

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100722\
 Data File : VN074803.D
 Acq On : 07 Oct 2022 11:54
 Operator : JC\MD
 Sample : N4963-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 257155-4

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: VN074803.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	53	rBV	251774	494498	16.80%	3.785%
2	2.777	119	123	126	rBV	45999	61647	2.09%	0.472%
3	2.848	126	135	138	rBV3	143141	438196	14.89%	3.354%
4	4.753	451	459	466	rBV4	33444	98717	3.35%	0.756%
5	5.518	582	589	591	rBV4	15843	31846	1.08%	0.244%
6	7.453	908	918	930	rBV2	51965	159390	5.42%	1.220%
7	8.177	1031	1041	1046	rBV2	380142	901103	30.62%	6.898%
8	8.230	1046	1050	1064	rVB	363292	833797	28.33%	6.383%
9	8.588	1101	1111	1122	rBV	462860	1065535	36.21%	8.157%
10	9.112	1187	1200	1210	rBV	586051	1230159	41.80%	9.417%
11	10.571	1440	1448	1463	rBV	1634375	2942986	100.00%	22.529%
12	11.870	1661	1669	1678	rBV	914141	1645283	55.91%	12.595%
13	12.853	1826	1836	1845	rBV	866876	1505798	51.17%	11.527%
14	13.794	1989	1996	2004	rBV	979405	1611592	54.76%	12.337%
15	15.641	2305	2310	2316	rVB3	21291	42788	1.45%	0.328%

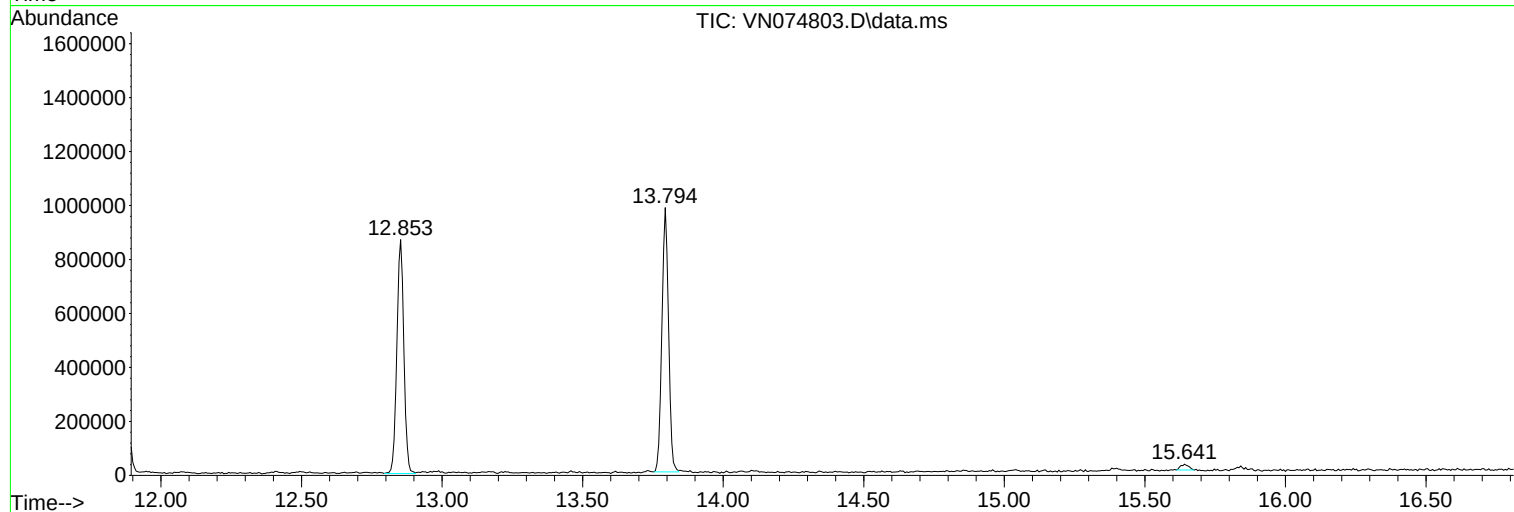
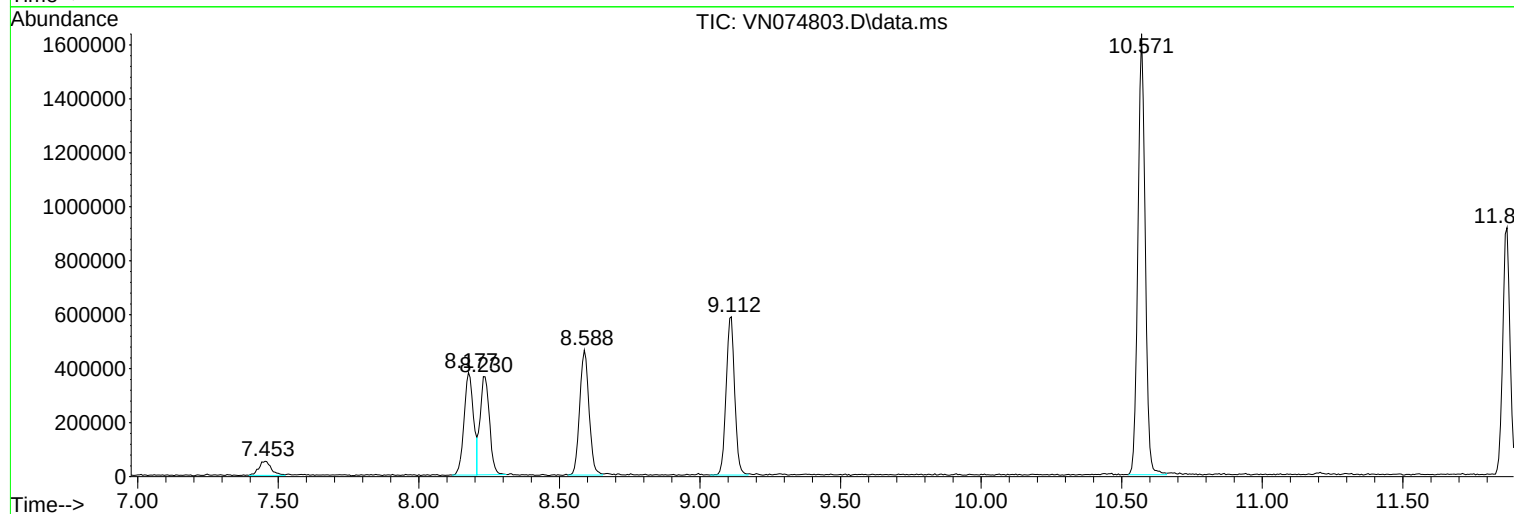
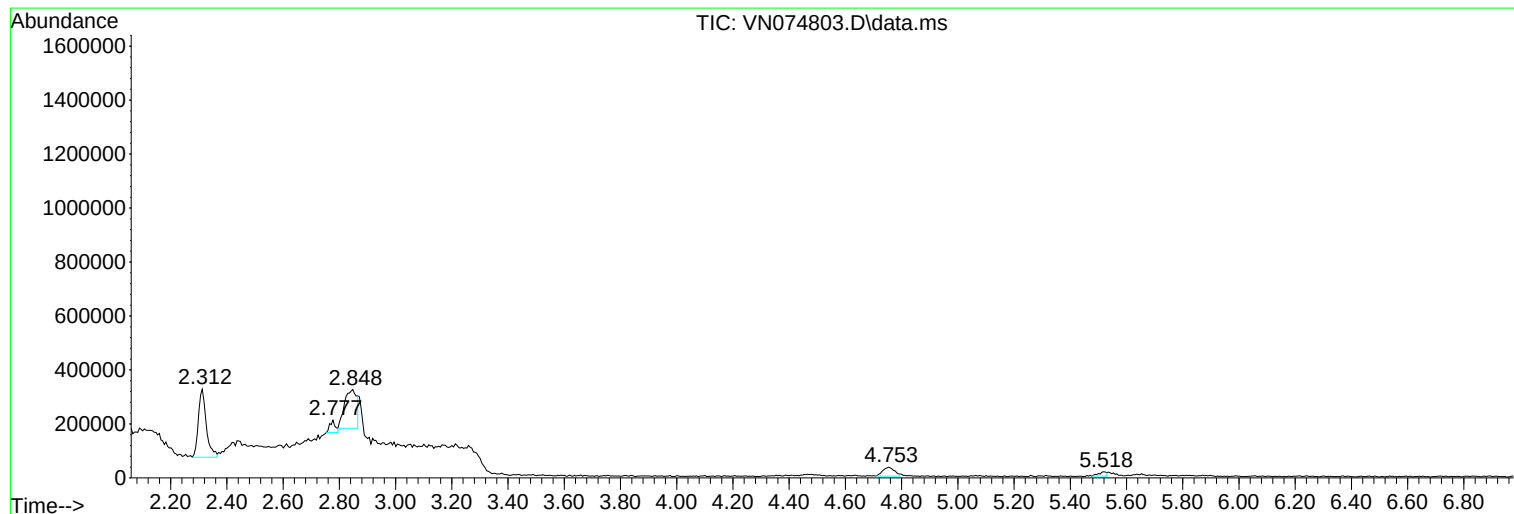
Sum of corrected areas: 13063335

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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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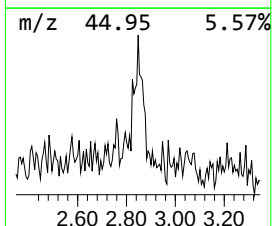
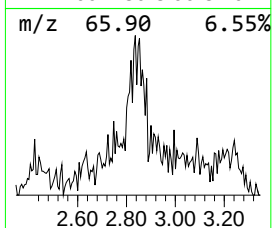
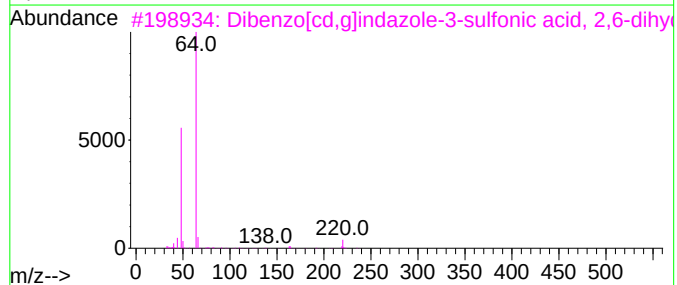
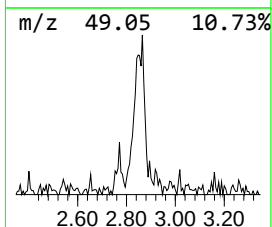
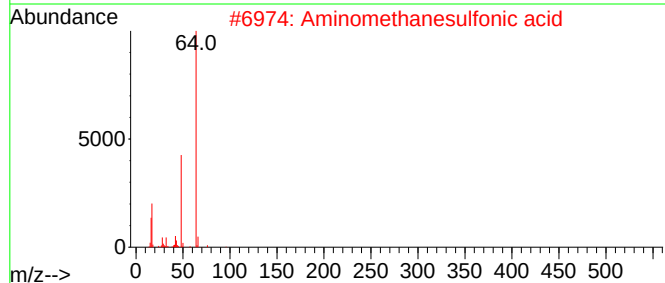
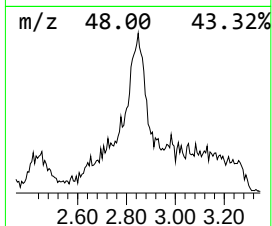
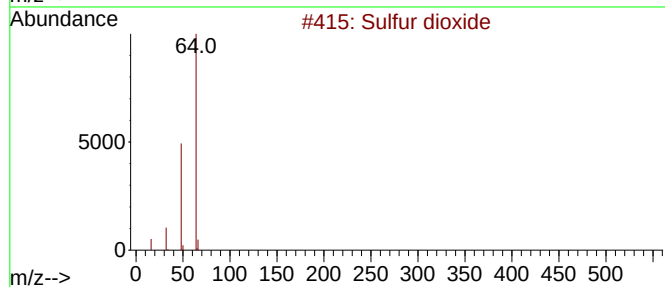
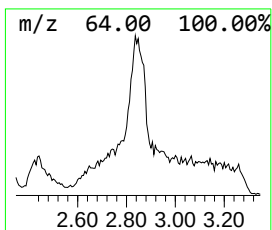
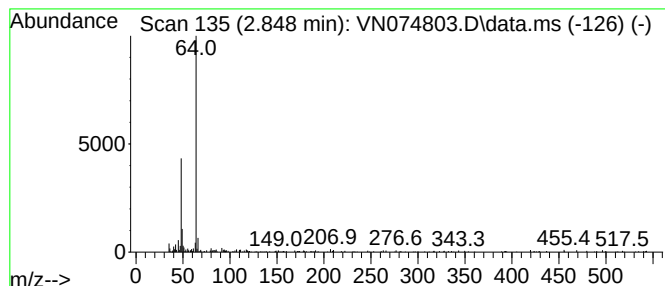
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Quant Title : SW846 8260

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

Peak Number 2 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.848	26.28 ug/l	438196	Pentafluorobenzene	8.235	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	86
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	64
4	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	64
5	2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	64



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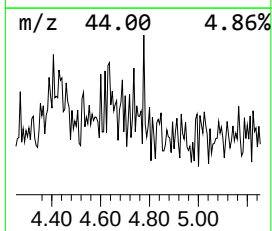
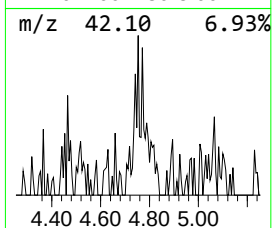
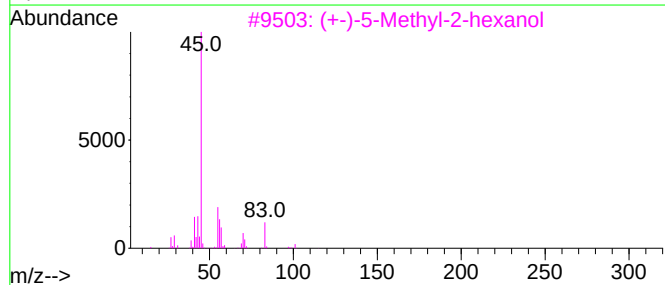
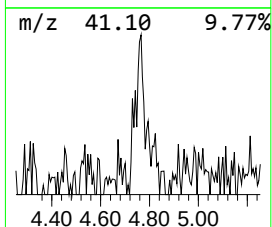
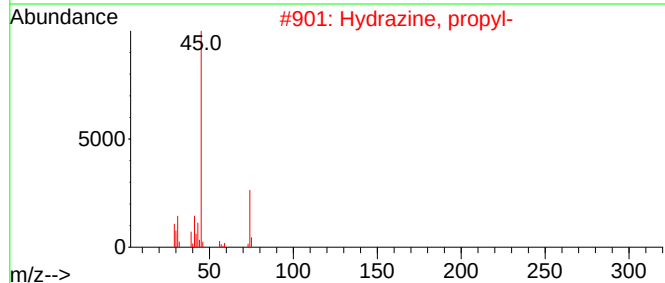
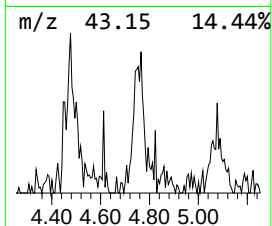
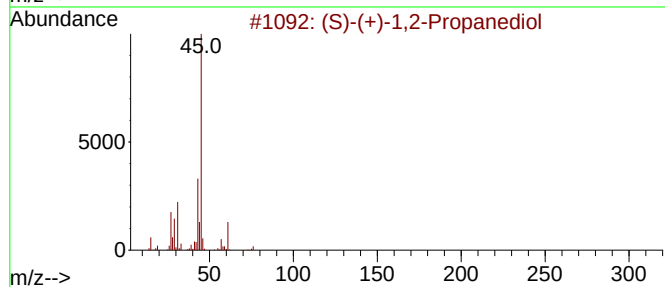
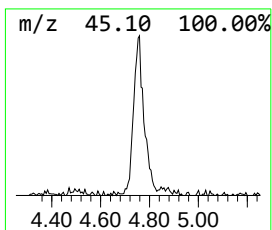
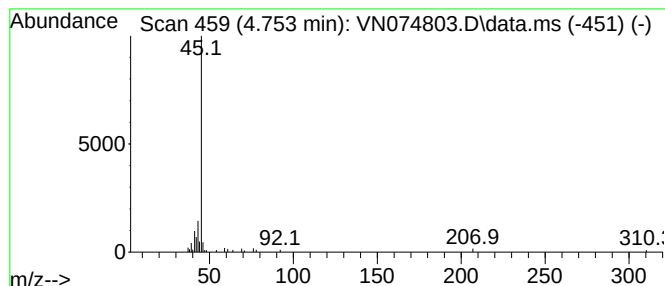
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Peak Number 3 unknown4.753 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.753	5.92 ug/l	98717	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	40
2	Hydrazine, propyl-			74	C3H10N2	005039-61-2	9
3	(+)-5-Methyl-2-hexanol			116	C7H16O	111768-09-3	9
4	1-Methoxy-5-heptafluorobutyrylox...			328	C11H15F7O3	1000216-63-3	9
5	Propane, 2-ethoxy-			88	C5H12O	000625-54-7	9



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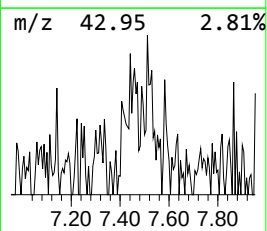
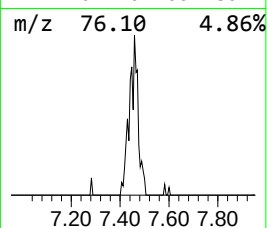
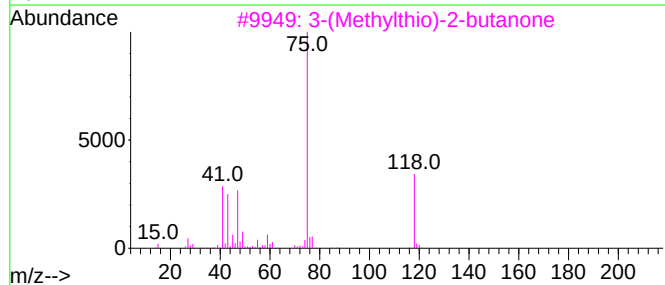
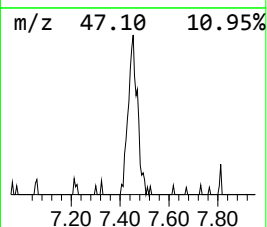
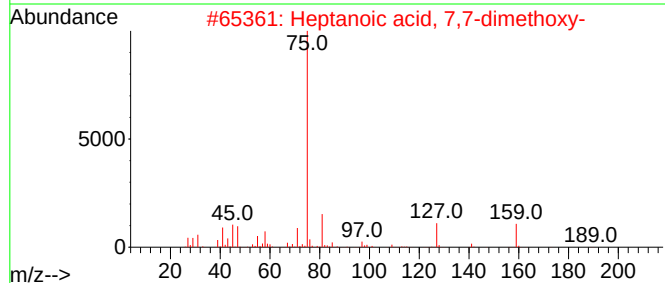
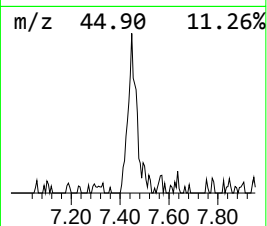
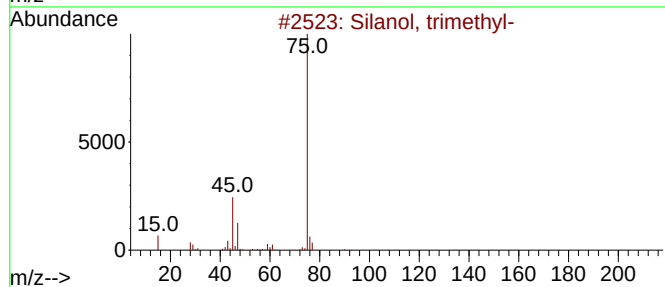
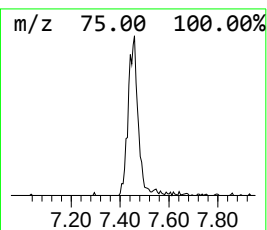
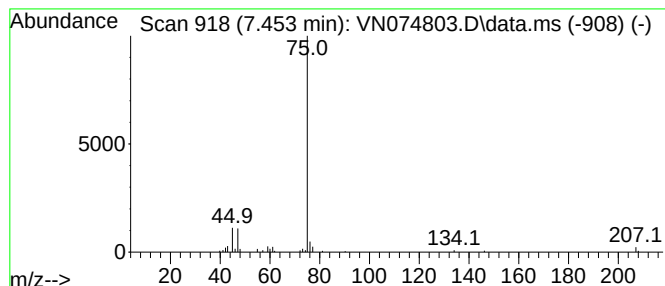
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Peak Number 4 Silanol, trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.453	9.56 ug/l	159390	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	80
2			Heptanoic acid, 7,7-dimethoxy-	190	C9H18O4	109137-93-1	64
3			3-(Methylthio)-2-butanone	118	C5H10OS	053475-15-3	56
4			Butane, 2-methyl-3-(methylthio)-	118	C6H14S	053897-51-1	43
5			2-Methylpropanoic acid, TBDMS de...	202	C10H22O2Si	111864-21-2	43



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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	2.848	26.3	ug/l	438196	1	8.235	833797	50.0
unknown4.753	4.753	5.9	ug/l	98717	1	8.235	833797	50.0
Silanol, trimet...	7.453	9.6	ug/l	159390	1	8.235	833797	50.0