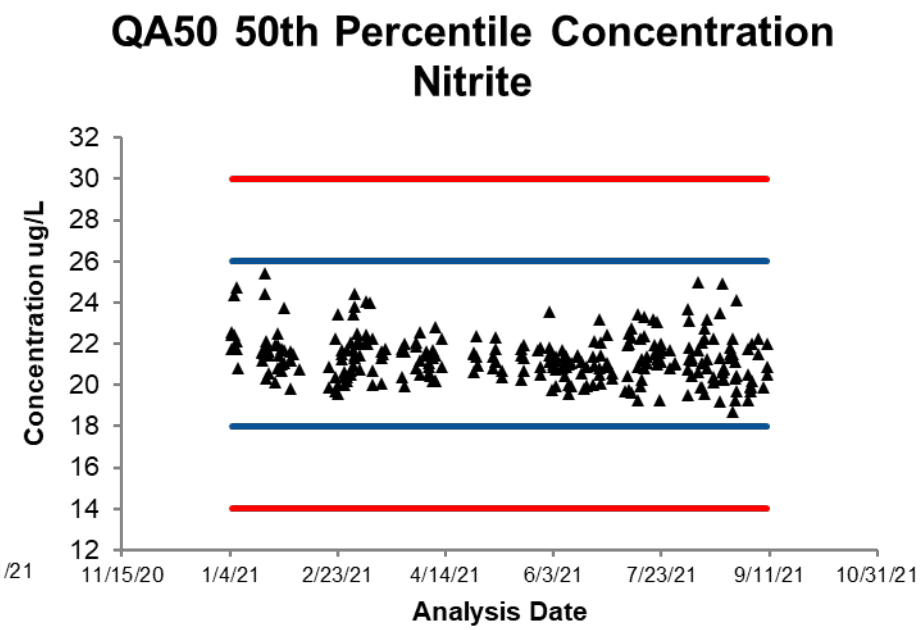
50th Chloride – 0.031 ug/m^3

75th Chloride - 0.061 ug/m^3



25th , 50th , & 75th Percentile Nitrite



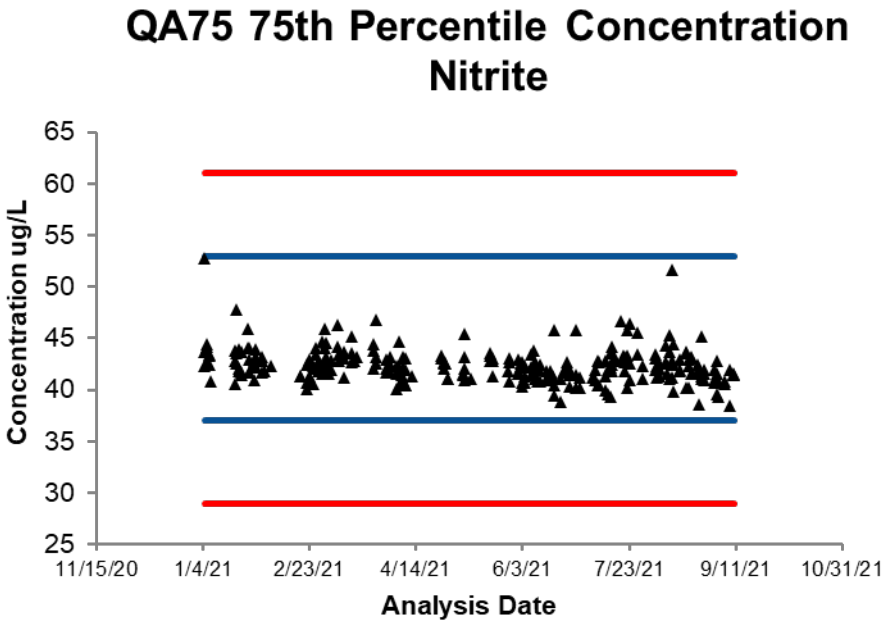


Approximate Air Concentration

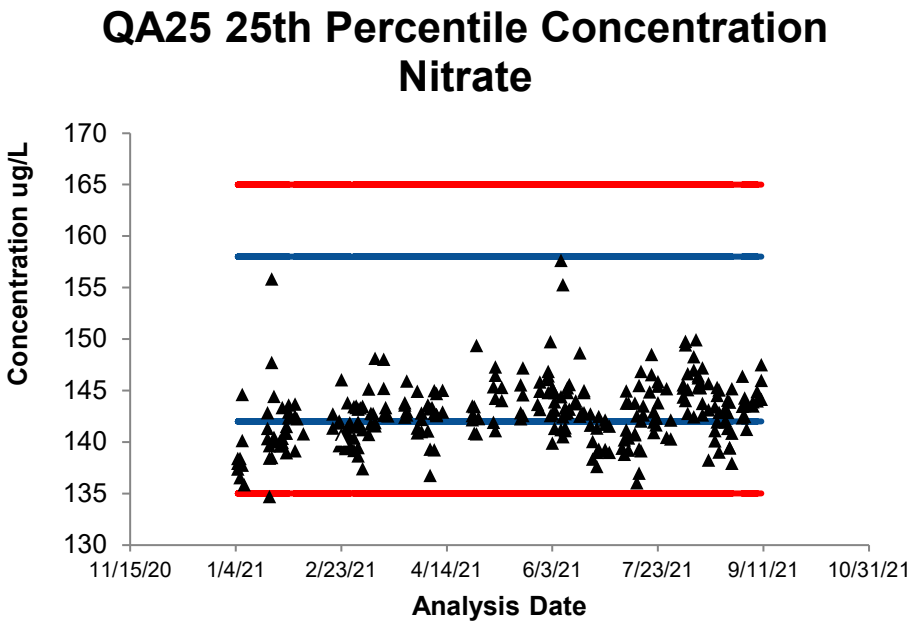
25th Nitrite – 0.007 ug/m3

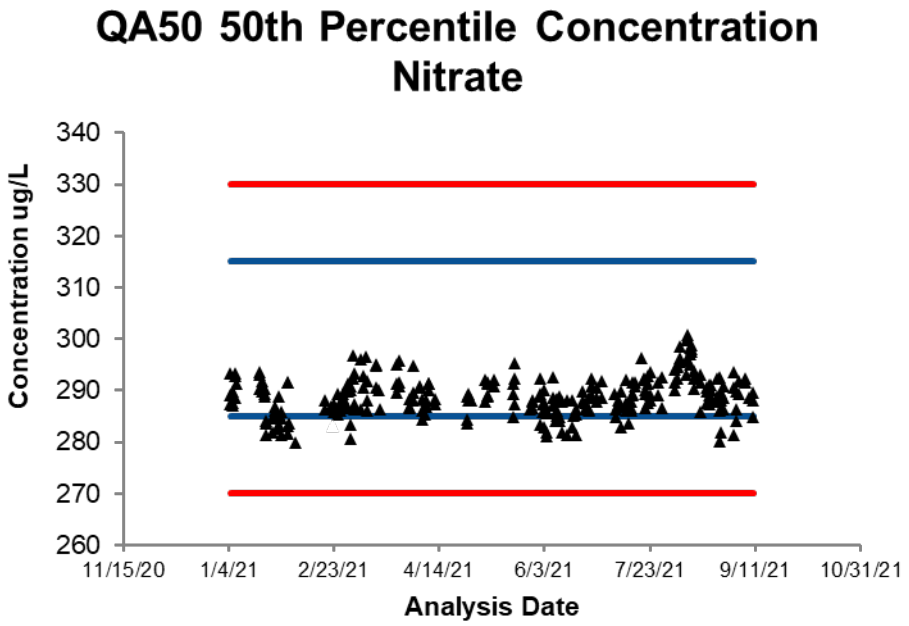
50th Nitrite – 0.013 ug/m3

75th Nitrite – 0.026 ug/m3



25th, 50th , & 75th Percentile Nitrate



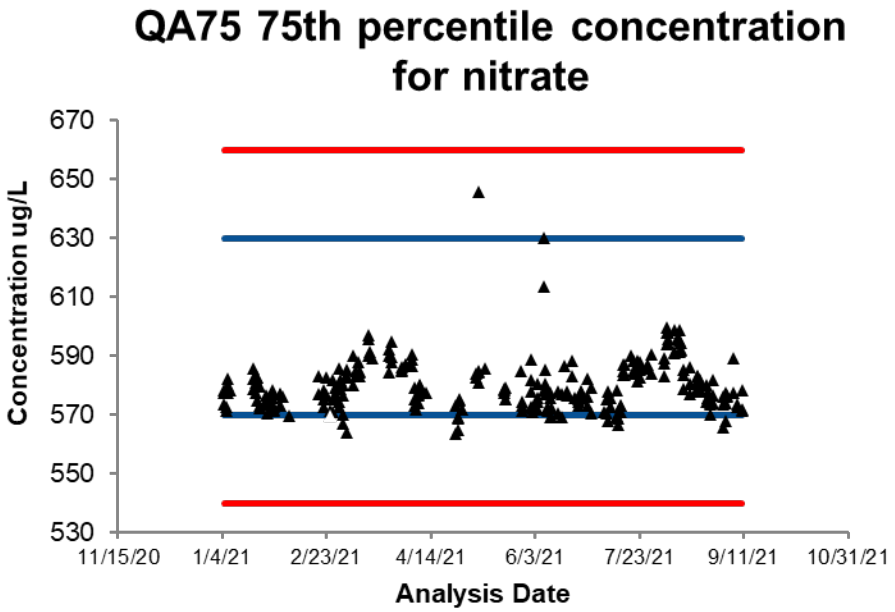


Approximate Air Concentration

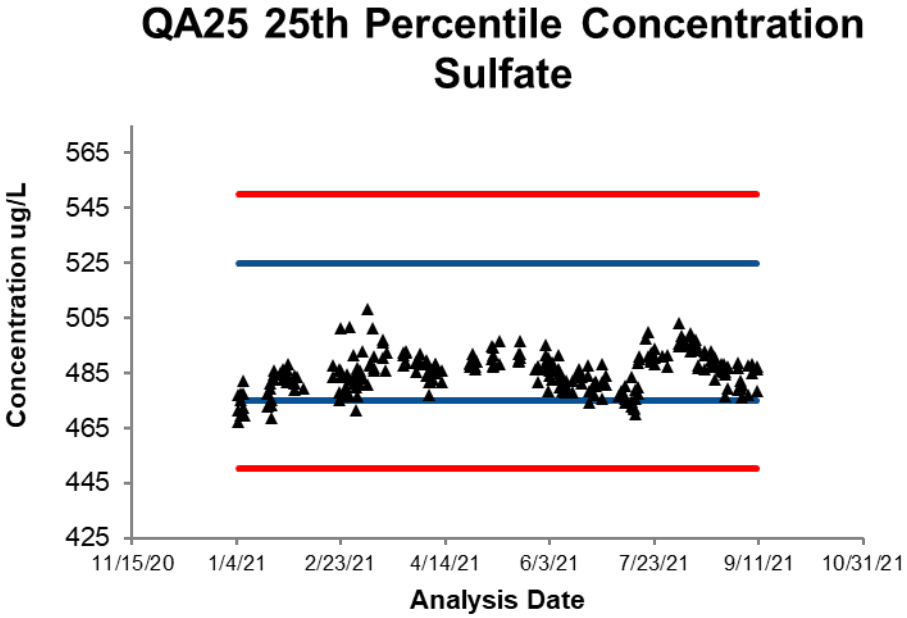
25th Nitrate – 0.092 ug/m3

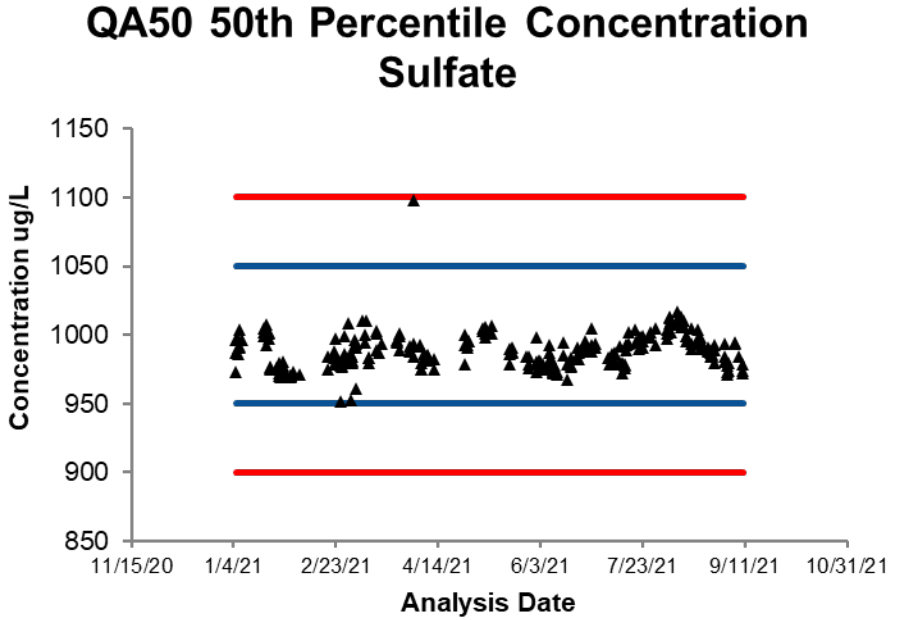
50th Nitrate – 0.18 ug/m3

75th Nitrate – 0.36 ug/m3



25th, 50th, & 75th Percentile Sulfate



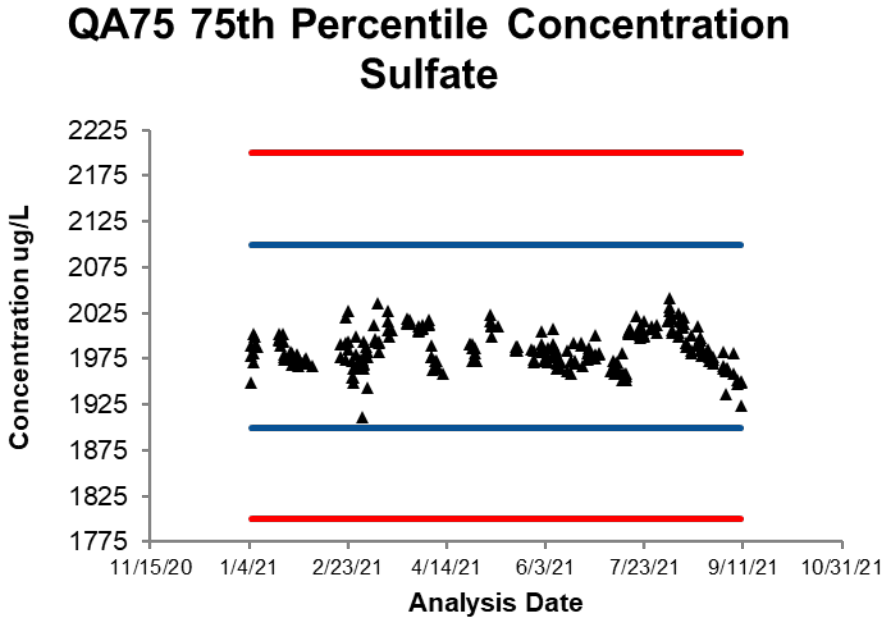


Approximate Air Concentration

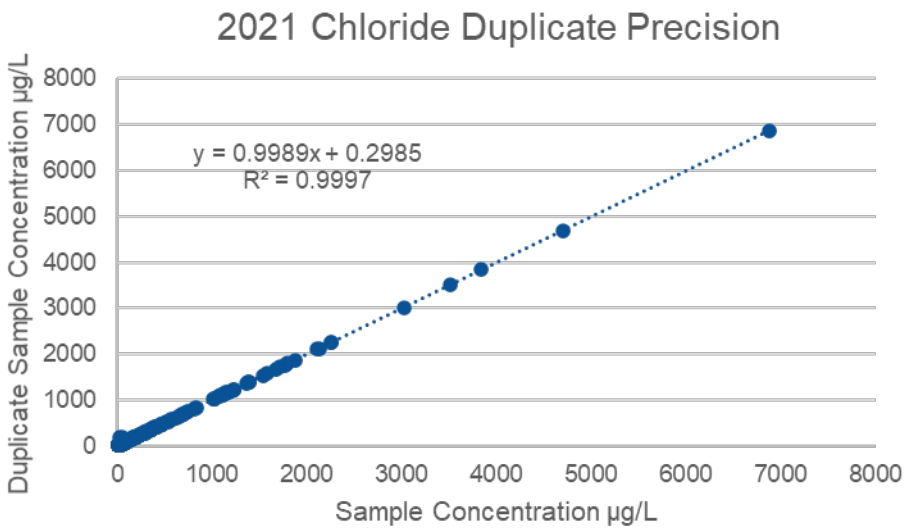
25th Sulfate – 0.30 ug/m3

50th Sulfate – 0.60 ug/m3

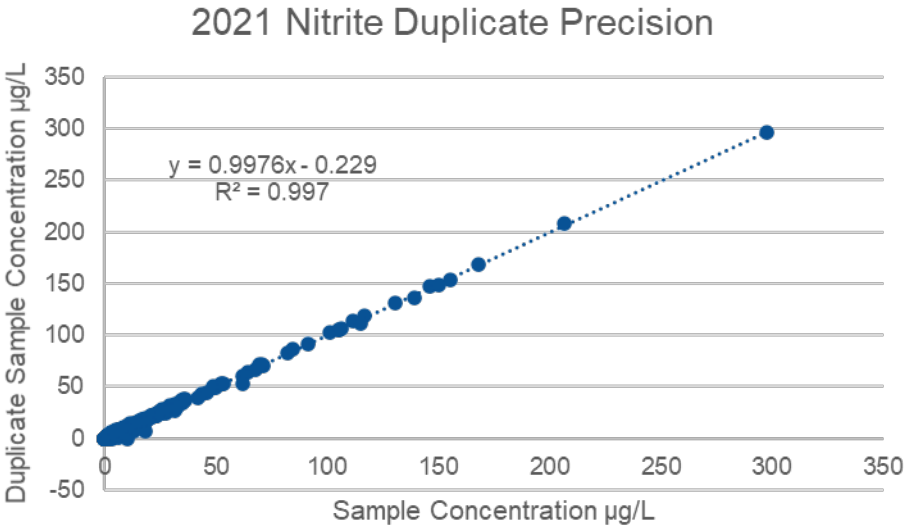
75th Sulfate – 1.2 ug/m3



Duplicate Precision

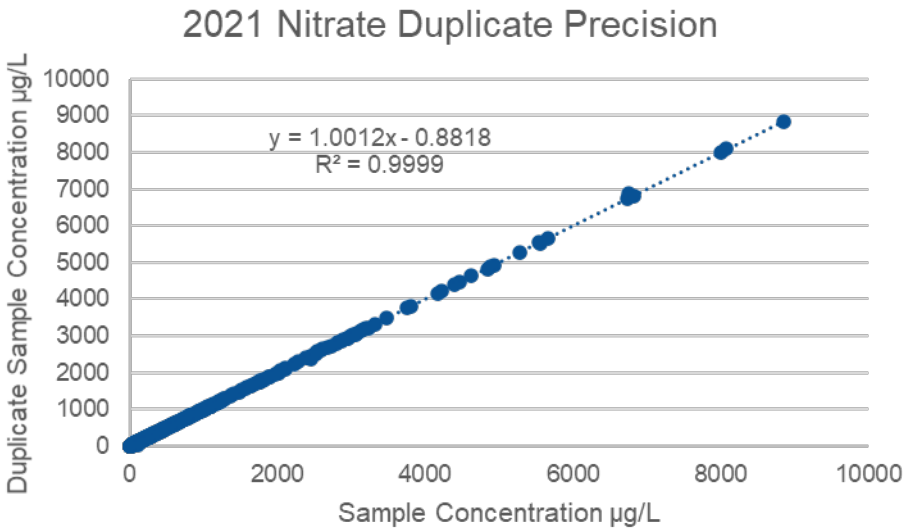


Chloride Percent Differences
Average = 0.28%
Median = 0.26%
Maximum = 72.5%
Minimum = -157%
Count = 726
Failures 0.83%

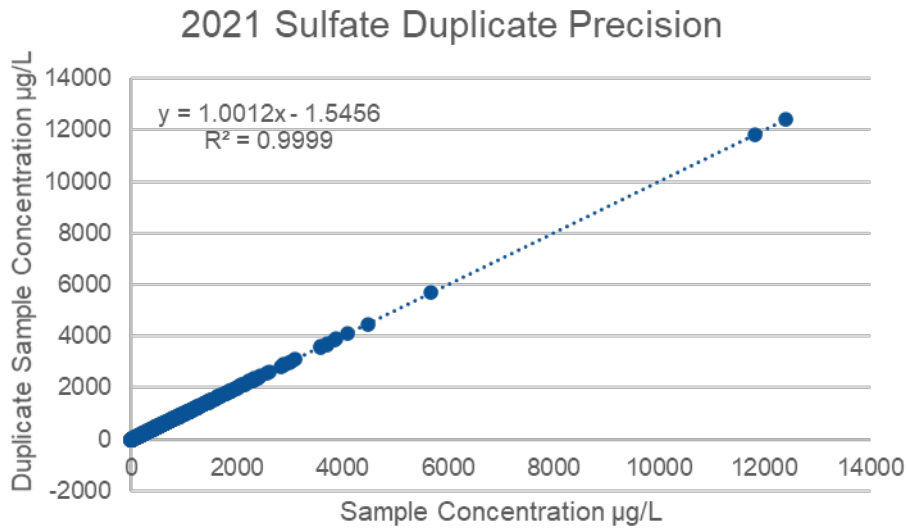


Nitrite Percent Differences
Average = 4.65%
Median = 0.75%
Maximum = 200%
Minimum = -87.3 %
Count = 726
Failures 0%

Duplicate Precision



Nitrate Percent Differences
Average = 0.49%
Median = 0.04%
Maximum = 106%
Minimum = -23.8 %
Count = 726
Failures 0.28%



Sulfate Percent Differences
Average = 1.12%
Median = 0.13%
Maximum = 200%
Minimum = -40.2%
Count = 726
Failures 0%

Reanalysis

	Chloride	Nitrite	Nitrate	Sulfate
2021 median RPD	-0.44%	0%	-0.04%	0%
2021Average RPD	-0.19%	2.35%	0.79%	-0.35%

- Roughly 5% of each batch of 400 NPS samples are reanalyzed after the original analysis.
- The Relative Percent Differences are calculated and verified against the DQO requirements.
- Any samples failing to meet DQO's are reanalyzed a third time to check.

Routine Filter Re-Extraction

- Extraction efficiencies were evaluated on nearly 486 samples.
- Efficiency is determined by dividing the result measured on the re-extracted filter by the sum of the original and re-extracted results.

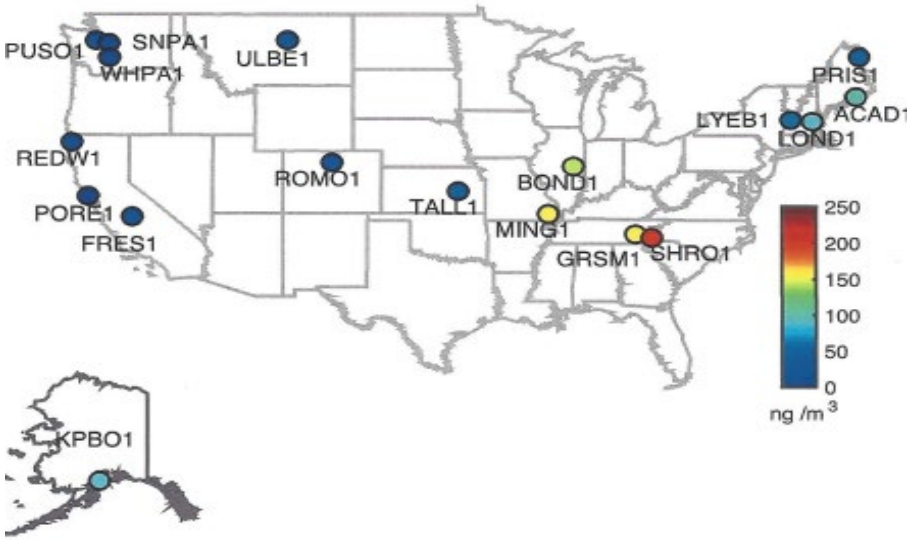
Chloride	Nitrite	Nitrate	Sulfate
100%		102%	100%

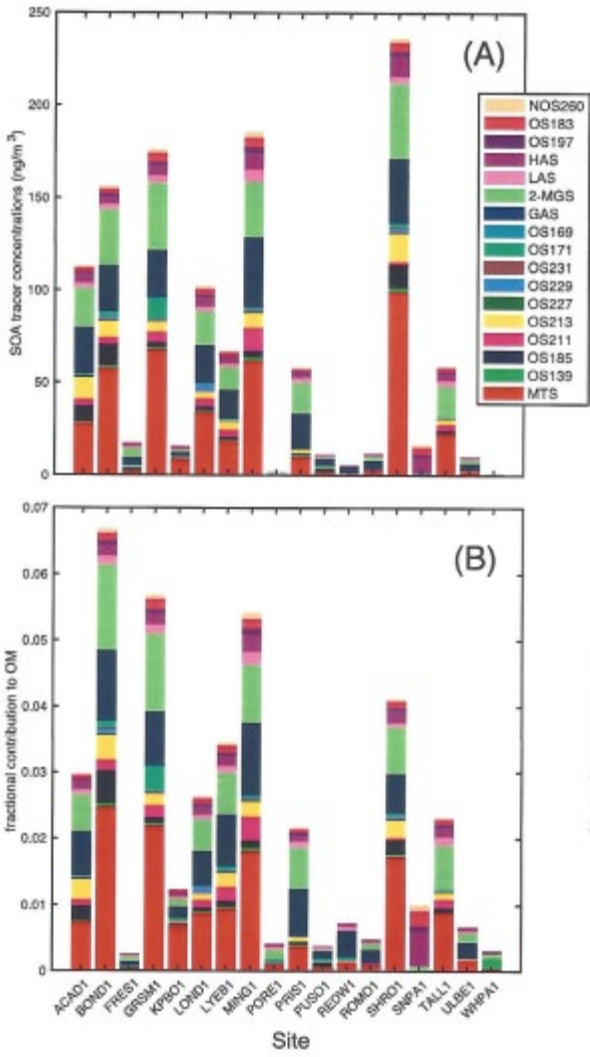
RTI International

Method Development and Research

Last year, RTI contributed to our research efforts by providing $50K to support research and method development.

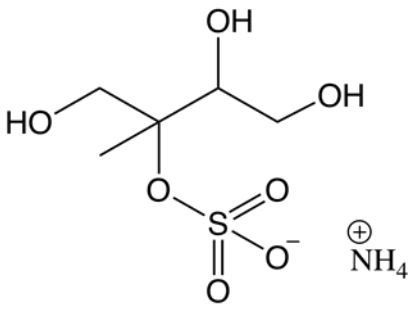
Indications of Water Soluble OS



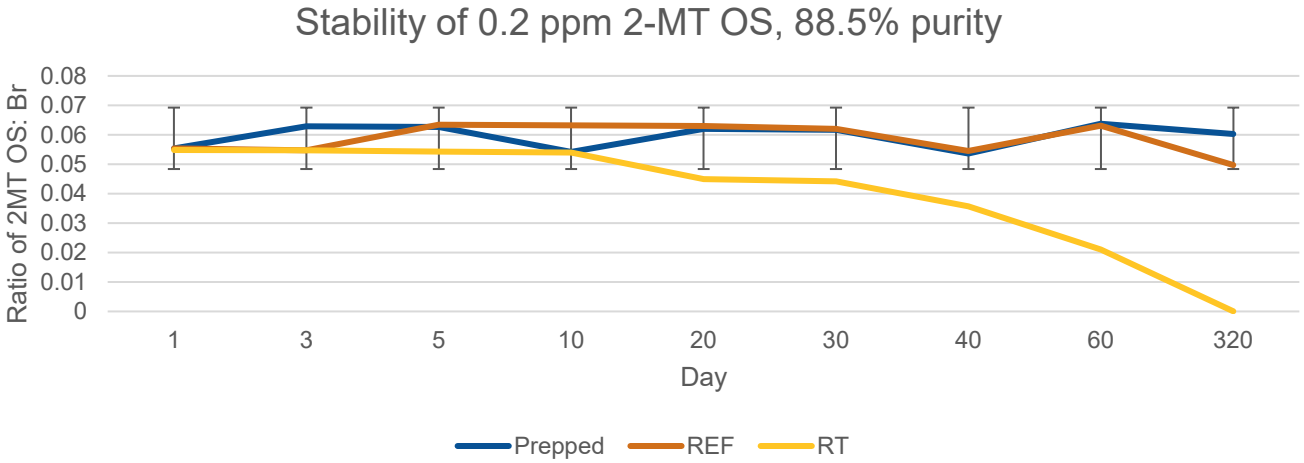


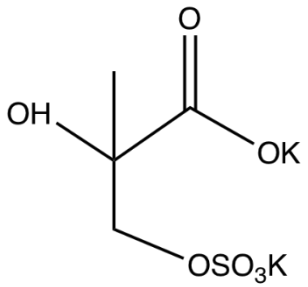
- We conducted analysis of IMPROVE extracts from filters collected during 2016 and we found differences between total water-soluble sulfur and inorganic sulfur measured by IC as Sulfate.
- We took a subset of sites distributed across the U.S and prepared composites of these samples which were analyzed using a HILIC/ESI-HR QTOFMS
- OS's were quantified using standards and through a surrogate stand when no standard was available.

Stability results evaluating most abundant OS species measured in IMPROVE samples

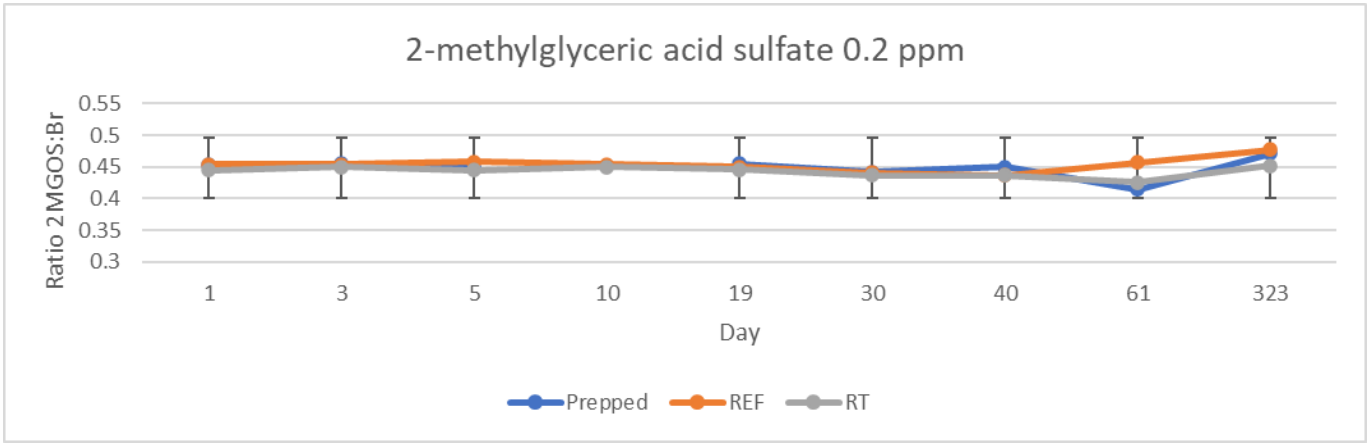


2-methyltetrol sulfate
Chemical Formula: $(NH_4)C_5H_{11}O_7S$





2-methylglyceric acid sulfate
Chemical Formula: $C_4H_6K_2O_7S$



Concentration samples for further analyses

- Evaluated OS matrix spikes with 37 and 47 mm Nylon filters to evaluate recovery through the freeze-drying process.

OS	Recovery of Spikes with filters freeze dried	Recovery of Spikes with no filters freeze dried	Recovery of Spikes with filters no freeze drying
2 MTOS	87.9% RSD 2.4%	78.9% RSD 1.6%	92.1% RSD 1.5%
2 MGOS	94.7% RSD	93.6% RSD 0.5%	96.9% RSD 1.4%

Yuzhi Chen, Dombek, T., Hand, J., Zhang, Z., Gold, A., Ault, A.P., Levine, K.E., Surratt, J.D., Seasonal Contribution of Isoprene-Derived Organosulfates to Total Water-Soluble Fine Particulate Organic Sulfur in the United States. ACS Earth Space Chem. 2021, 5, 9, 2419-2432.

Acknowledgements

- Dr. Jason D. Surratt, Ph.D. Professor Dept of Environmental Sciences and Engineering and Department of Chemistry, Gillings School of Public Health, University of North Carolina, Chapel Hill

- Yuzhi Chen, PHD Candidate, Environmental Sciences and Engineering and Department of Chemistry, Gillings School of Public Health, University of North Carolina, Chapel Hill

- Dr. Ann Dillner, Ph.D. Research Engineer, Air Quality Research Center, University of California, Davis

- Dr. Keith Levine, Ph.D., Senior Director Analytical Sciences, RTI/

- IC lab team, Miranda De Boskey, Kat Lindskog, Sophie Brenner, and Nicole Manalis, Laurie Stella, Ellen Colcough, Eric Poitras and Laura Haines

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delivering **the promise of science**
for global good

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