

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072321\
 Data File : VY005425.D
 Acq On : 23 Jul 2021 18:59
 Operator : SY/MD
 Sample : M3137-05
 Misc : 10.49G/5ML/MSVOA_Y/SOIL
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20210726-15

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_Y\methods\82Y072221S.M

Title : SW846 8260

Signal : TIC: VY005425.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.869	3	8	18	rVB3	33919	64038	2.13%	0.689%
2	2.223	62	66	76	rVB2	15260	31965	1.07%	0.344%
3	3.960	339	351	358	rBV	61330	166676	5.55%	1.794%
4	4.046	358	365	376	rVV	20496	59407	1.98%	0.639%
5	4.204	379	391	403	rBV	24329	67810	2.26%	0.730%
6	4.729	467	477	493	rBV	11633	39690	1.32%	0.427%
7	7.003	841	850	861	rBV2	18734	52277	1.74%	0.563%
8	7.728	958	969	974	rBV	162105	386323	12.87%	4.158%
9	7.795	974	980	994	rVB	250629	583155	19.43%	6.276%
10	8.149	1027	1038	1051	rBV	176319	396141	13.20%	4.264%
11	8.697	1118	1128	1139	rBV	434508	832782	27.75%	8.963%
12	10.185	1363	1372	1381	rBV	714292	1215295	40.50%	13.080%
13	11.496	1579	1587	1595	rBV	681785	1106563	36.87%	11.910%
14	12.496	1741	1751	1760	rBV2	1681902	3001066	100.00%	32.299%
15	13.428	1894	1904	1910	rBV	729151	1096015	36.52%	11.796%
16	13.971	1986	1993	2000	rVB2	113961	192178	6.40%	2.068%

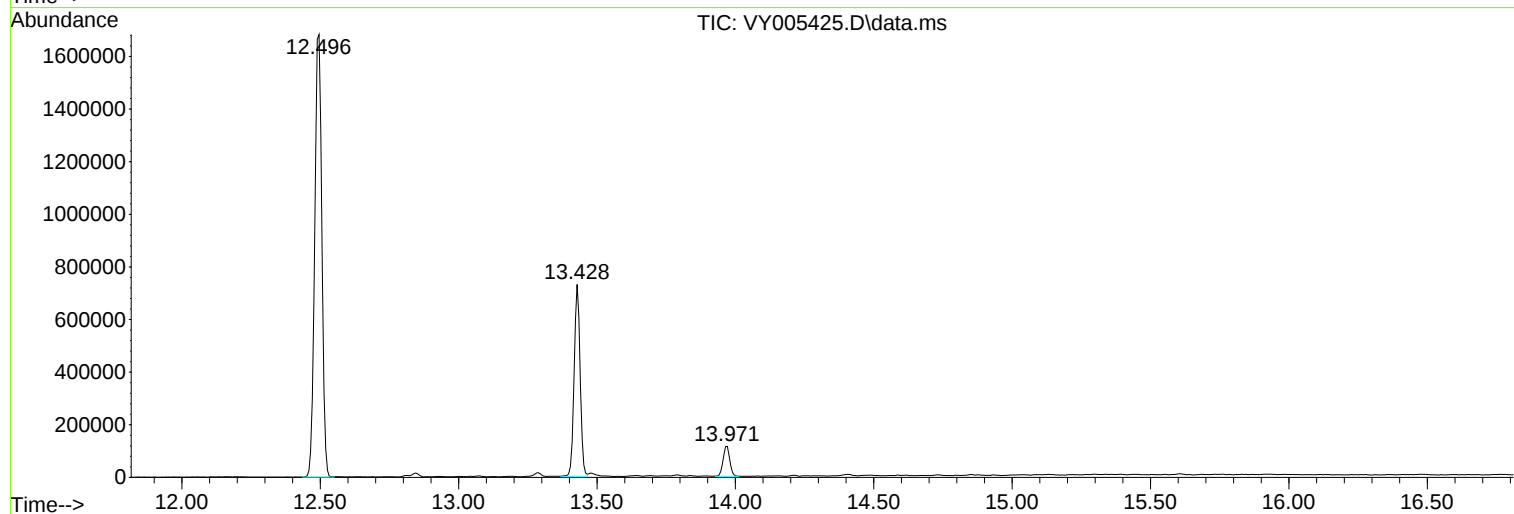
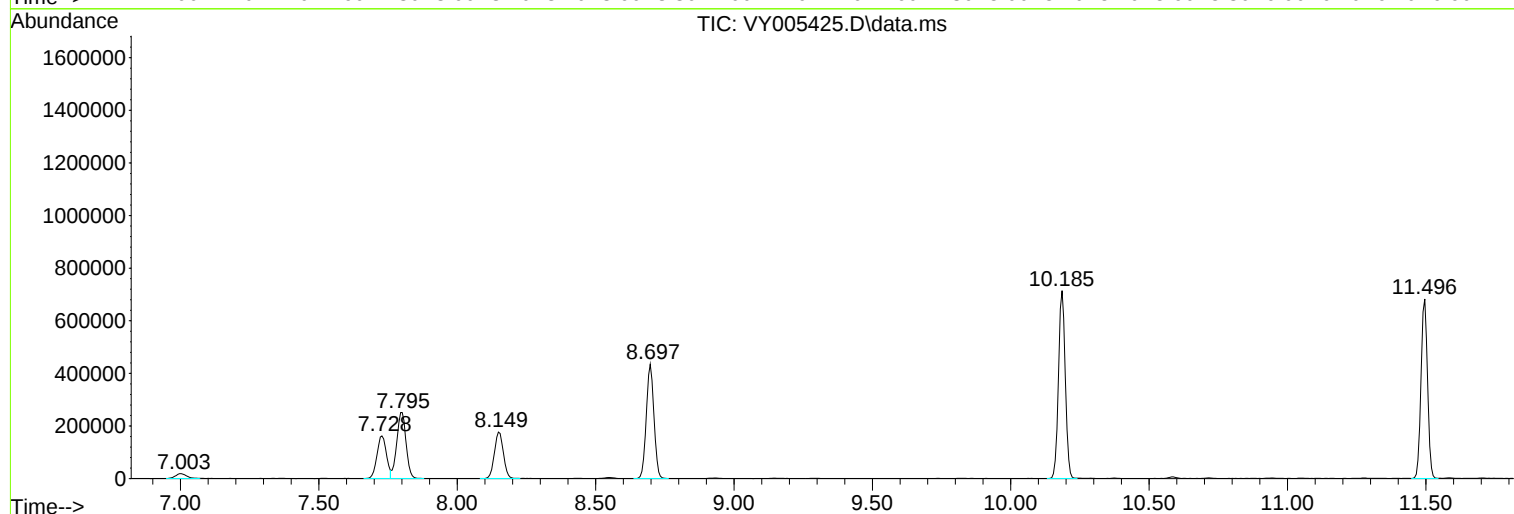
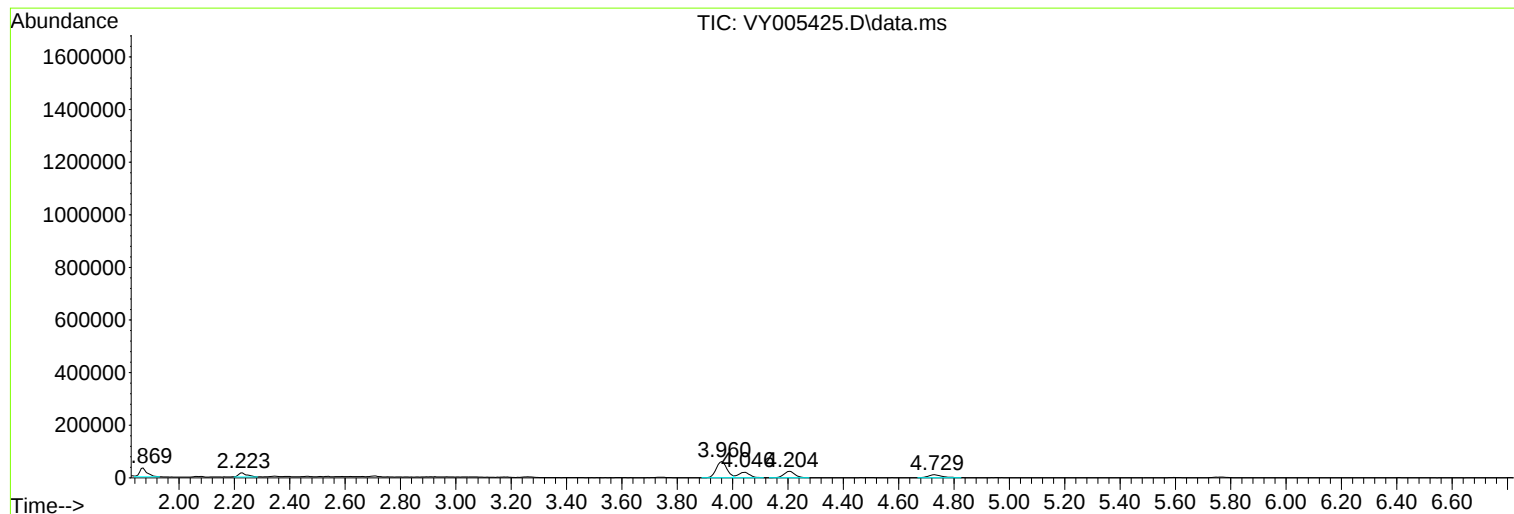
Sum of corrected areas: 9291381

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072221S.M
Quant Title : SW846 8260

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



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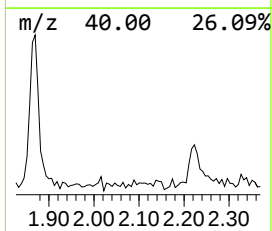
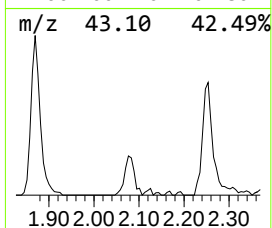
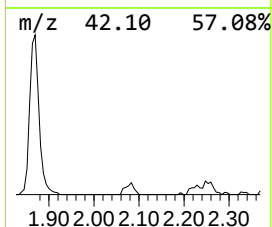
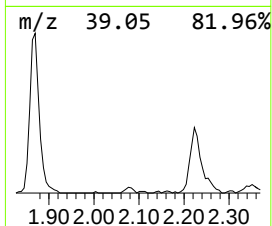
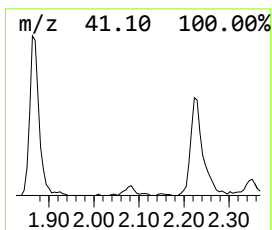
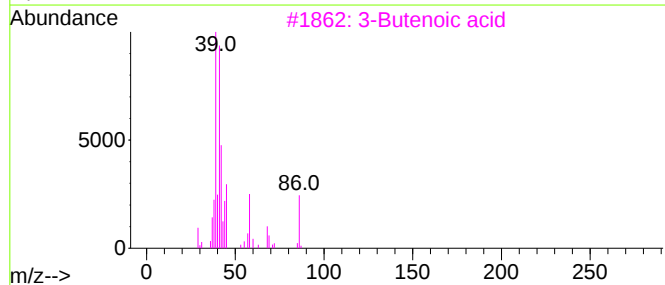
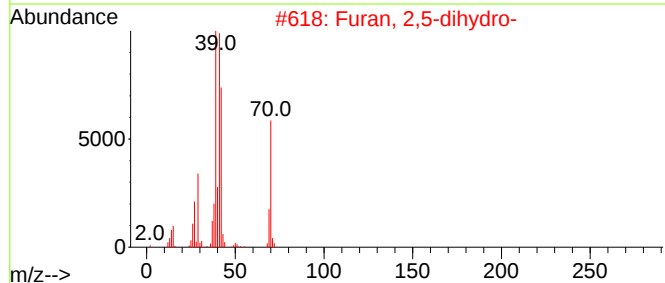
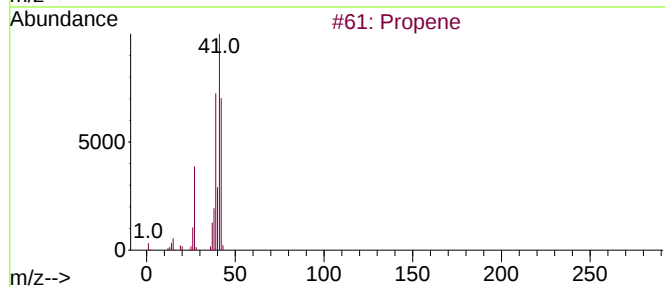
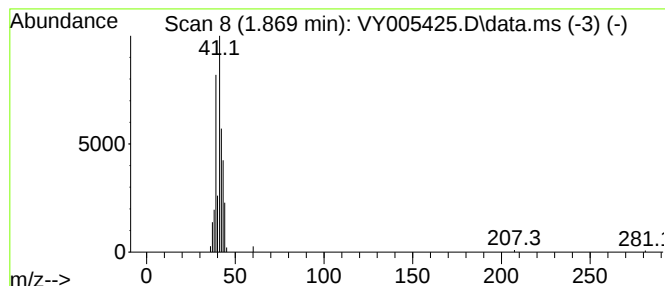
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072221S.M
Quant Title : SW846 8260

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

Peak Number 1 Propene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.869	5.49 ug/l	64038	Pentafluorobenzene	7.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	83
3			3-Butenoic acid	86	C4H6O2	000625-38-7	78
4			2-Butenal, (E)-	70	C4H6O	000123-73-9	78
5			Pyrimidin-4(3H)-one, 3-amino-2,6...	139	C6H9N3O	093098-74-9	78



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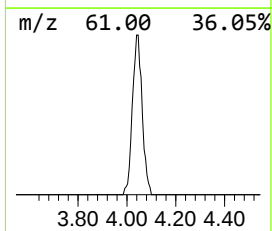
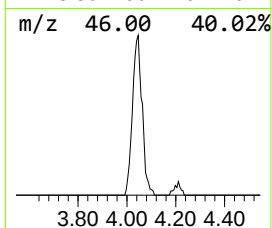
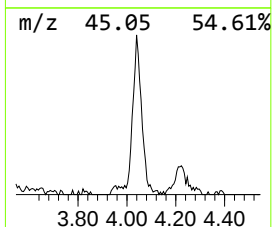
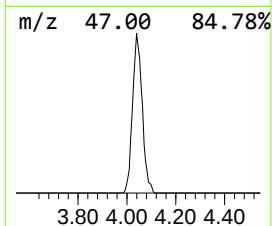
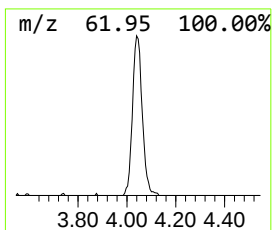
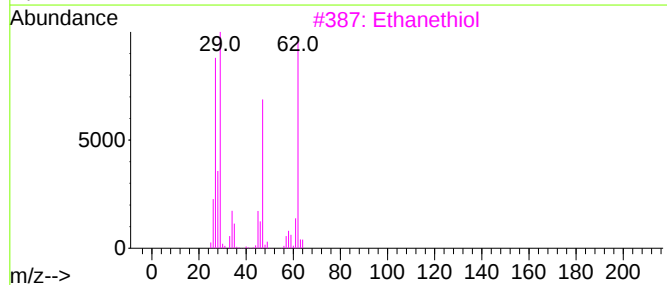
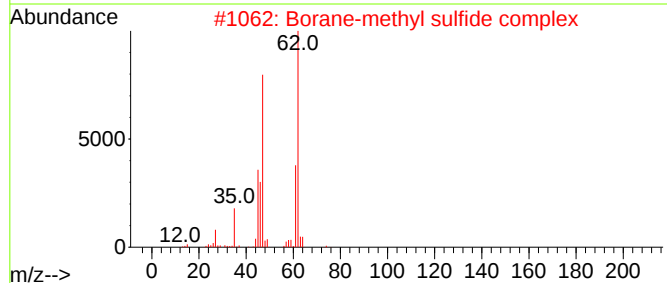
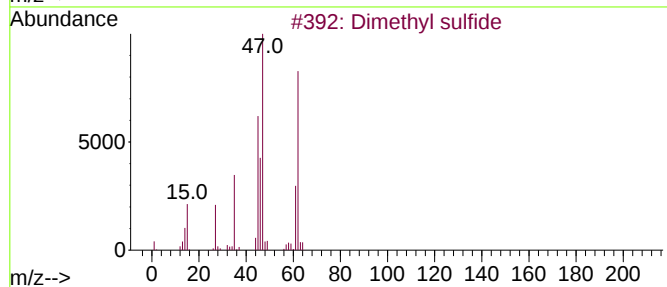
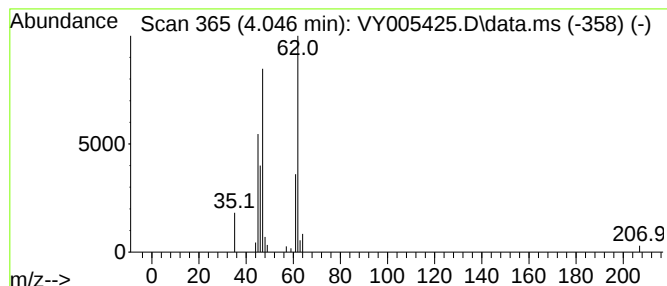
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Peak Number 2 Dimethyl sulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.046	5.09 ug/l	59407	Pentafluorobenzene	7.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	91
2			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90
3			Ethanethiol	62	C2H6S	000075-08-1	72
4			Sulfonium, dimethyl-, cyanonitro...	146	C4H6N2O2S	058992-18-0	38
5			Acetic acid, mercapto-, methyl e...	106	C3H6O2S	002365-48-2	22



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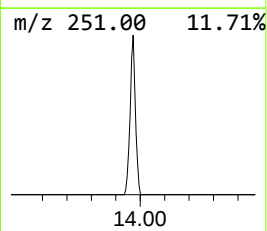
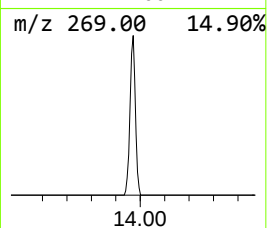
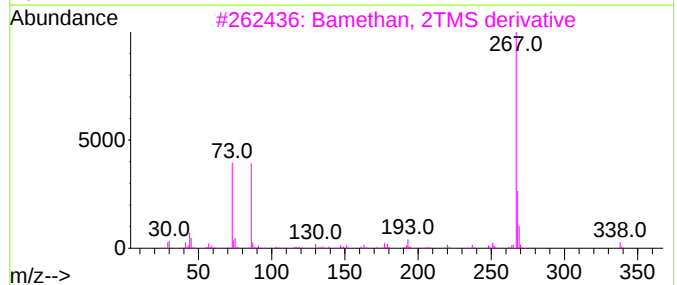
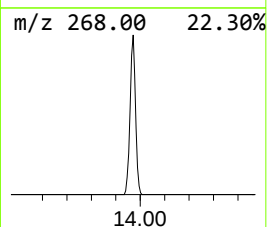
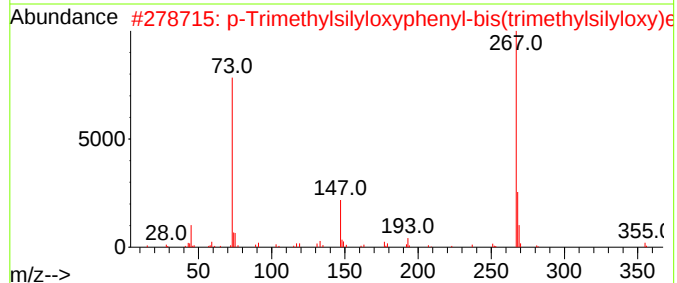
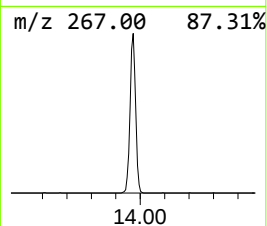
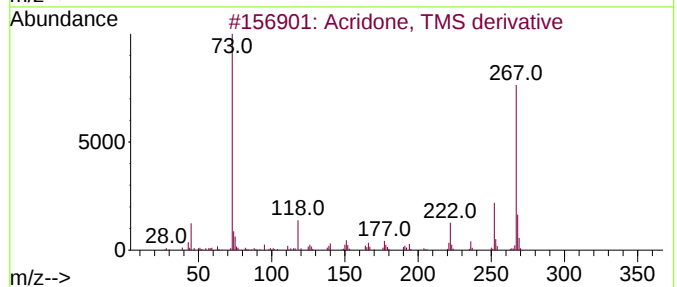
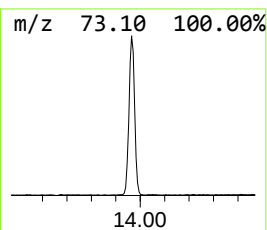
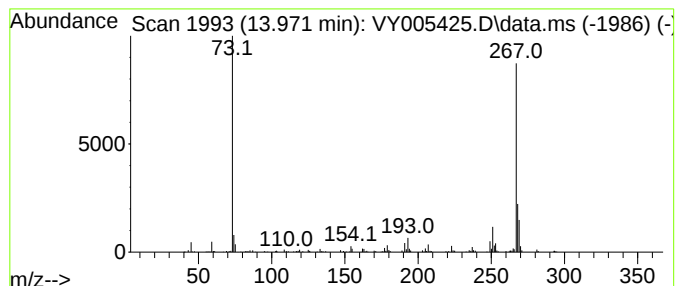
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Peak Number 3 Acridone, TMS derivative Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.971	8.77 ug/l	192178	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acridone, TMS derivative	267	C16H17NOSi	1000478-16-0	72
2			p-Trimethylsilyloxyphenyl-bis(tr...	370	C17H34O3Si3	1000079-08-1	72
3			Bamethan, 2TMS derivative	353	C18H35NO2Si2	040629-66-1	72
4			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	72
5			4-(2-Acetylamino-1-(trimethylsil...	339	C16H29NO3Si2	1000373-43-5	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propene	1.869	5.5	ug/l	64038	1	7.801	583155	50.0
Dimethyl sulfide	4.046	5.1	ug/l	59407	1	7.801	583155	50.0
Acridone, TMS d...	13.971	8.8	ug/l	192178	4	13.428	1096020	50.0