

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100622\
 Data File : VN074784.D
 Acq On : 06 Oct 2022 15:27
 Operator : JC\MD
 Sample : N4910-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-5

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M

Title : SW846 8260

Signal : TIC: VN074784.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.312	39	44	49	rVB2	83346	144939	5.33%	1.124%
2	2.424	59	63	64	rBV2	28573	33500	1.23%	0.260%
3	2.836	126	133	135	rBV3	132359	295072	10.85%	2.288%
4	7.447	906	917	924	rBV2	103569	276022	10.15%	2.140%
5	8.177	1031	1041	1046	rBV2	341414	832309	30.62%	6.454%
6	8.235	1046	1051	1061	rVB2	346566	770418	28.34%	5.974%
7	8.588	1102	1111	1126	rBV2	425342	999757	36.78%	7.752%
8	9.106	1189	1199	1213	rVB	532968	1119602	41.19%	8.681%
9	9.359	1235	1242	1249	rVB6	51441	104486	3.84%	0.810%
10	10.570	1440	1448	1459	rBV	1465326	2718411	100.00%	21.078%
11	11.106	1532	1539	1552	rBV	686105	1247112	45.88%	9.670%
12	11.870	1660	1669	1677	rBV	812232	1487068	54.70%	11.530%
13	12.853	1828	1836	1846	rVB	783888	1400931	51.53%	10.863%
14	13.794	1988	1996	2005	rBV	890175	1467264	53.98%	11.377%

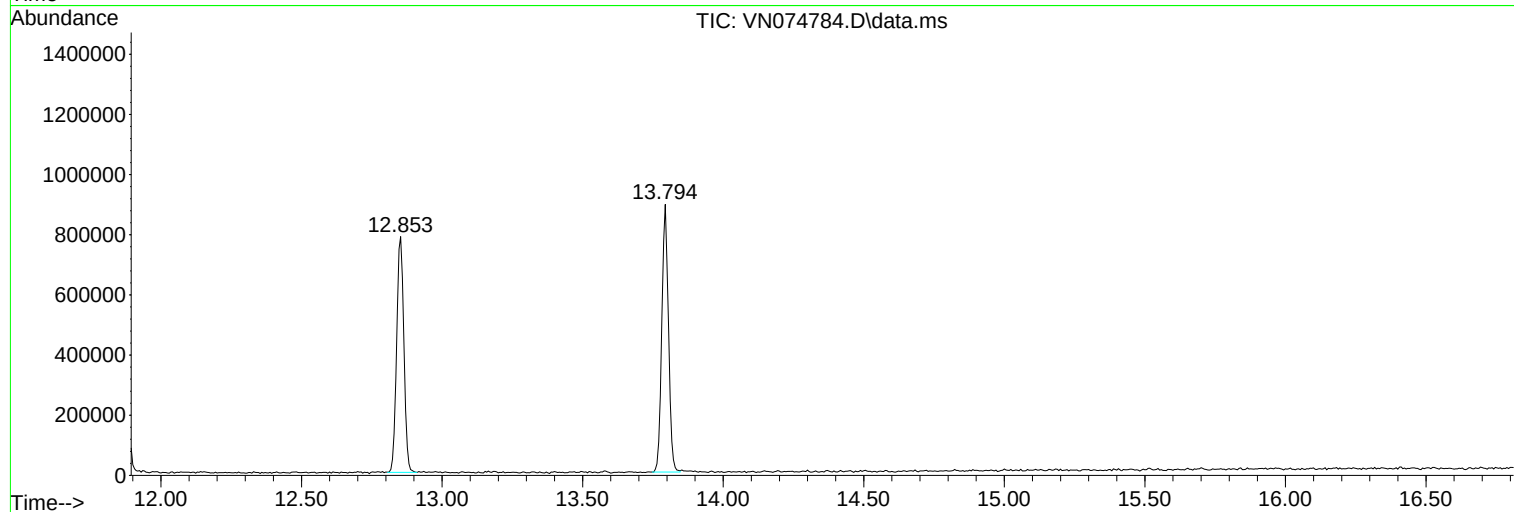
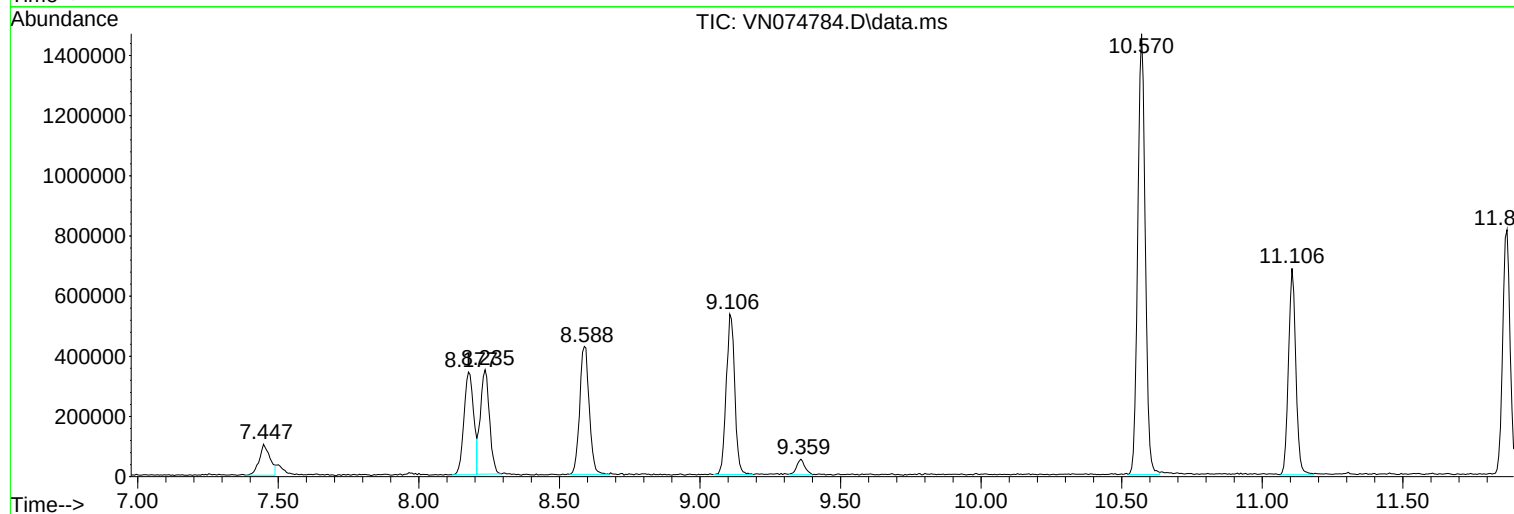
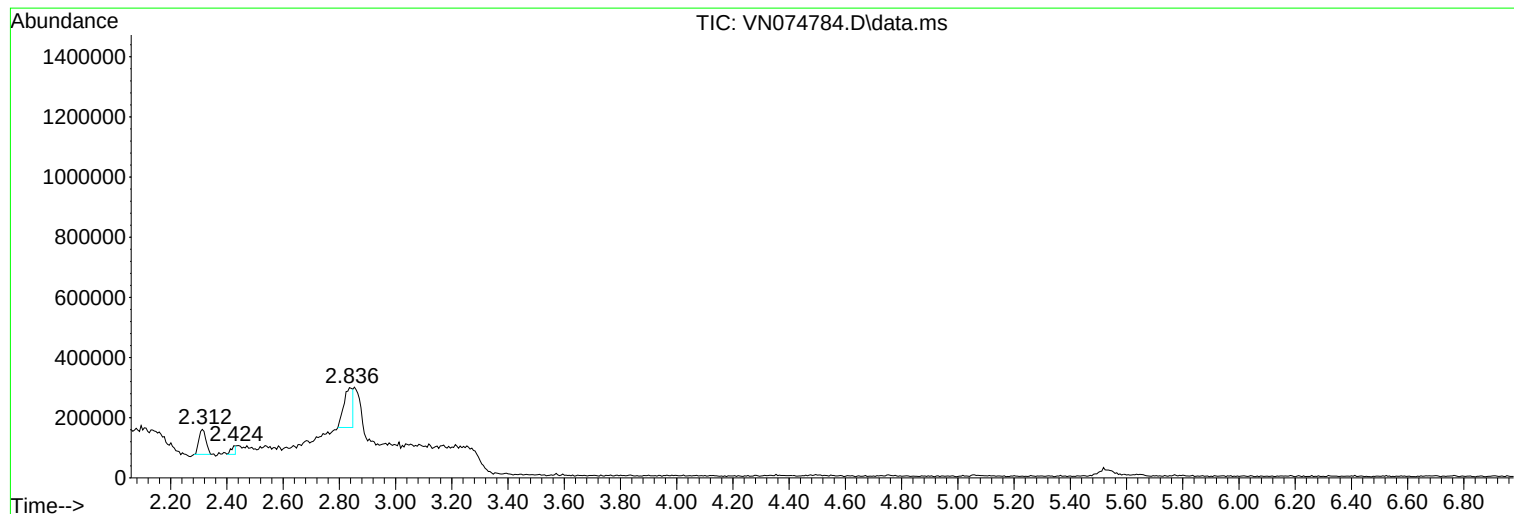
Sum of corrected areas: 12896891

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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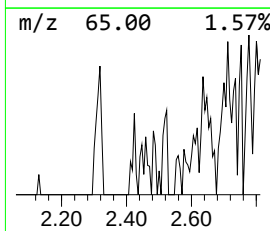
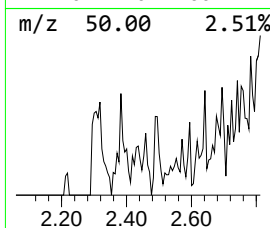
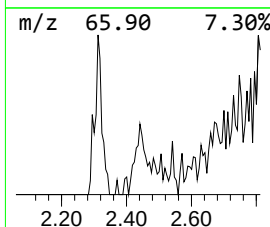
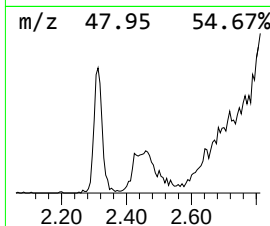
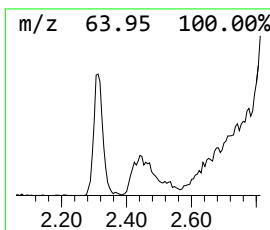
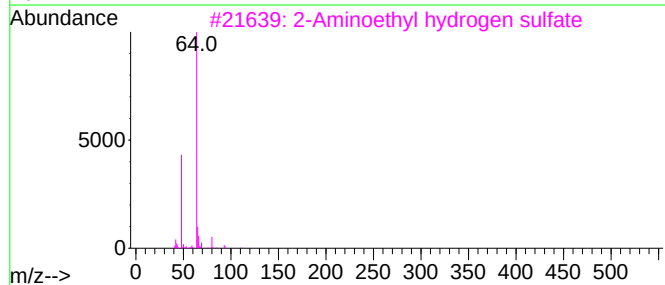
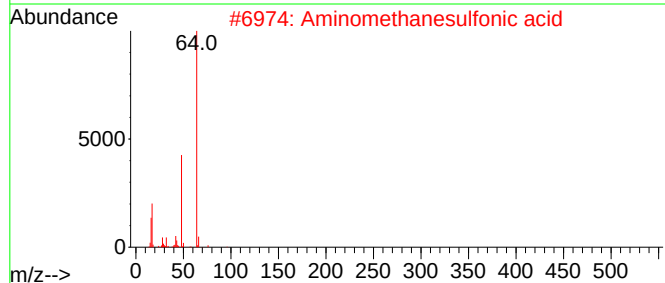
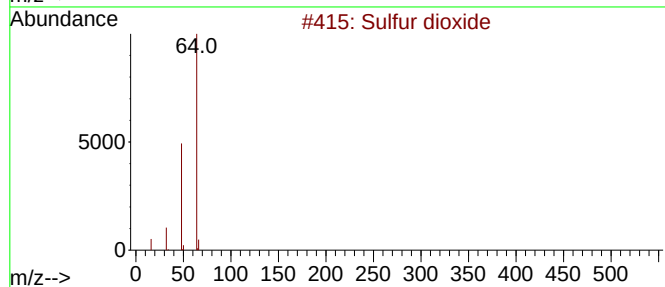
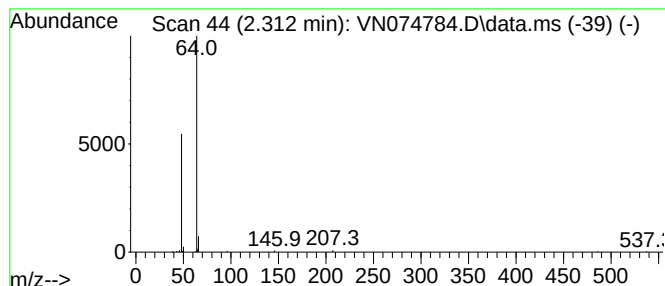
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.312	9.41 ug/l	144939	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4			1,1,1,2,2,3,3,4,4,5,5-Undecafluoro...	602	C10F22O2S	1000486-78-5	64
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	64



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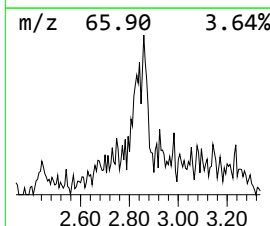
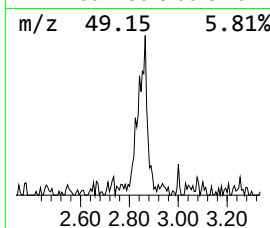
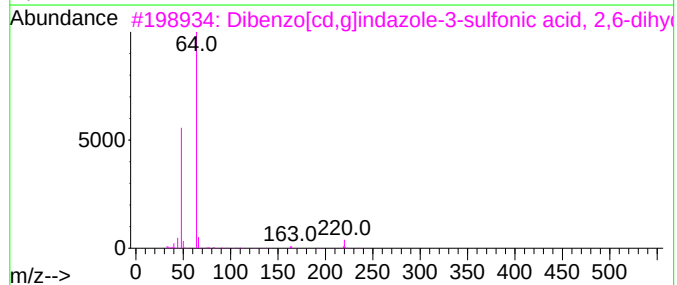
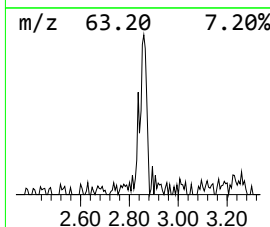
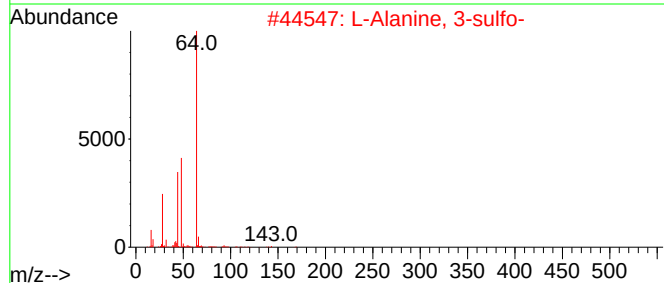
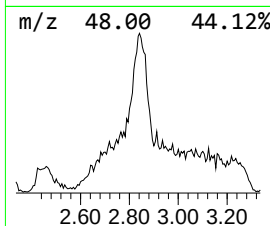
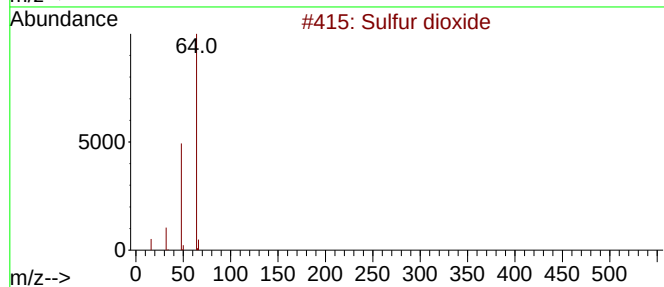
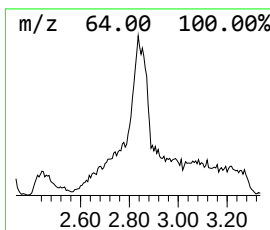
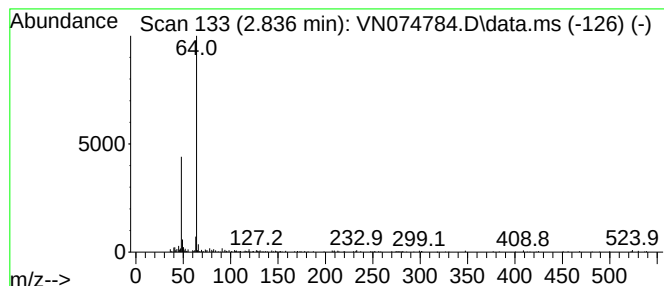
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Peak Number 2 L-Alanine, 3-sulfo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.836	19.15 ug/l	295072	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	74
3			Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	64
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	64



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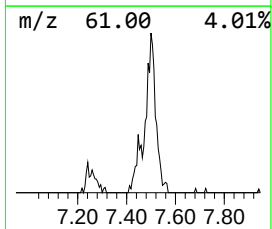
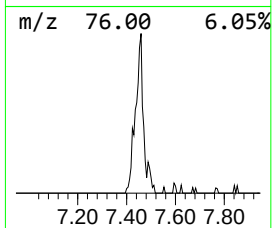
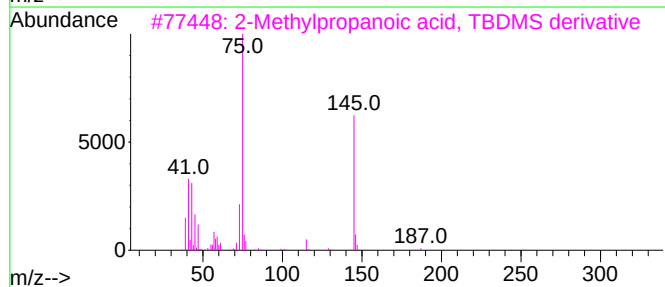
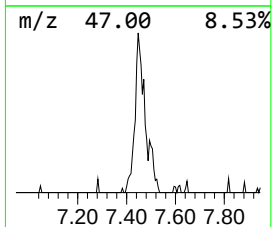
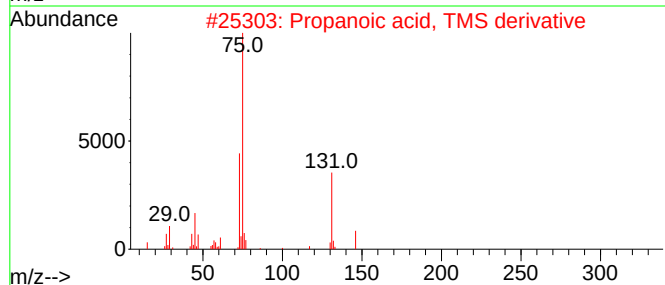
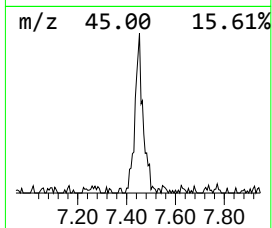
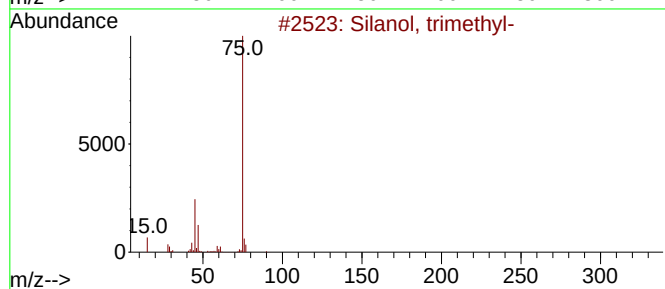
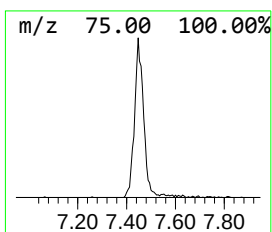
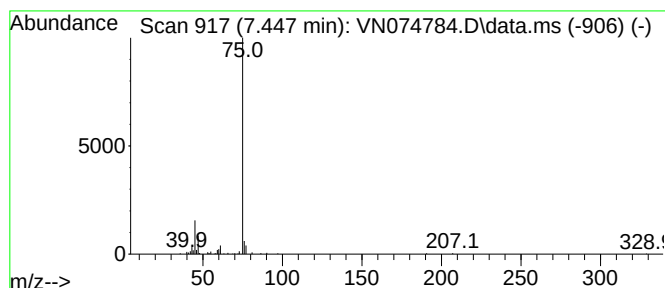
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Peak Number 3 Silanol, trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.447	17.91 ug/l	276022	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	86
2			Propanoic acid, TMS derivative	146	C6H14O2Si	016844-98-7	78
3			2-Methylpropanoic acid, TBDMS de...	202	C10H22O2Si	111864-21-2	74
4			Silanol, dimethyl(1,1,2-trimethy...	160	C8H20O2Si	055644-10-5	64
5			Formamide, N-methylthio	75	C2H5NS	018952-41-5	64



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.312	9.4	ug/l	144939	1	8.235	770418	50.0
L-Alanine, 3-su...	2.836	19.1	ug/l	295072	1	8.235	770418	50.0
Silanol, trimet...	7.447	17.9	ug/l	276022	1	8.235	770418	50.0