

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
 Data File : VN074587.D
 Acq On : 19 Sep 2022 15:39
 Operator : JC\MD
 Sample : N4647-08
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1039-FB090822

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\82N091522W.M

Title : SW846 8260

Signal : TIC: VN074587.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	46	53	60	rBV	184941	367242	19.99%	3.049%
2	2.416	86	90	91	rBV4	17695	23515	1.28%	0.195%
3	2.693	131	137	140	rBV2	52380	117734	6.41%	0.977%
4	4.222	391	397	406	rBV3	39644	112932	6.15%	0.937%
5	7.257	907	913	922	rVB4	13579	41338	2.25%	0.343%
6	7.951	1023	1031	1036	rBV2	240878	558567	30.41%	4.637%
7	8.016	1036	1042	1053	rVB2	359418	820048	44.64%	6.808%
8	8.369	1092	1102	1113	rBV2	267045	612841	33.36%	5.087%
9	8.904	1184	1193	1203	rBV	595336	1203912	65.53%	9.994%
10	9.098	1221	1226	1234	rVB2	10260	20683	1.13%	0.172%
11	10.380	1435	1444	1451	rBV	902288	1668040	90.80%	13.847%
12	10.439	1451	1454	1463	rVB2	28580	56664	3.08%	0.470%
13	11.127	1565	1571	1578	rVB4	15075	25039	1.36%	0.208%
14	11.686	1658	1666	1676	rBV	941488	1648153	89.72%	13.682%
15	12.216	1751	1756	1760	rBV2	13518	21986	1.20%	0.183%
16	12.674	1826	1834	1842	rBV	778760	1264775	68.85%	10.499%
17	13.321	1938	1944	1948	rBV5	14044	25260	1.38%	0.210%
18	13.616	1987	1994	2001	rBV	917319	1501317	81.72%	12.463%
19	13.715	2003	2011	2025	rBV	1150164	1837059	100.00%	15.250%
20	14.086	2069	2074	2078	rBV6	15884	25870	1.41%	0.215%
21	14.363	2116	2121	2130	rVB3	34213	68476	3.73%	0.568%
22	14.592	2155	2160	2166	rVB4	13863	24701	1.34%	0.205%

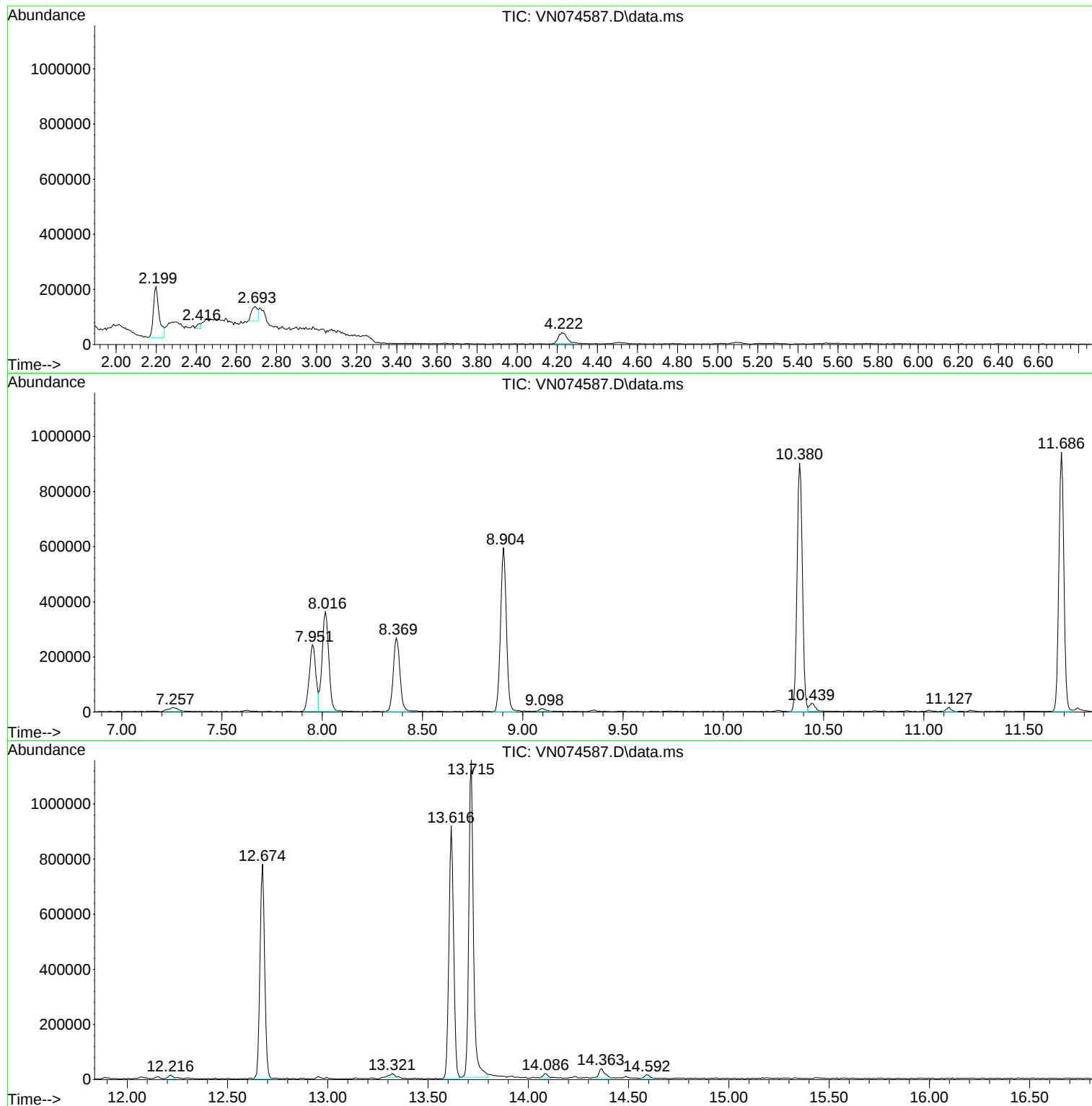
Sum of corrected areas: 12046152

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Quant Title : SW846 8260

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



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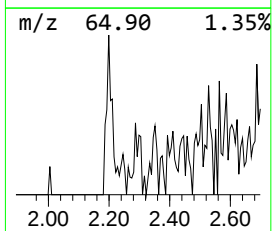
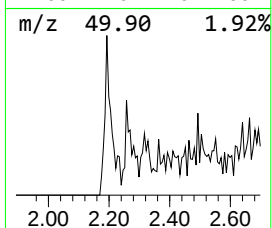
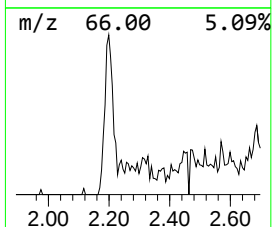
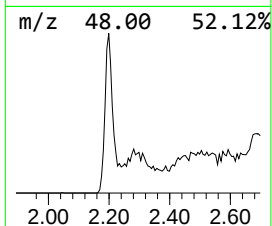
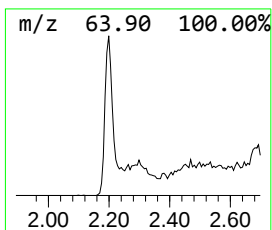
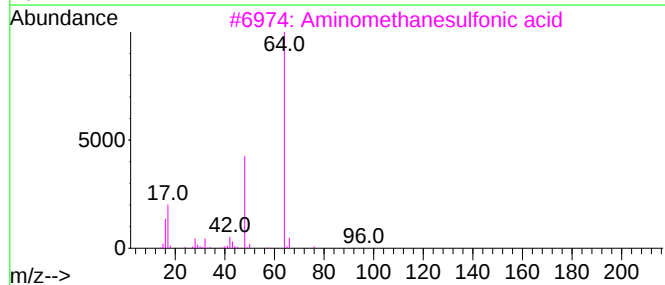
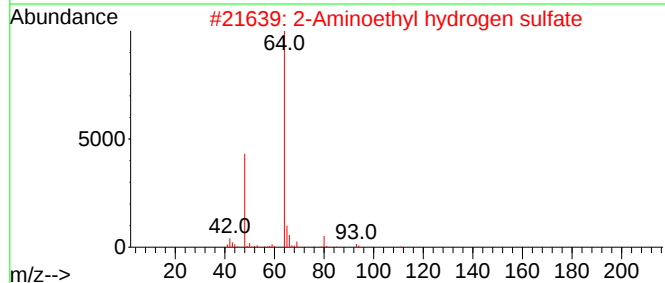
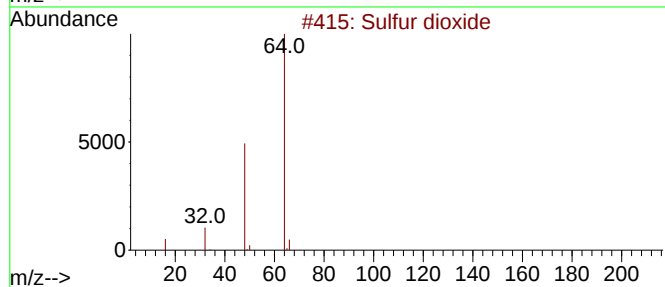
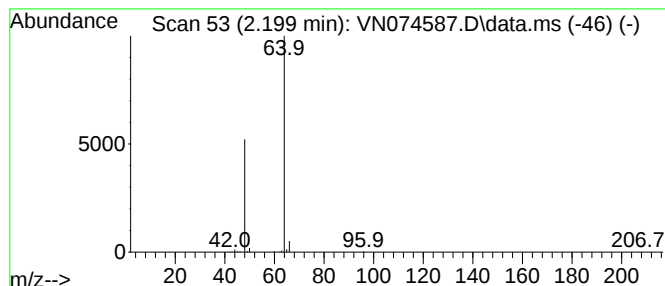
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	22.39 ug/l	367242	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			2-Aminoethyl hydrogen sulfate	141	C2H7N04S	000926-39-6	83
3			Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	74
4			L-Alanine, 3-sulfo-	169	C3H7N05S	000498-40-8	64
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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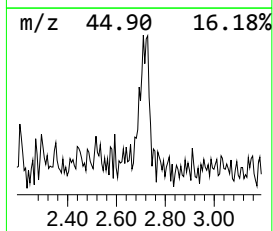
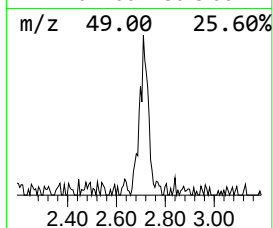
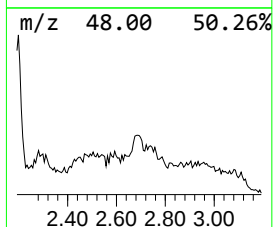
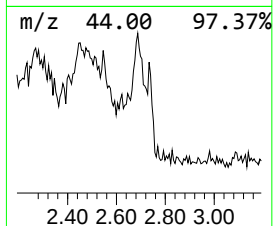
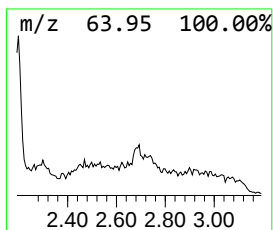
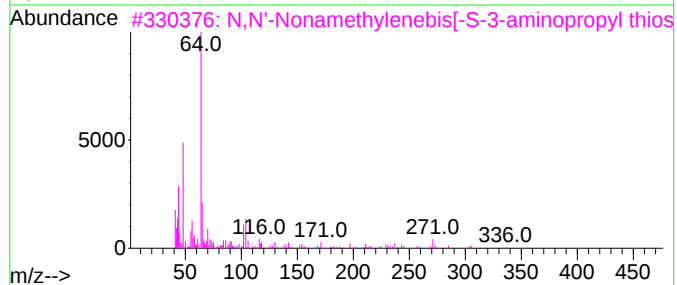
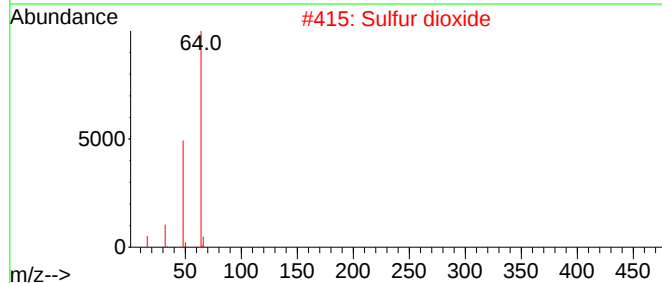
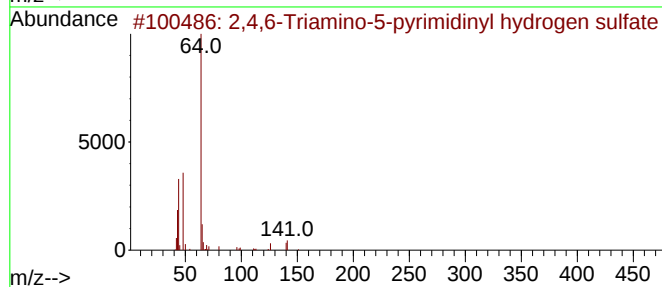
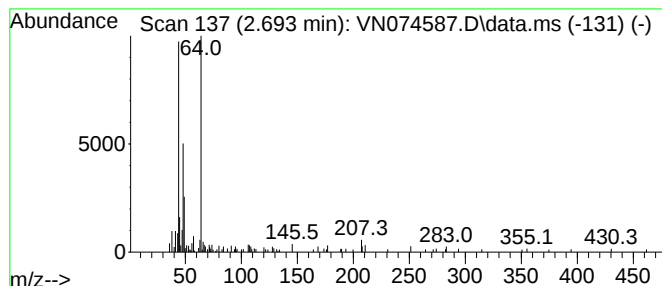
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Peak Number 2 2,4,6-Triamino-5-pyrimidiny... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.693	7.18 ug/l	117734	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	53		
2	Sulfur dioxide	64	O2S	007446-09-5	52		
3	N,N'-Nonamethylenebis[-S-3-amino...	466	C15H34N2O6S4	035871-58-0	42		
4	2-[N-[1,4-Benzodioxan-2-methyl]]...	305	C11H15NO5S2	060311-26-4	39		
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	38		



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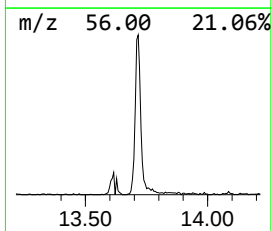
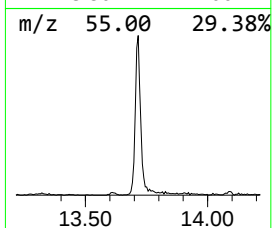
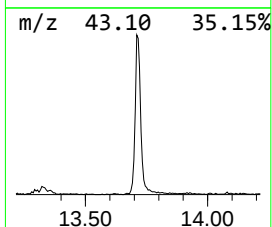
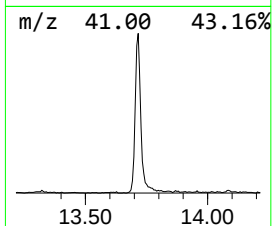
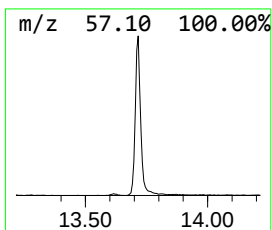
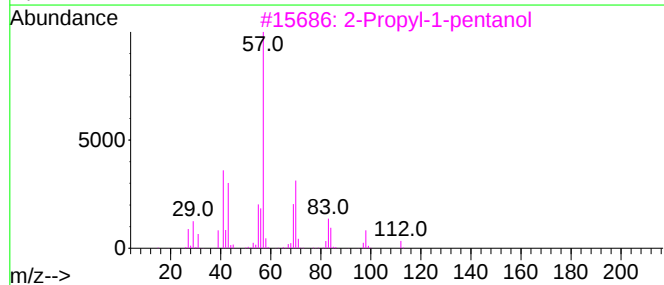
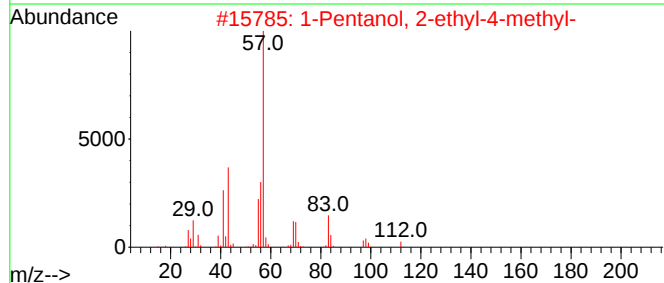
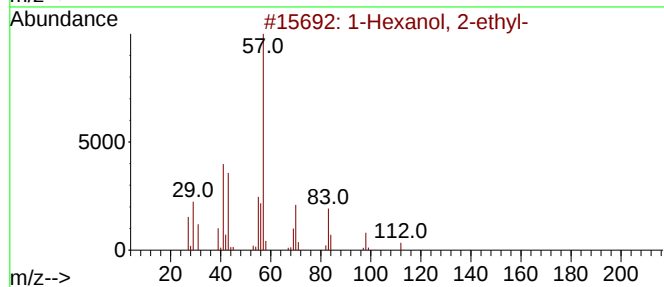
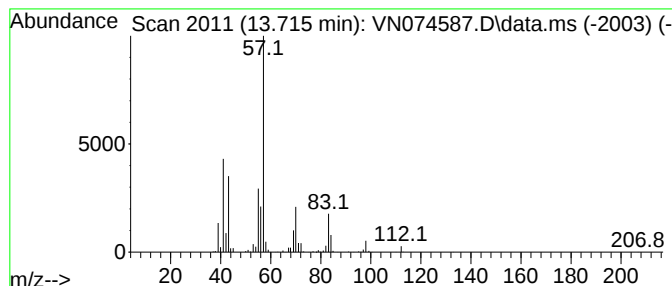
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.716	61.18 ug/l	1837060	1,4-Dichlorobenzene-d4			13.616
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-		130	C8H18O	000106-67-2	50
3	2-Propyl-1-pentanol		130	C8H18O	058175-57-8	50
4	Octane, 2,3-dimethyl-		142	C10H22	007146-60-3	45
5	Heptane, 1,1'-oxybis-		214	C14H30O	000629-64-1	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	22.4	ug/l	367242	1	8.022	820048	50.0
2,4,6-Triamino-...	2.693	7.2	ug/l	117734	1	8.022	820048	50.0
1-Hexanol, 2-et...	13.716	61.2	ug/l	1837060	4	13.616	1501320	50.0