

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100522\
 Data File : VN074745.D
 Acq On : 05 Oct 2022 18:24
 Operator : JC\MD
 Sample : VN1005WBL01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VN1005WBL01

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: VN074745.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	38	44	51	rBV	207365	372165	10.92%	2.617%
2	2.724	110	114	115	rBV	54327	63768	1.87%	0.448%
3	2.836	127	133	135	rBV2	138033	307124	9.01%	2.159%
4	7.447	908	917	926	rBV3	41416	120868	3.55%	0.850%
5	8.177	1031	1041	1046	rBV	421824	1026474	30.11%	7.217%
6	8.235	1046	1051	1059	rVB	419249	920156	26.99%	6.469%
7	8.588	1098	1111	1123	rBV	529018	1240816	36.40%	8.724%
8	9.106	1191	1199	1211	rBV	653012	1372891	40.28%	9.652%
9	10.571	1440	1448	1460	rBV	1843651	3408626	100.00%	23.965%
10	11.871	1661	1669	1678	rBV	1003792	1853170	54.37%	13.029%
11	12.853	1829	1836	1847	rBV	996326	1730094	50.76%	12.164%
12	13.794	1989	1996	2006	rVB	1057862	1807317	53.02%	12.707%

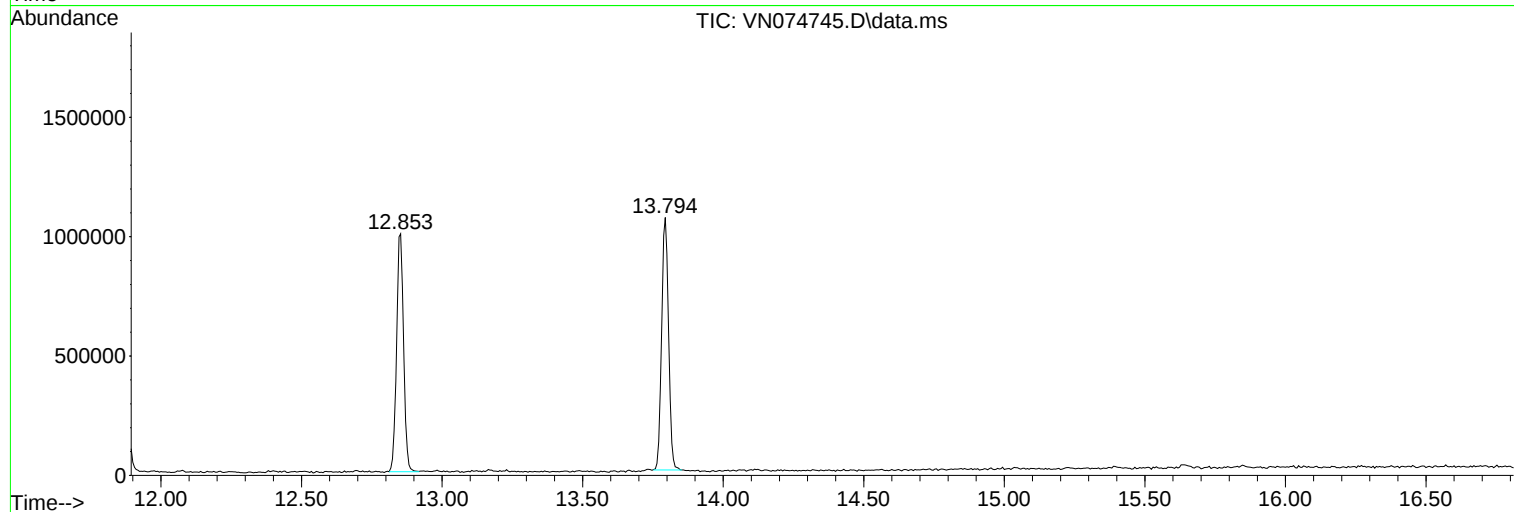
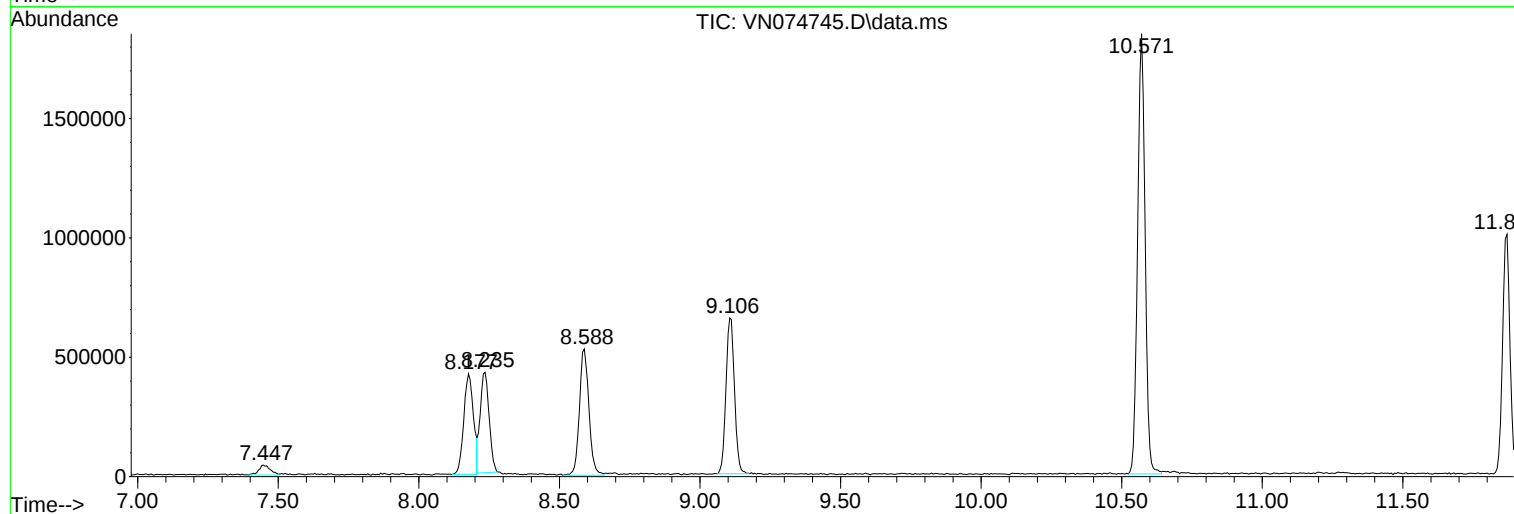
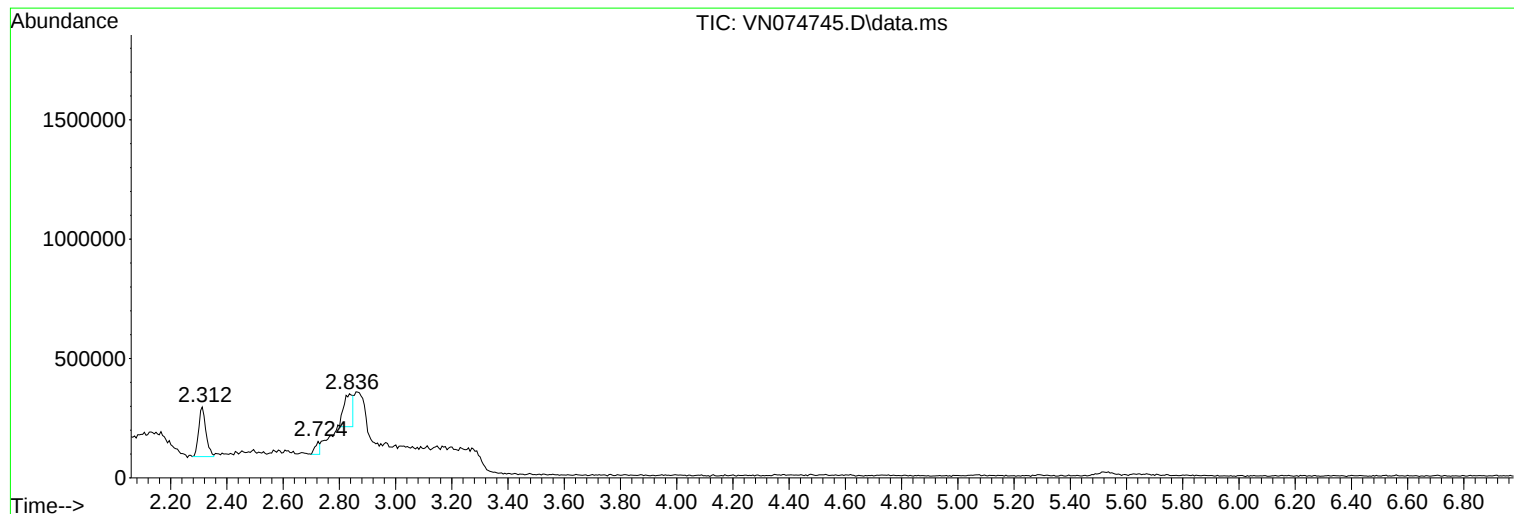
Sum of corrected areas: 14223469

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Instrument :
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ClientSampleId :
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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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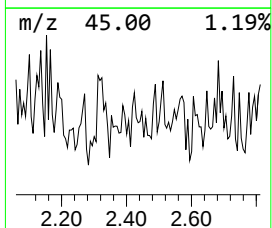
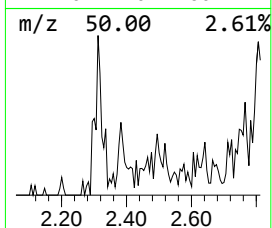
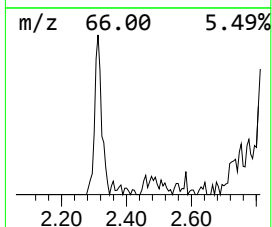
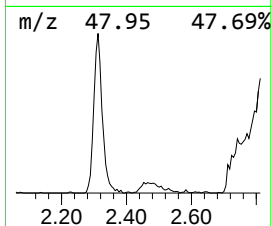
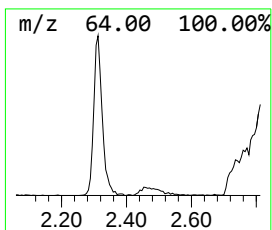
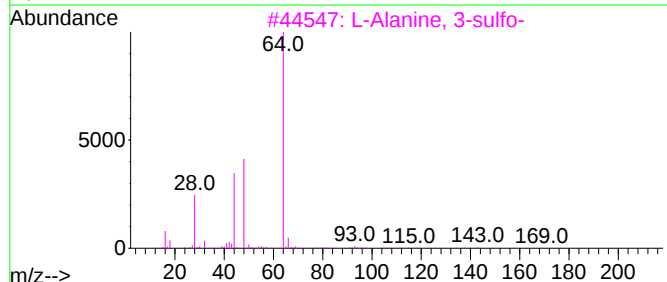
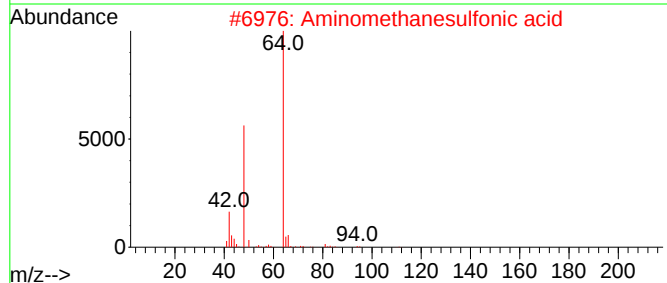
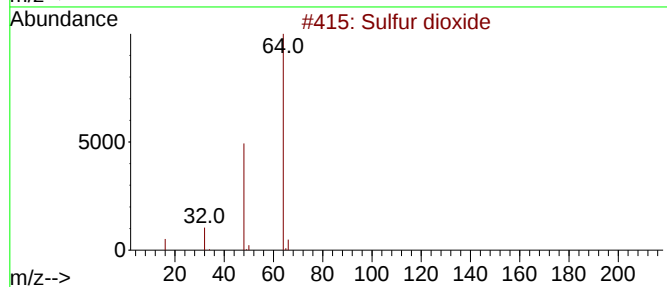
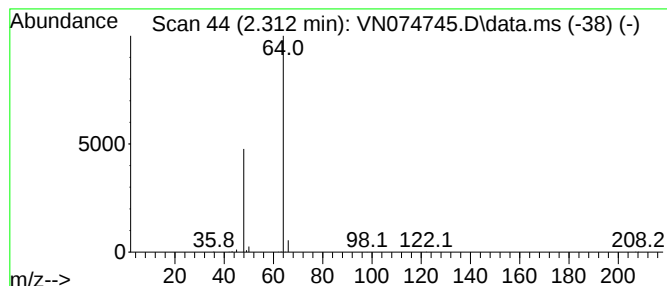
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.312	20.22 ug/l	372165	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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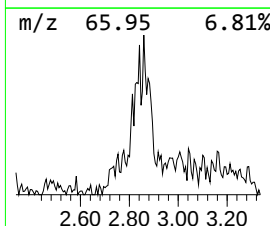
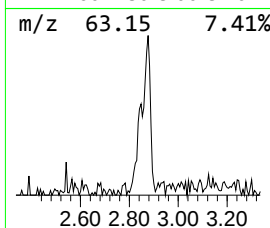
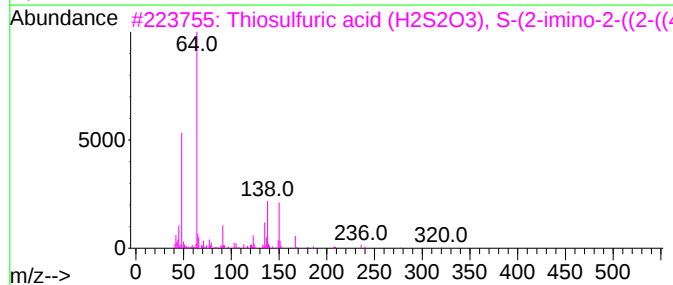
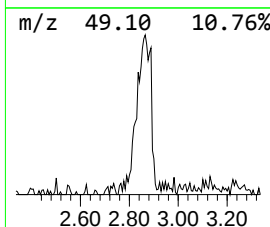
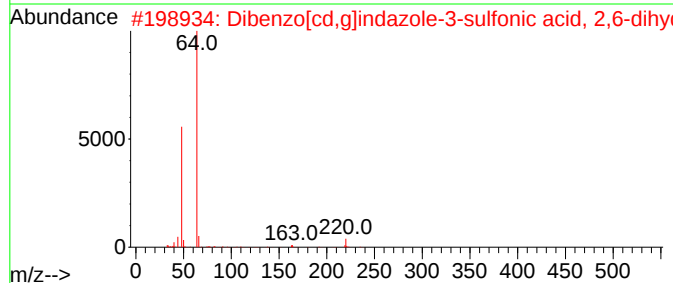
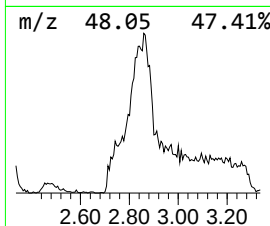
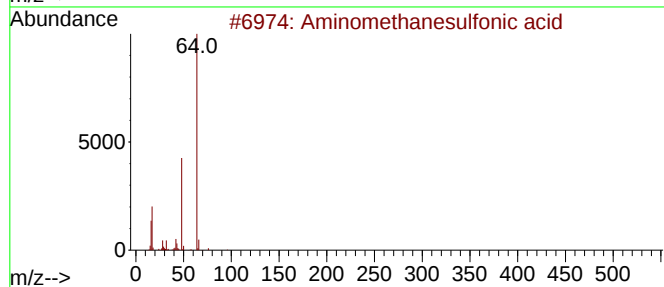
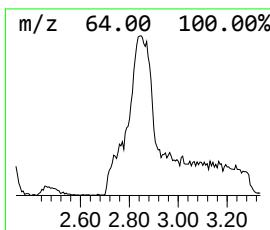
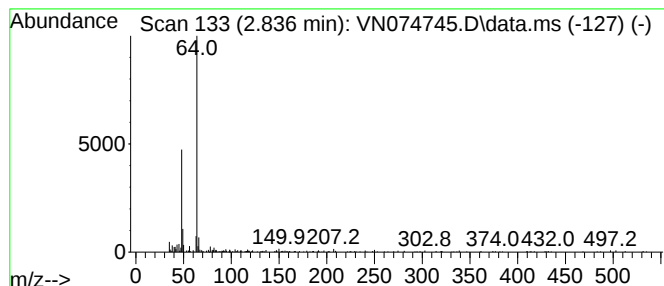
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Peak Number 2 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.836	16.69 ug/l	307124	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
2			Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	64
3			Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	64
4			Vinylsulfonamide	107	C2H5NO2S	002386-58-5	64
5			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	64



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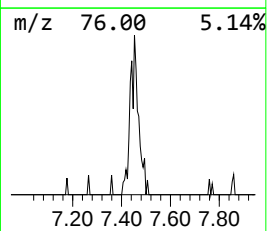
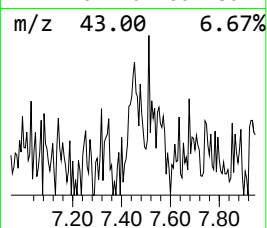
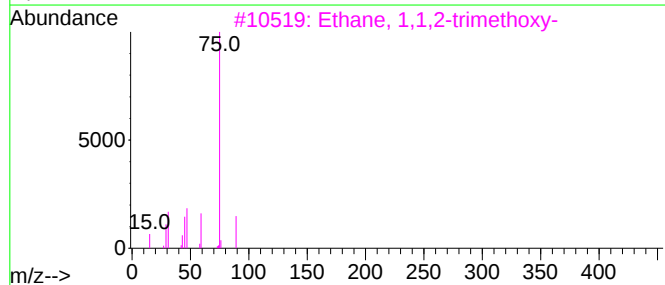
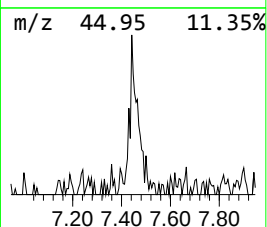
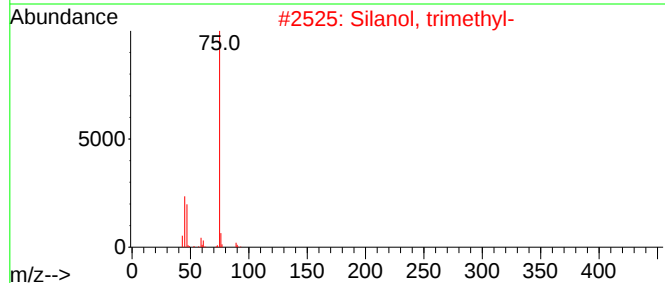
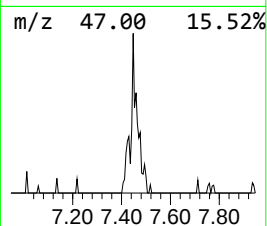
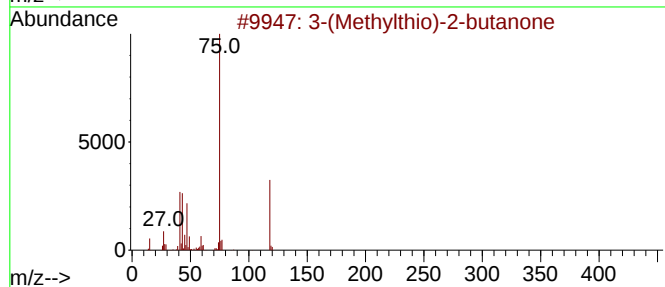
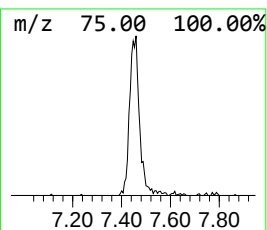
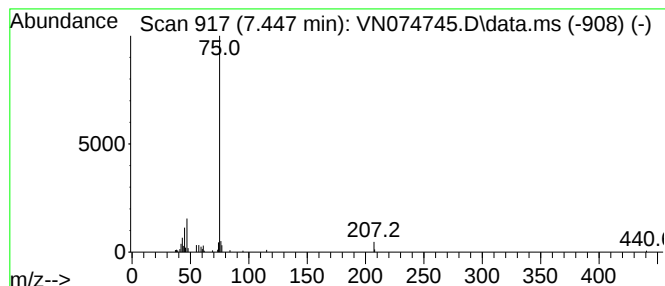
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Peak Number 3 3-(Methylthio)-2-butanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.447	6.57 ug/l	120868	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(Methylthio)-2-butanone	118	C5H10OS	053475-15-3	72
2			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	64
3			Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	56
4			Silanol, dimethyl(1,1,2-trimethy...	160	C8H20OSi	055644-10-5	56
5			Propanoic acid, TMS derivative	146	C6H14O2Si	016844-98-7	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.312	20.2	ug/l	372165	1	8.235	920156	50.0
Aminomethanesul...	2.836	16.7	ug/l	307124	1	8.235	920156	50.0
3-(Methylthio)-...	7.447	6.6	ug/l	120868	1	8.235	920156	50.0