

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
 Data File : VN074695.D
 Acq On : 01 Oct 2022 07:14
 Operator : JC\MD
 Sample : N4882-07
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-108

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\82N092922W.M
 Title : SW846 8260

Signal : TIC: VN074695.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	39	45	52	rBV	423798	802283	14.98%	3.163%
2	2.240	53	60	61	rBV3	90280	170018	3.17%	0.670%
3	4.128	372	381	393	rBV2	103675	302013	5.64%	1.191%
4	4.404	418	428	439	rBV	85763	274842	5.13%	1.083%
5	5.416	585	600	615	rBV3	279096	1037112	19.37%	4.088%
6	7.869	1004	1017	1023	rBV	717808	1794140	33.50%	7.073%
7	7.934	1023	1028	1040	rVB	668865	1505652	28.12%	5.935%
8	8.292	1079	1089	1099	rBV	873504	2034985	38.00%	8.022%
9	8.392	1099	1106	1114	rVB3	115421	274350	5.12%	1.081%
10	8.828	1170	1180	1191	rBV	1075500	2256058	42.13%	8.893%
11	10.075	1384	1392	1395	rBV6	29487	60918	1.14%	0.240%
12	10.110	1395	1398	1403	rVB4	33544	55986	1.05%	0.221%
13	10.310	1424	1432	1445	rBV	2915551	5355206	100.00%	21.110%
14	10.422	1445	1451	1462	rVB5	44022	100611	1.88%	0.397%
15	11.616	1647	1654	1667	rBV	1721848	3025291	56.49%	11.926%
16	12.604	1815	1822	1837	rBV	2102071	3552465	66.34%	14.004%
17	13.551	1974	1983	1995	rBV	1637352	2765855	51.65%	10.903%

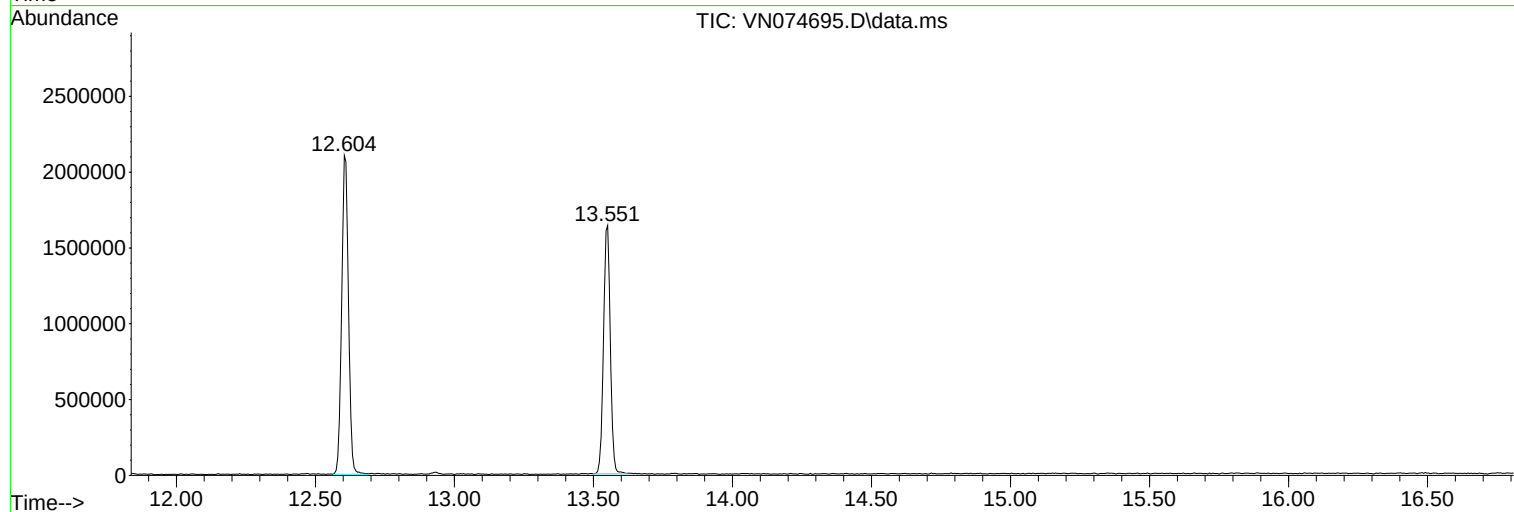
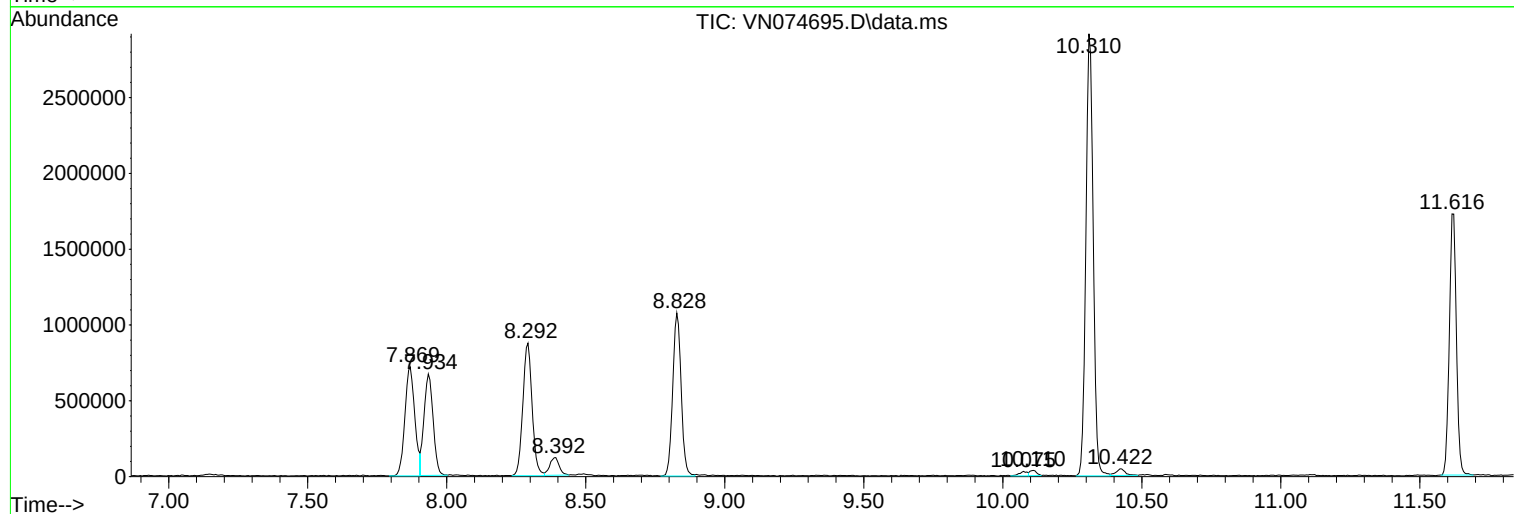
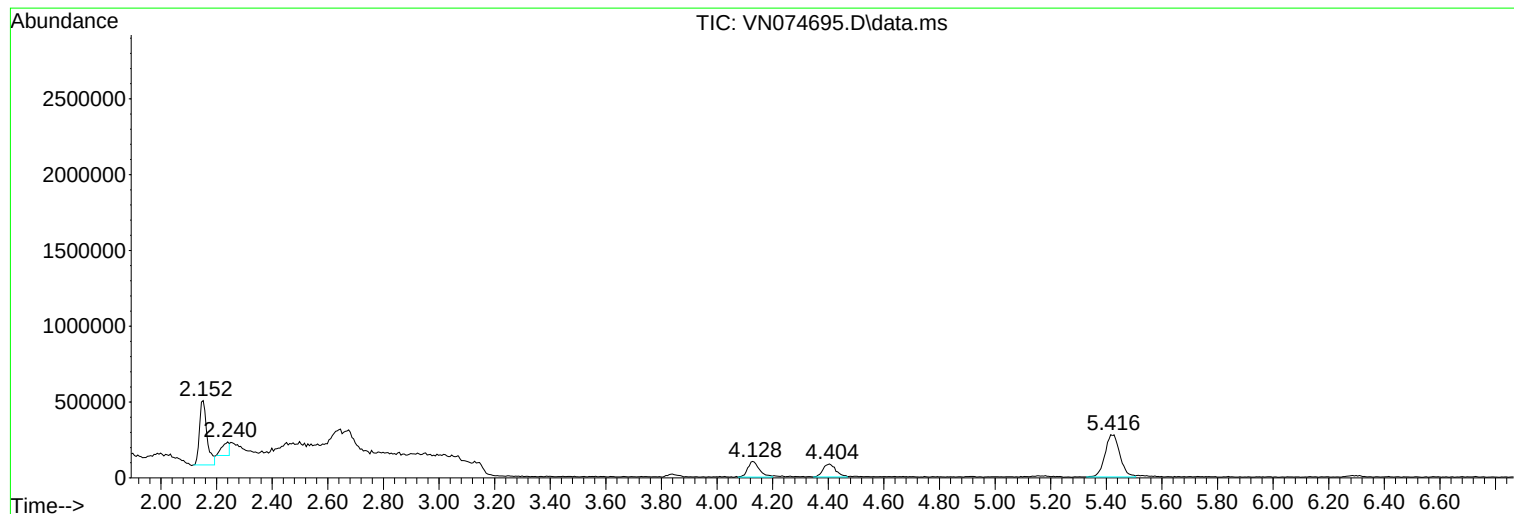
Sum of corrected areas: 25367785

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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



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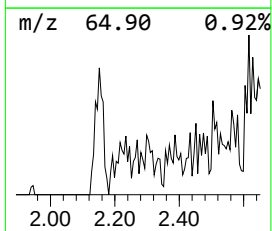
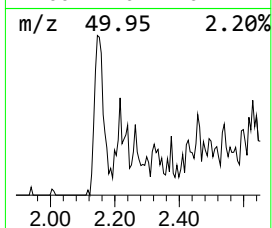
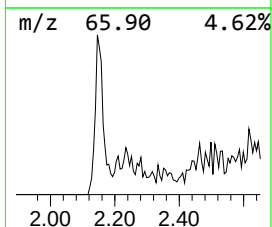
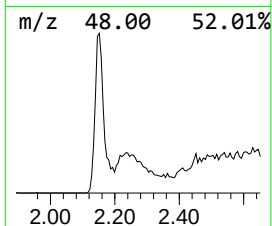
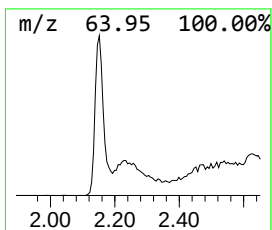
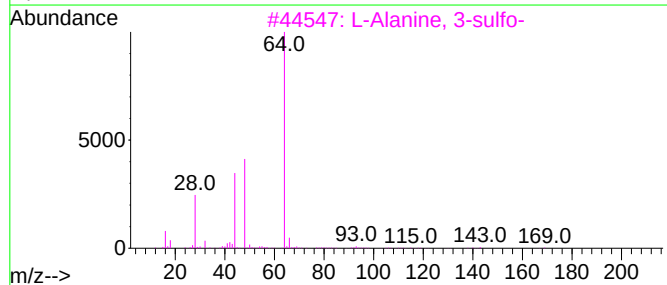
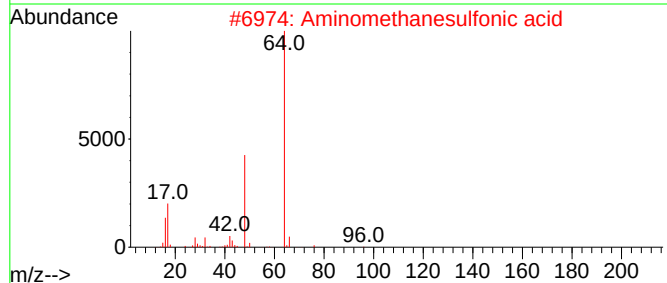
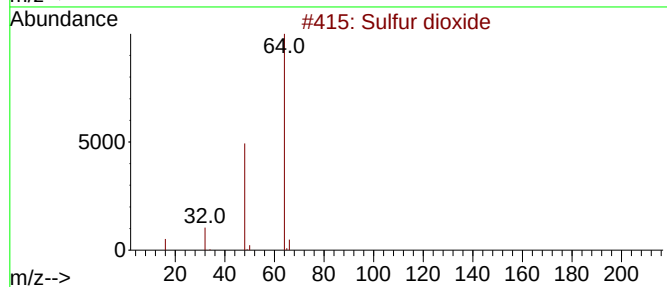
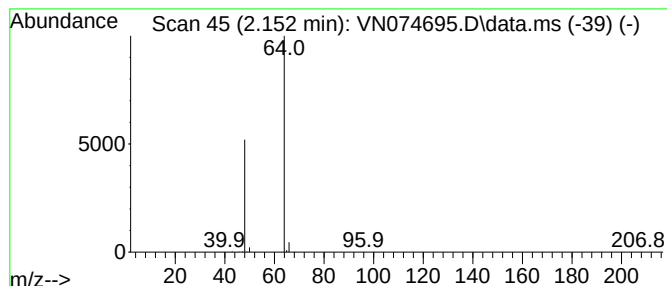
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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.
2.152	26.64 ug/l	802283	Pentafluorobenzene	7.939

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	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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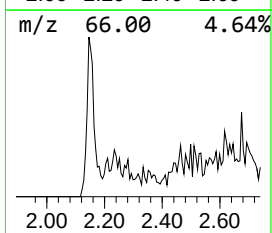
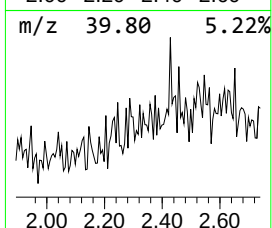
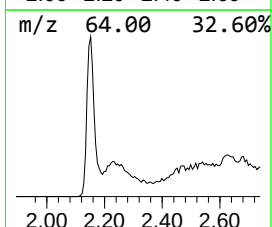
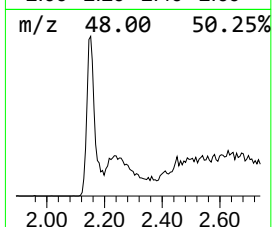
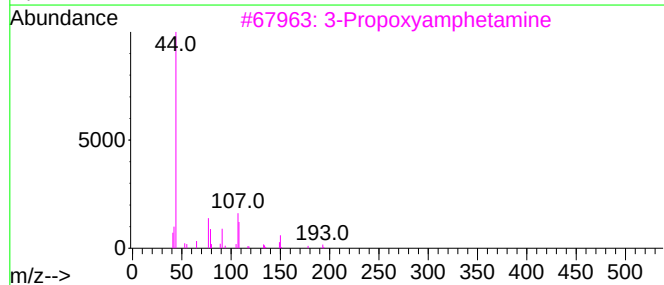
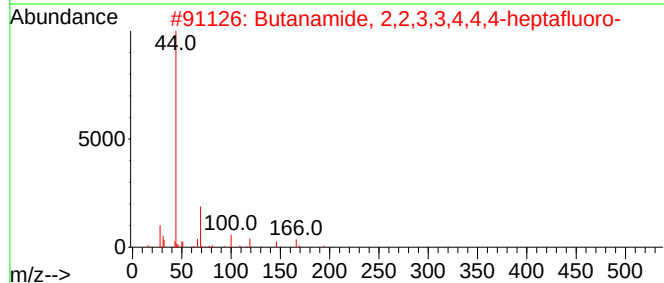
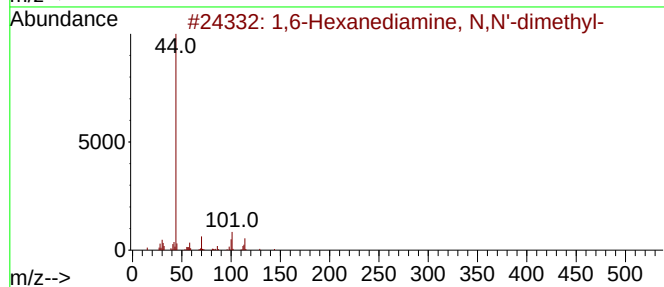
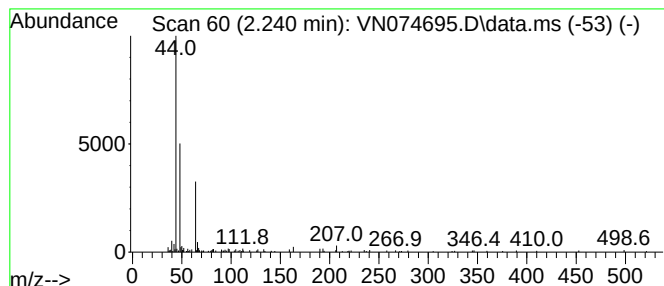
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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Peak Number 2 unknown2.240 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	5.65 ug/l	170018	Pentafluorobenzene	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,6-Hexanediamine, N,N'-dimethyl-	144	C8H20N2	013093-04-4	23
2			Butanamide, 2,2,3,3,4,4,4-heptafluoro-	213	C4H2F7NO	000662-50-0	23
3			3-Propoxyamphetamine	193	C12H19NO	1000124-04-4	9
4			Propanamide, 3,3,3-trifluoro-2-(2,2,2-trifluoroethyl)-	195	C4H3F6NO	1000351-46-4	9
5			(S)-(+)-1-Cyclohexylethylamine	127	C8H17N	017430-98-7	9



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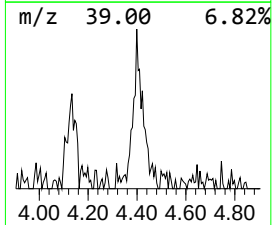
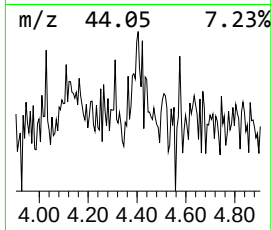
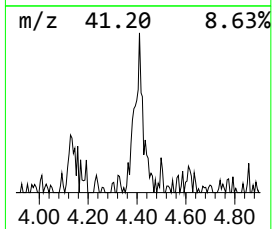
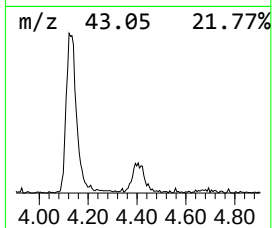
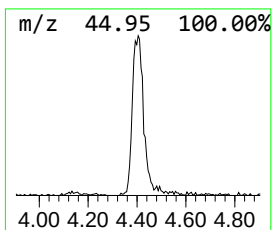
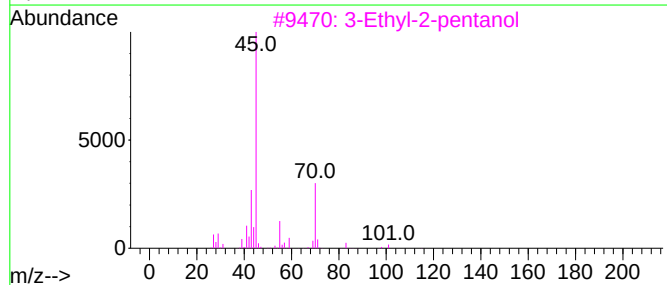
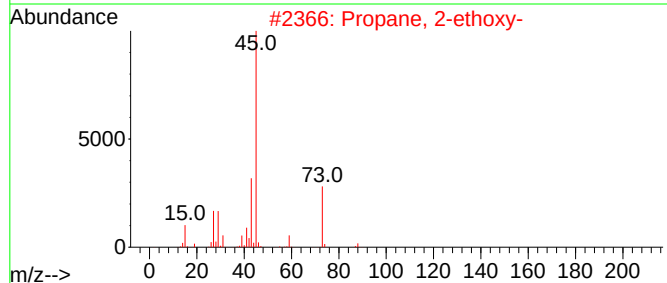
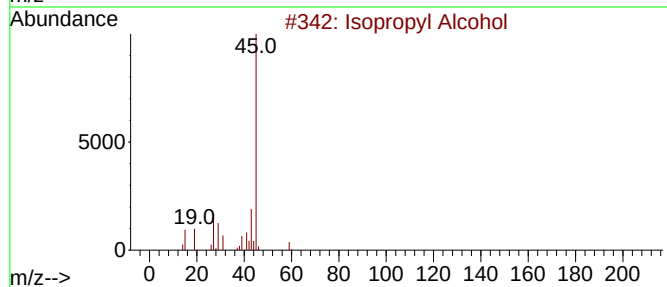
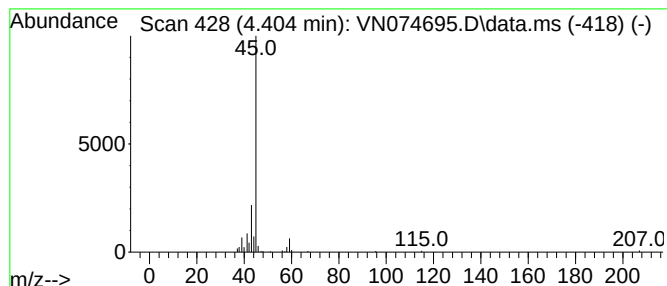
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Peak Number 3 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.404	9.13 ug/l	274842	Pentafluorobenzene	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	80
2			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	56
3			3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	43
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40



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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	2.152	26.6	ug/l	802283	1	7.939	1505650	50.0
unknown2.240	2.240	5.7	ug/l	170018	1	7.939	1505650	50.0
Isopropyl Alcohol	4.404	9.1	ug/l	274842	1	7.939	1505650	50.0