

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091522\
 Data File : VN074474.D
 Acq On : 15 Sep 2022 20:24
 Operator : JC\MD
 Sample : N4555-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 257248-3

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\82N091522W.M
 Title : SW846 8260

Signal : TIC: VN074474.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	48	53	60	rBV	87039	194042	7.44%	1.250%
2	2.287	63	68	80	rVB3	40047	160333	6.15%	1.033%
3	2.628	121	126	132	rBV	131202	241729	9.27%	1.557%
4	4.222	393	397	404	rBV6	12844	29567	1.13%	0.190%
5	4.499	437	444	453	rBV3	29914	90793	3.48%	0.585%
6	7.228	900	908	920	rBV2	79572	234525	9.00%	1.510%
7	7.951	1021	1031	1036	rBV2	350885	853024	32.73%	5.494%
8	8.016	1036	1042	1052	rVB	574380	1326251	50.88%	8.542%
9	8.369	1093	1102	1113	rBV	387115	904307	34.69%	5.824%
10	8.563	1128	1135	1137	rBV5	20781	40607	1.56%	0.262%
11	8.904	1181	1193	1203	rBV	960306	1975908	75.80%	12.726%
12	10.380	1435	1444	1454	rBV	1413771	2570325	98.61%	16.554%
13	11.686	1657	1666	1675	rBV	1492755	2606577	100.00%	16.787%
14	12.674	1827	1834	1843	rBV	1170667	1939962	74.43%	12.494%
15	13.616	1987	1994	2004	rBV	1421661	2359025	90.50%	15.193%

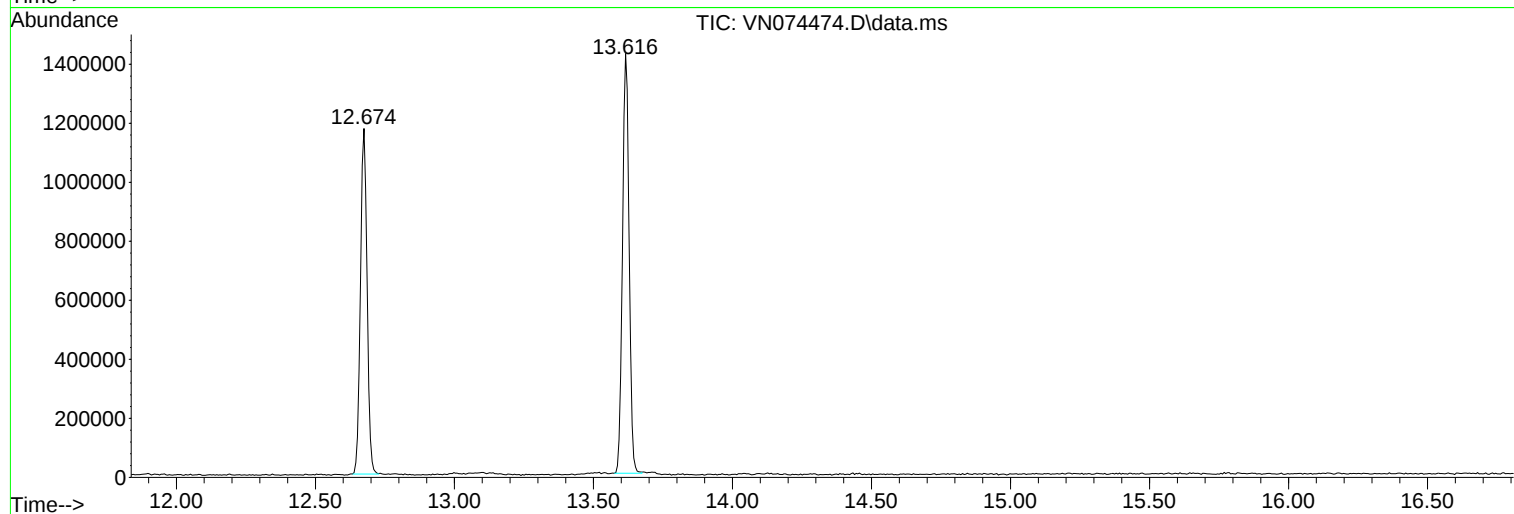
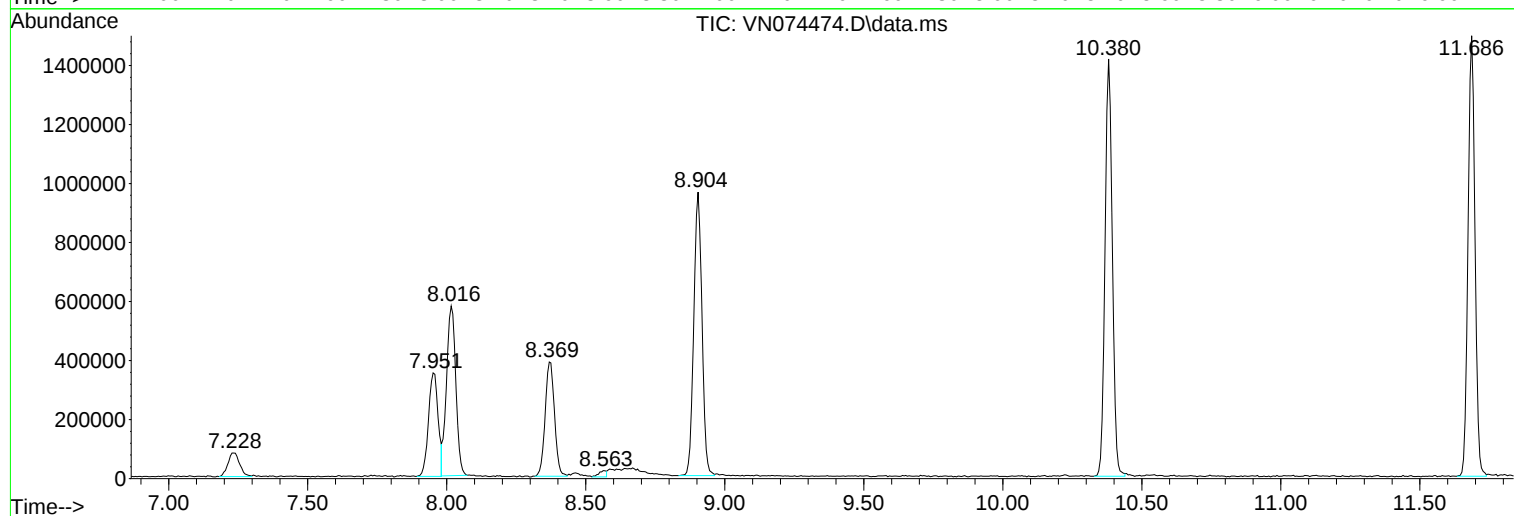
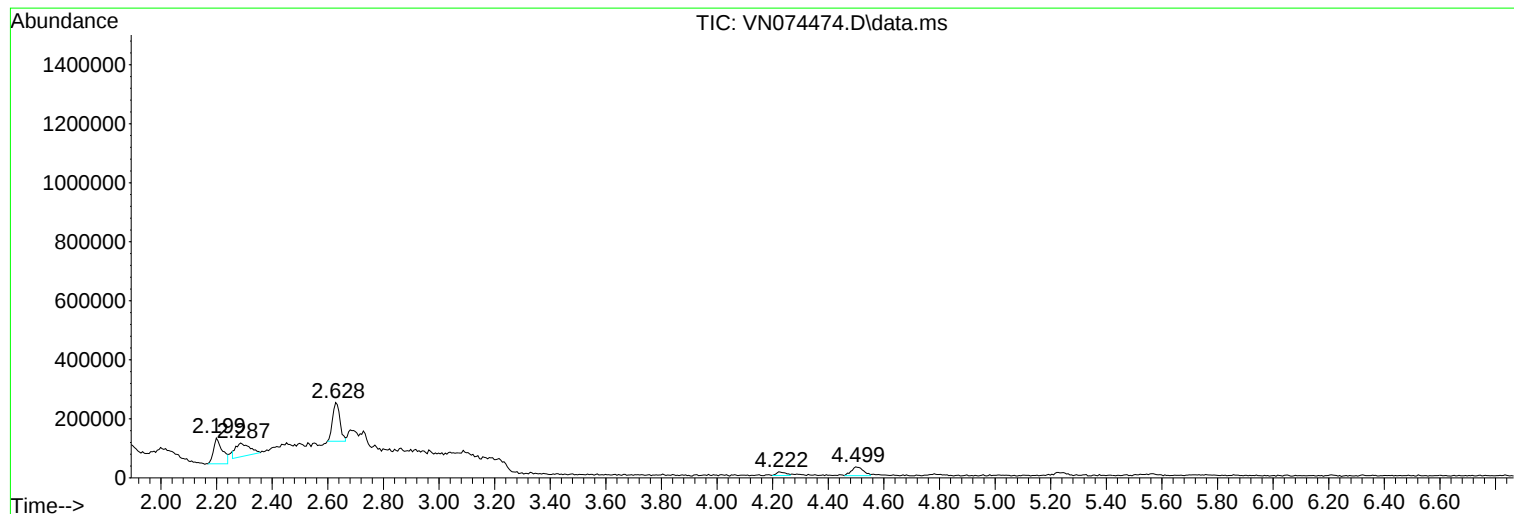
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



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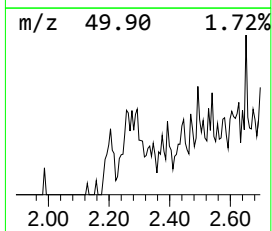
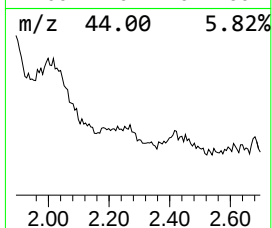
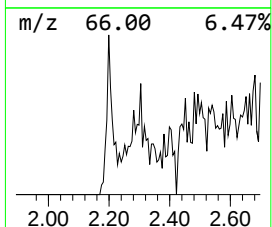
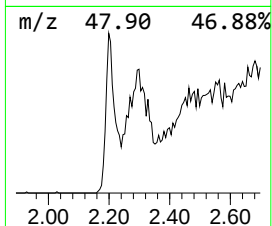
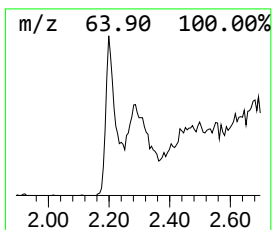
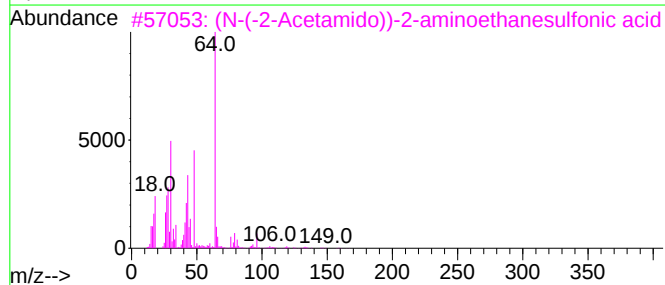
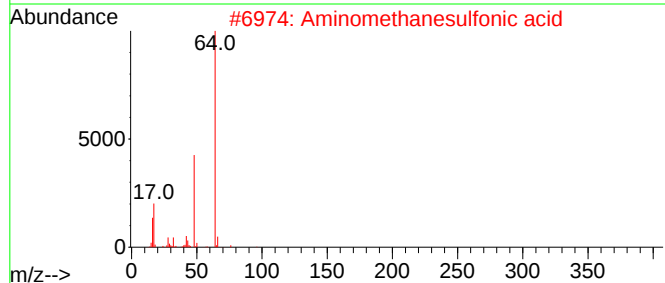
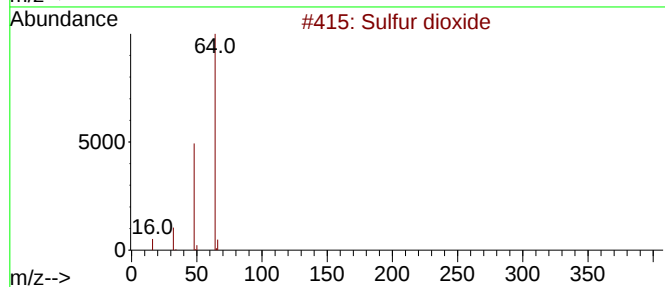
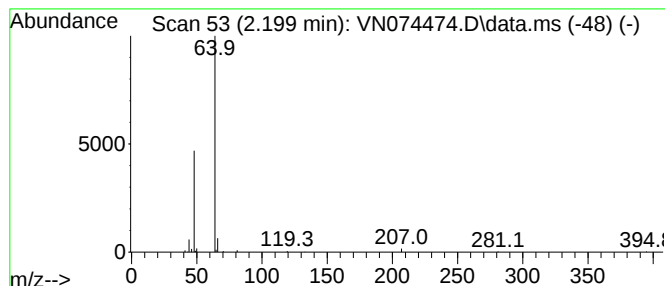
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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.
2.199	7.32 ug/l	194042	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
3			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	74
4			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
5			Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	74



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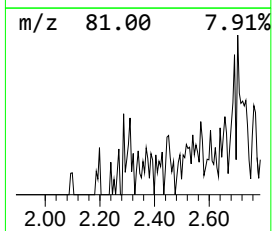
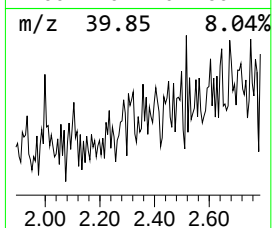
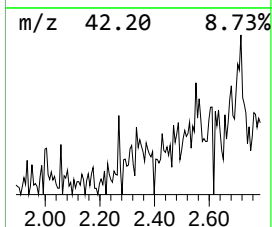
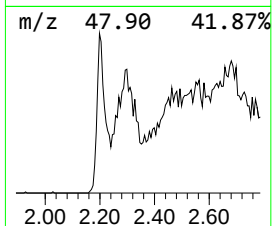
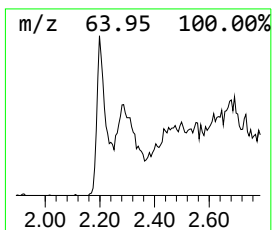
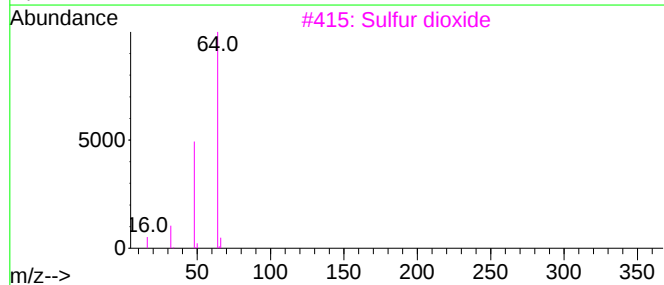
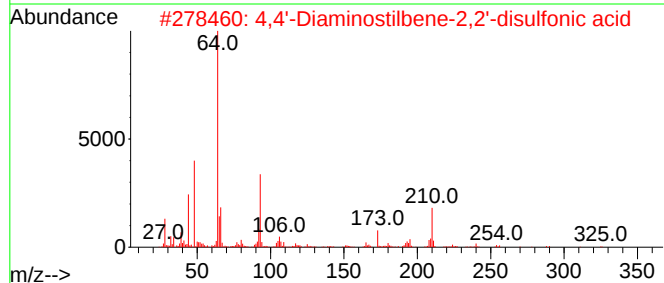
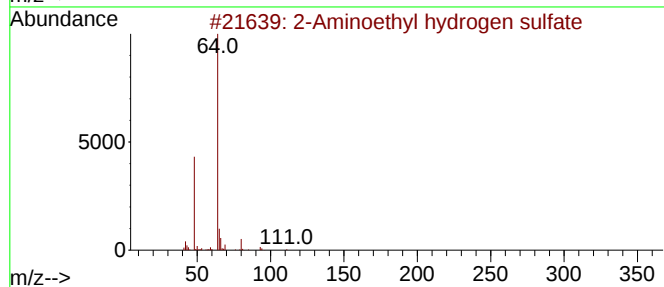
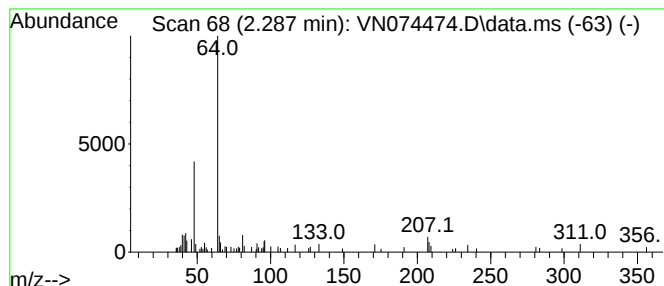
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Peak Number 2 2-Aminoethyl hydrogen sulfate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	6.04 ug/l	160333	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	78
2			4,4'-Diaminostilbene-2,2'-disulf...	370	C14H14N2O6S2	000081-11-8	64
3			Sulfur dioxide	64	O2S	007446-09-5	64
4			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	64
5			Methanethiol, N-(p-methoxyphenet...	304	C11H16N2O4S2	040283-94-1	43



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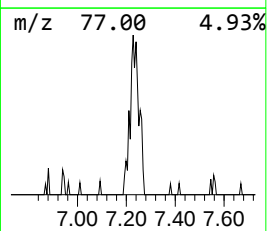
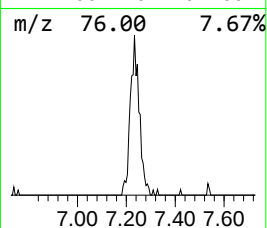
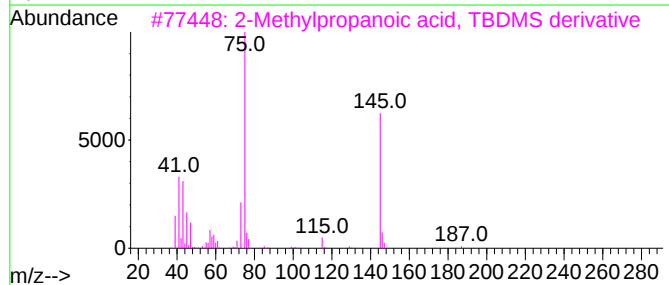
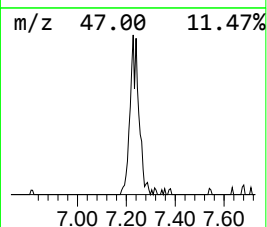
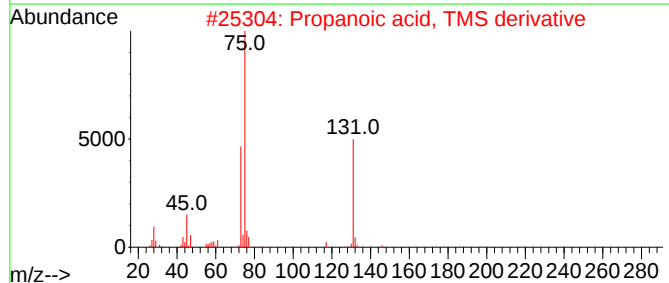
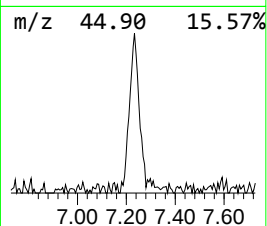
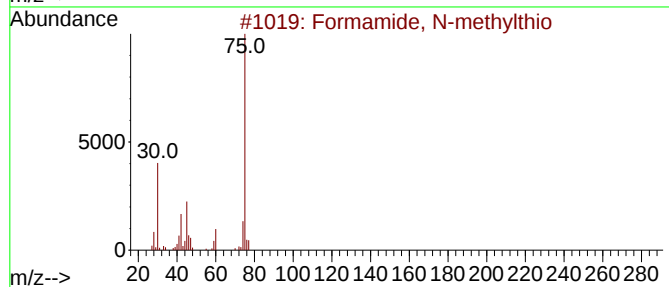
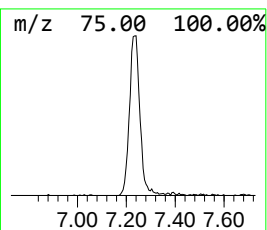
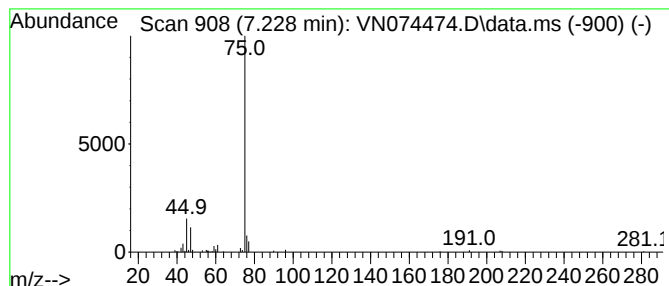
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Peak Number 4 Formamide, N-methylthio Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.228	8.84 ug/l	234525	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formamide, N-methylthio	75	C2H5NS	018952-41-5	80
2			Propanoic acid, TMS derivative	146	C6H14O2Si	016844-98-7	78
3			2-Methylpropanoic acid, TBDMS de...	202	C10H22O2Si	111864-21-2	78
4			Silanol, trimethyl-	90	C3H10O5Si	001066-40-6	74
5			Ethylene glycol, TMS derivative	134	C5H14O2Si	004403-13-8	56



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	7.3	ug/l	194042	1	8.016	1326250	50.0
2-Aminoethyl hy...	2.287	6.0	ug/l	160333	1	8.016	1326250	50.0
Formamide, N-me...	7.228	8.8	ug/l	234525	1	8.016	1326250	50.0