

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091322\
 Data File : VN074433.D
 Acq On : 13 Sep 2022 15:13
 Operator : JC\MD
 Sample : N4580-01 50X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 CO-1

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\82N090922W.M

Title : SW846 8260

Signal : TIC: VN074433.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	61	rBV	46187	106428	8.37%	1.374%
2	2.287	62	68	69	rBV4	20185	29729	2.34%	0.384%
3	2.699	132	138	142	rBV3	36456	88590	6.97%	1.144%
4	4.228	389	398	408	rBV2	22265	63473	4.99%	0.820%
5	5.293	572	579	589	rVB	13090	39764	3.13%	0.513%
6	7.245	898	911	922	rBV4	20145	71498	5.62%	0.923%
7	7.951	1021	1031	1037	rBV2	187519	479112	37.68%	6.187%
8	8.016	1037	1042	1055	rVB	294008	645483	50.77%	8.336%
9	8.375	1092	1103	1115	rBV2	210006	486911	38.30%	6.288%
10	8.904	1182	1193	1203	rBV	461515	916450	72.08%	11.835%
11	9.098	1218	1226	1232	rBV4	14263	33114	2.60%	0.428%
12	10.380	1436	1444	1454	rBV	681787	1271470	100.00%	16.419%
13	10.892	1526	1531	1542	rVB6	5198	14092	1.11%	0.182%
14	11.686	1656	1666	1677	rBV	705981	1224932	96.34%	15.818%
15	11.933	1699	1708	1714	rVB3	20557	36972	2.91%	0.477%
16	12.674	1827	1834	1844	rVB	575092	973412	76.56%	12.570%
17	13.616	1987	1994	2005	rBV	672174	1133981	89.19%	14.644%
18	13.716	2005	2011	2020	rBV2	59838	113942	8.96%	1.471%
19	15.439	2298	2304	2310	rVB6	7843	14381	1.13%	0.186%

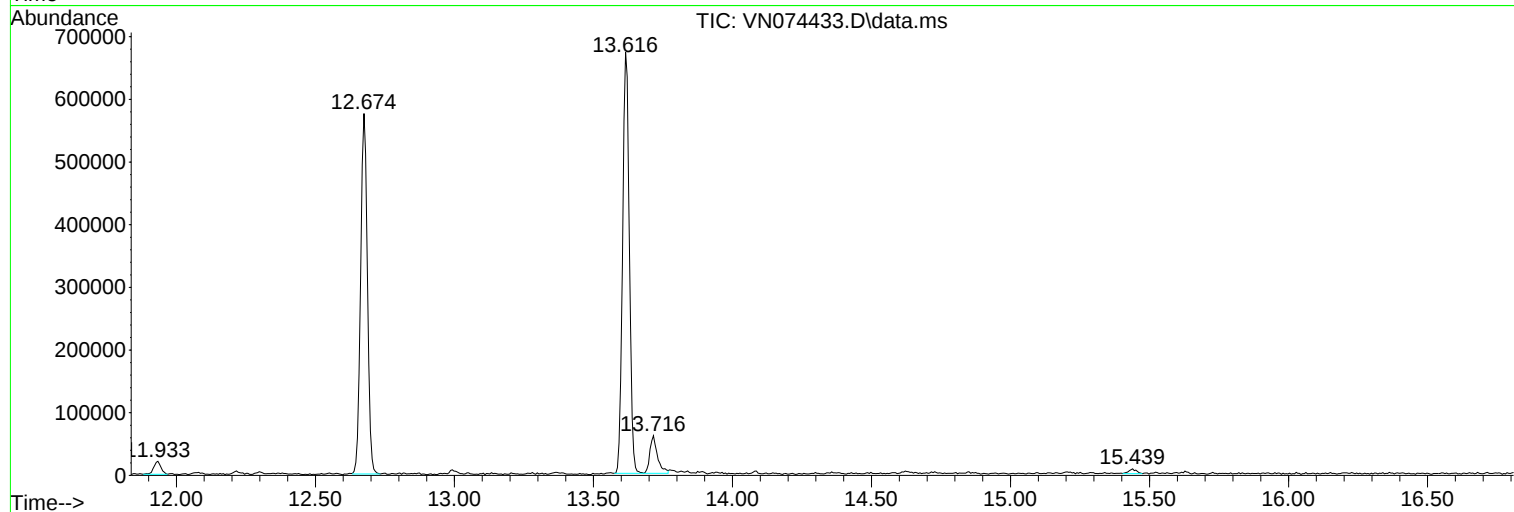
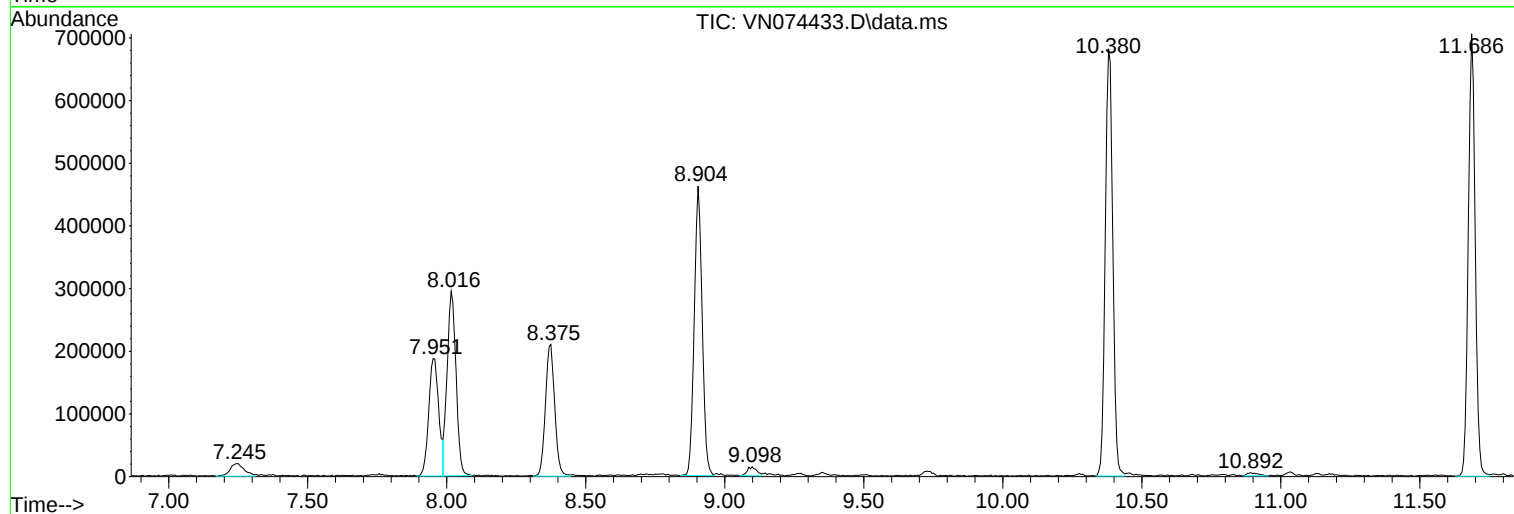
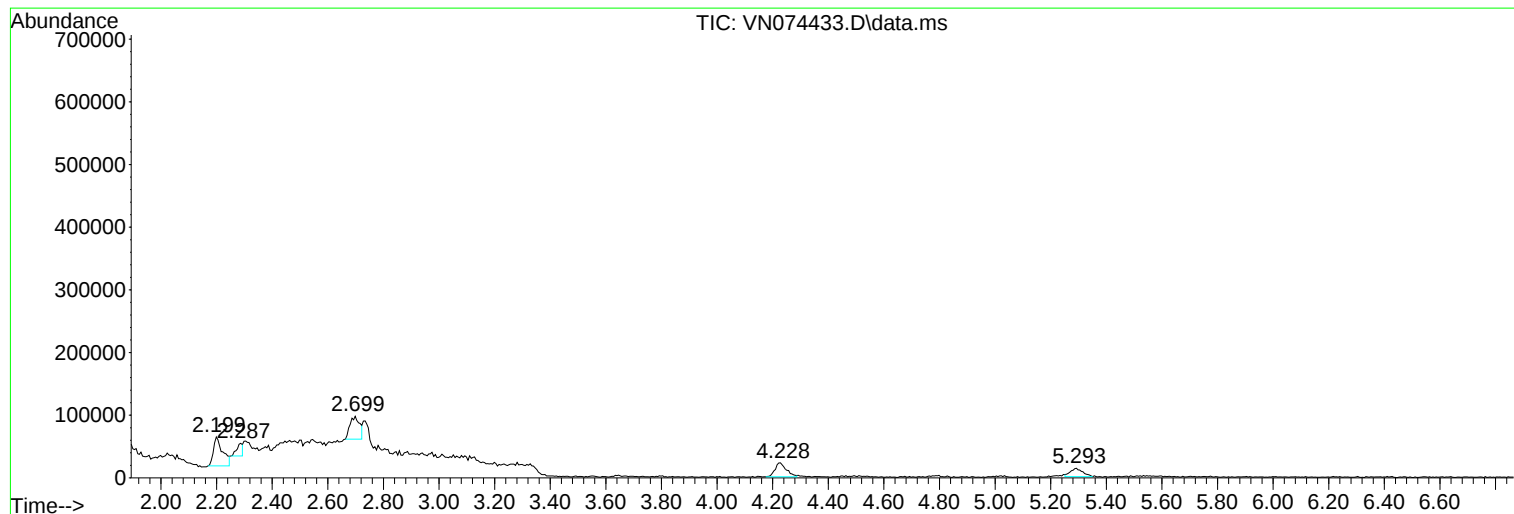
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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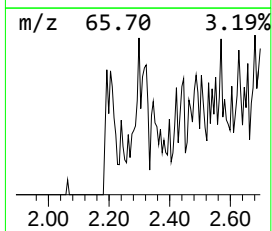
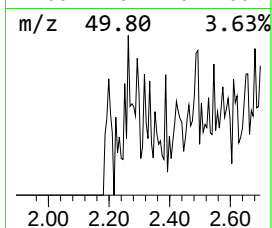
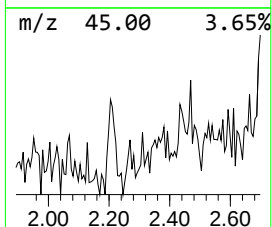
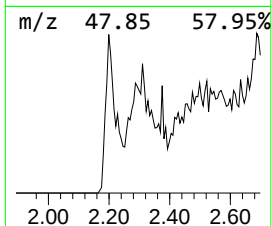
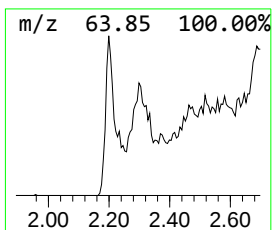
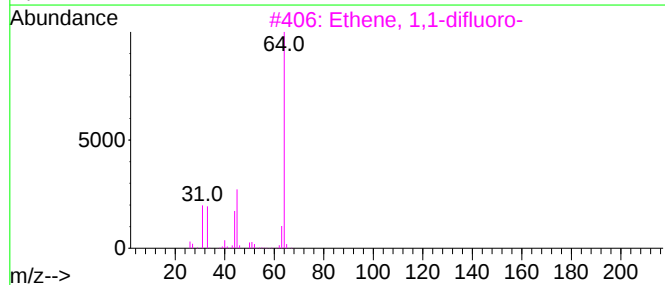
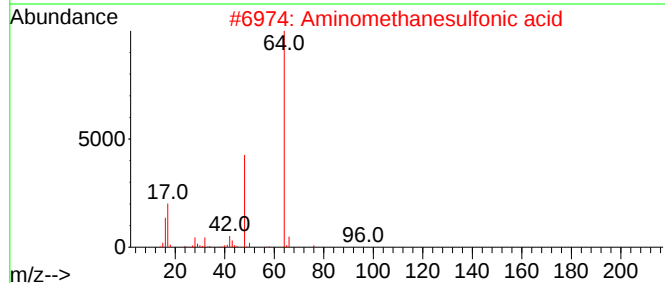
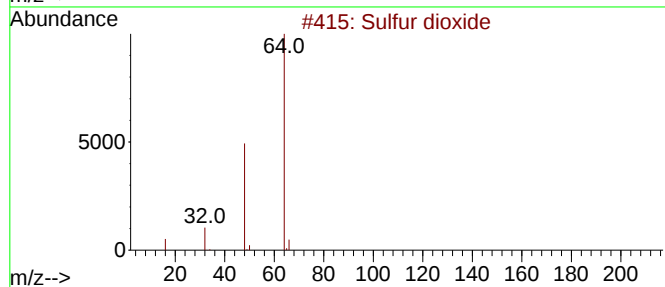
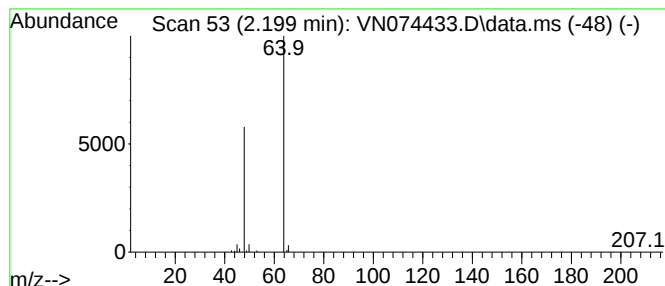
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090922W.M
Quant Title : SW846 8260

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.
2.199	8.24 ug/l	106428	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	74
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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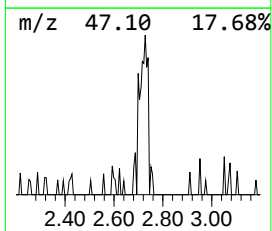
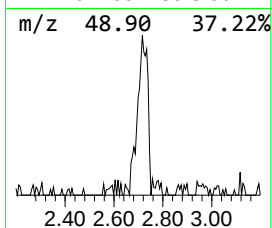
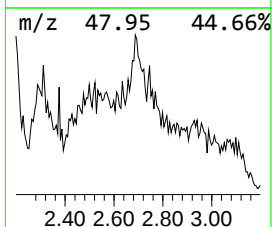
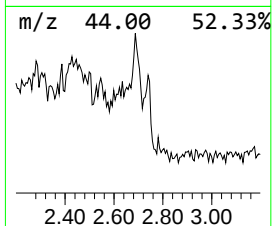
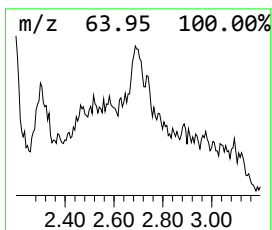
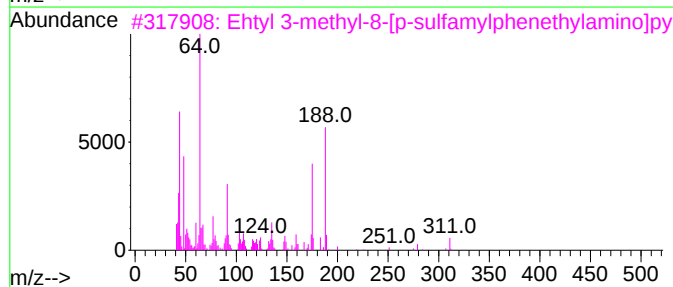
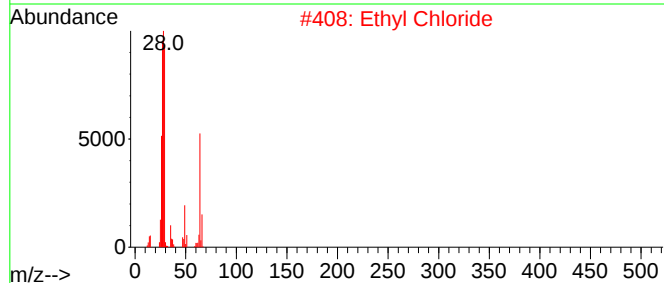
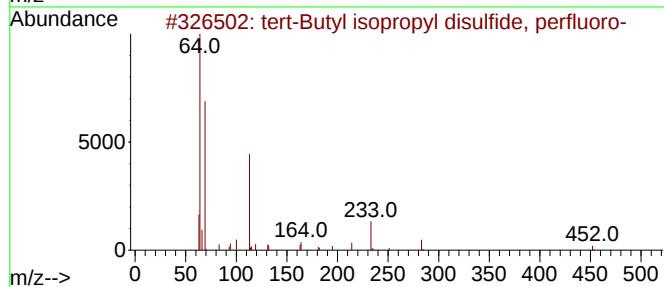
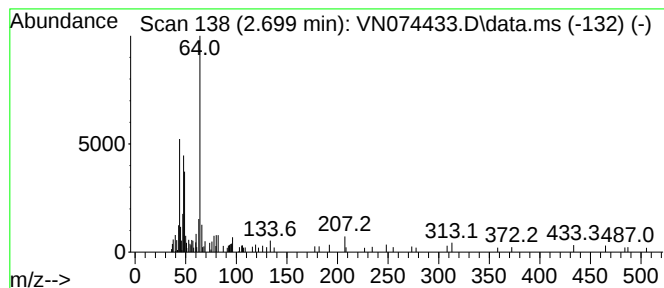
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Peak Number 2 tert-Butyl isopropyl disulf... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.699	6.86 ug/l	88590	Pentafluorobenzene	8.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	tert-Butyl isopropyl disulfide, ...	452	C7F16S2	1000226-69-7	64
2	Ethyl Chloride	64	C2H5Cl	000075-00-3	56
3	Ehtyl 3-methyl-8-[p-sulfamylphen...	430	C19H22N6O4S	021271-93-2	50
4	(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	40
5	4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	39



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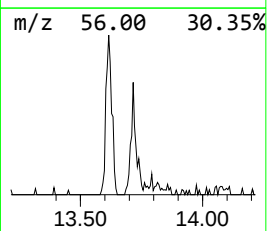
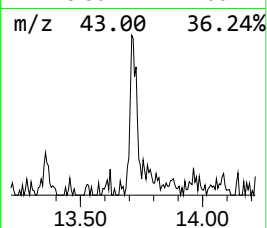
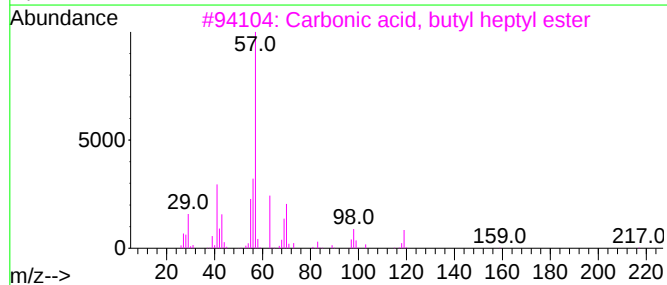
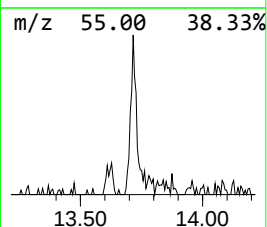
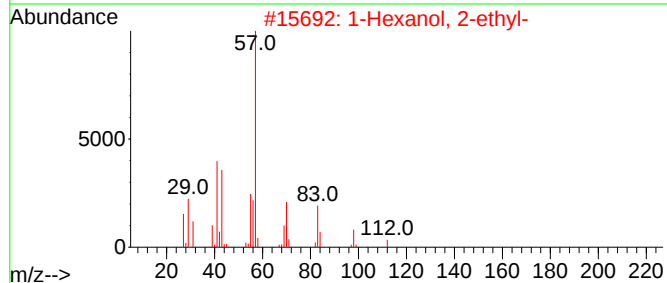
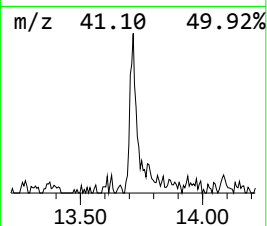
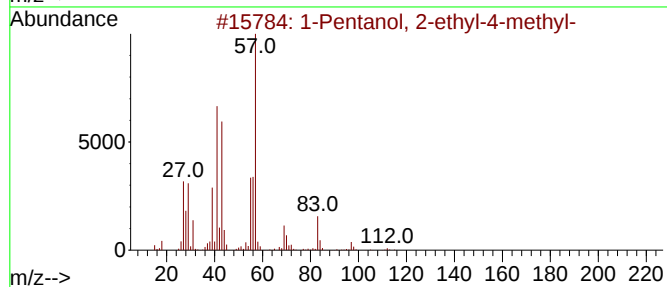
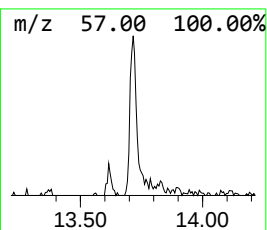
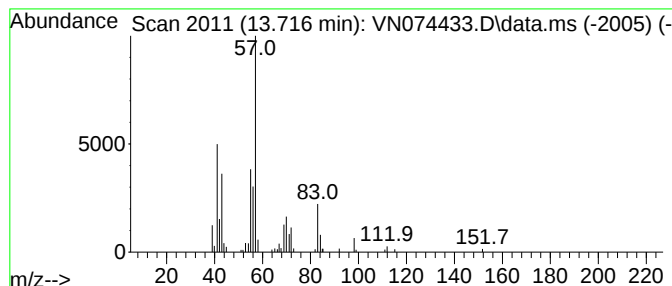
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Peak Number 3 1-Pentanol, 2-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.716	5.02 ug/l	113942	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
3			Carbonic acid, butyl heptyl ester	216	C12H24O3	1000314-63-4	47
4			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	43
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	8.2	ug/l	106428	1	8.016	645483	50.0
tert-Butyl isop...	2.699	6.9	ug/l	88590	1	8.016	645483	50.0
1-Pentanol, 2-e...	13.716	5.0	ug/l	113942	4	13.616	1133980	50.0