

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
 Data File : VN074679.D
 Acq On : 30 Sep 2022 20:06
 Operator : JC\MD
 Sample : N4860-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-03

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: VN074679.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	53	rBV	547370	1003663	16.61%	3.510%
2	2.634	122	127	132	rBV4	92539	241600	4.00%	0.845%
3	7.869	1004	1017	1023	rBV	795974	1998709	33.09%	6.989%
4	7.933	1023	1028	1046	rVB2	770968	1757404	29.09%	6.145%
5	8.292	1076	1089	1102	rBV	945117	2189718	36.25%	7.657%
6	8.828	1171	1180	1195	rBV	1294443	2648477	43.84%	9.261%
7	9.080	1216	1223	1229	rVB6	41424	86413	1.43%	0.302%
8	10.310	1421	1432	1451	rBV	3298001	6041035	100.00%	21.124%
9	11.616	1646	1654	1666	rBV	2097941	3683488	60.97%	12.880%
10	12.610	1814	1823	1833	rBV	2442800	4163448	68.92%	14.559%
11	13.551	1975	1983	1990	rBV	2109223	3511621	58.13%	12.279%
12	13.645	1995	1999	2005	rVB4	52433	90142	1.49%	0.315%
13	13.751	2012	2017	2021	rVB2	54226	76235	1.26%	0.267%
14	14.204	2089	2094	2099	rVB4	36240	62818	1.04%	0.220%
15	14.339	2110	2117	2122	rBV	63450	112494	1.86%	0.393%
16	14.533	2144	2150	2157	rVB3	41511	67523	1.12%	0.236%
17	14.698	2172	2178	2183	rBV4	53666	89248	1.48%	0.312%
18	15.180	2249	2260	2267	rBV2	242471	553292	9.16%	1.935%
19	15.498	2305	2314	2324	rBV5	55765	151617	2.51%	0.530%
20	16.651	2502	2510	2518	rBV9	29099	68903	1.14%	0.241%

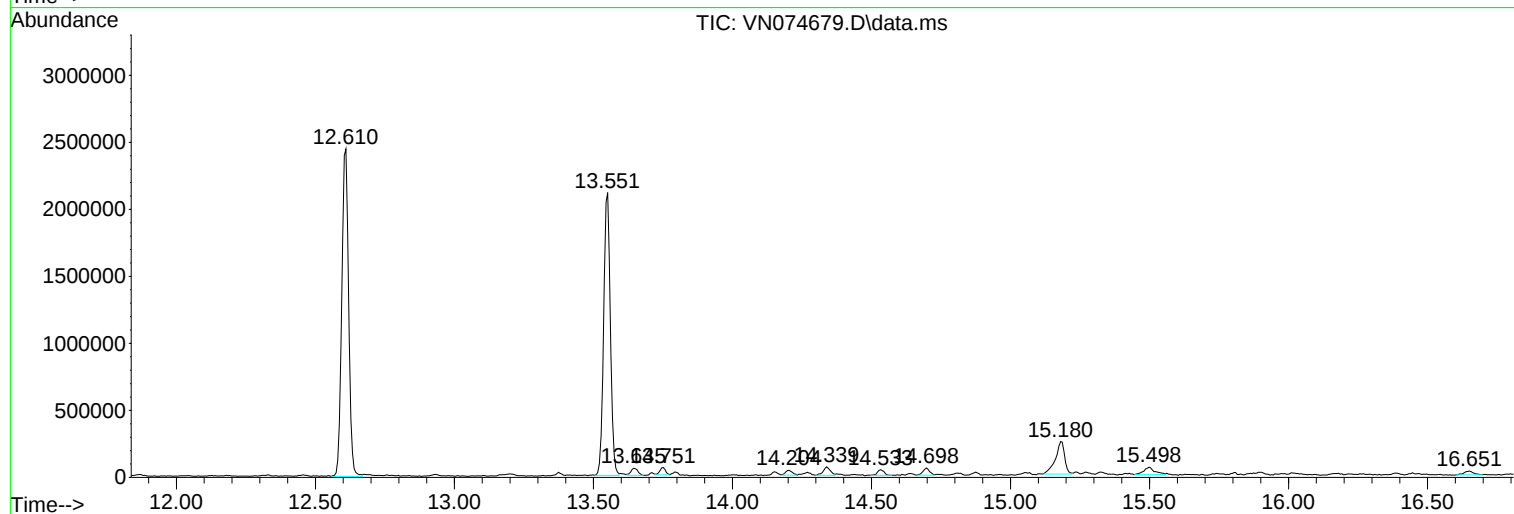
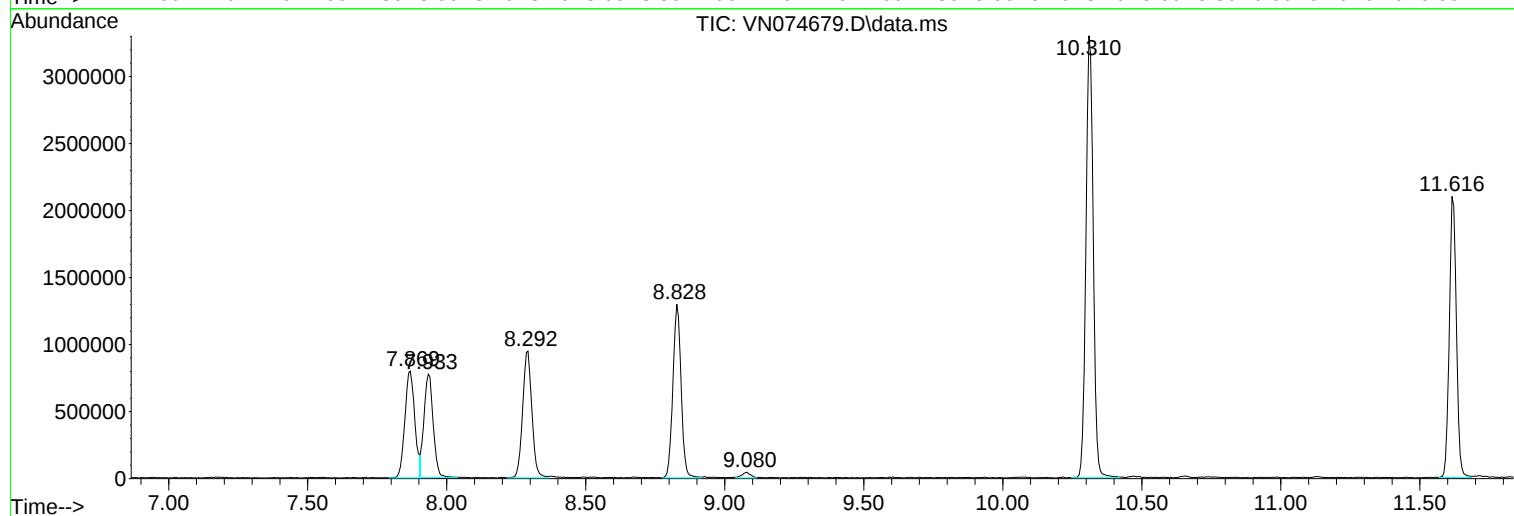
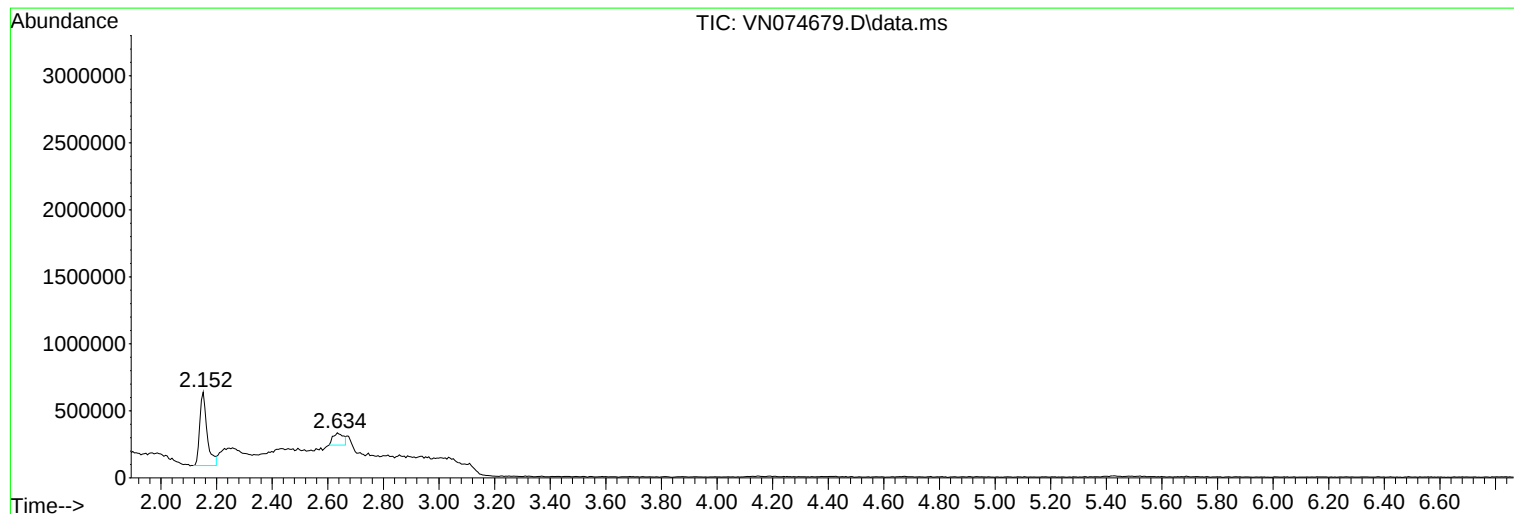
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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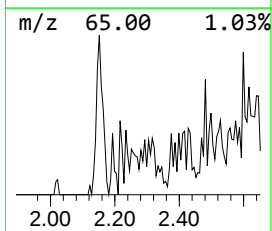
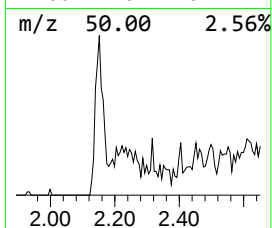
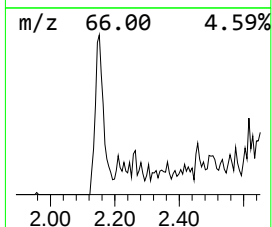
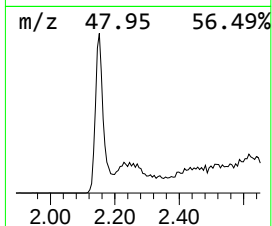
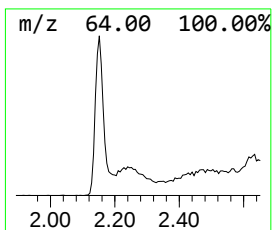
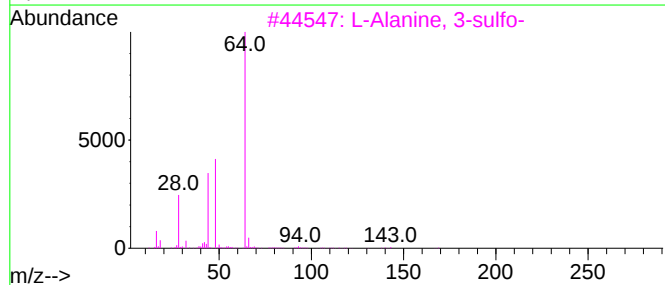
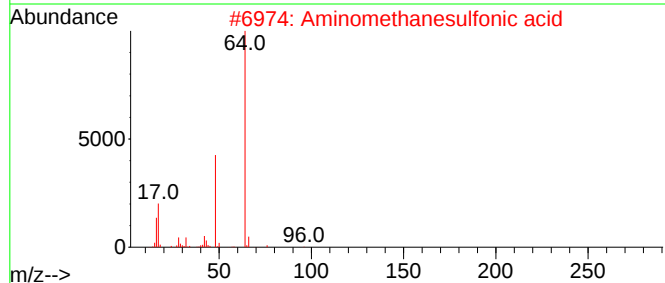
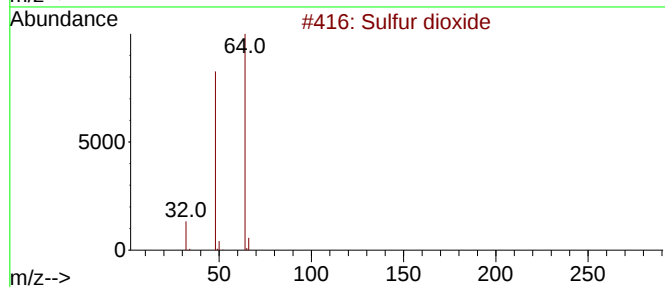
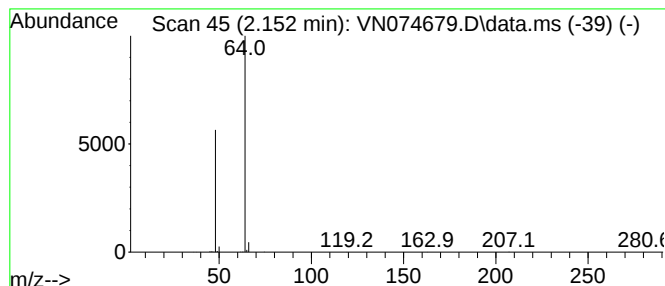
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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	28.56 ug/l	1003660	Pentafluorobenzene	7.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
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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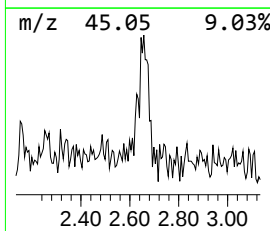
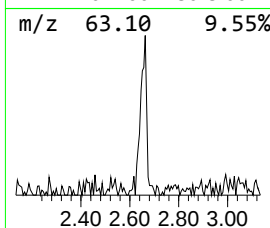
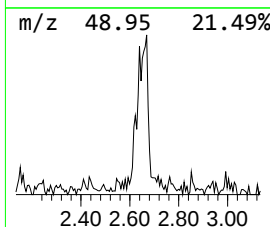
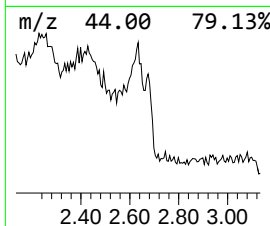
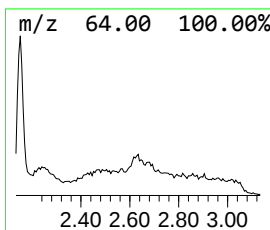
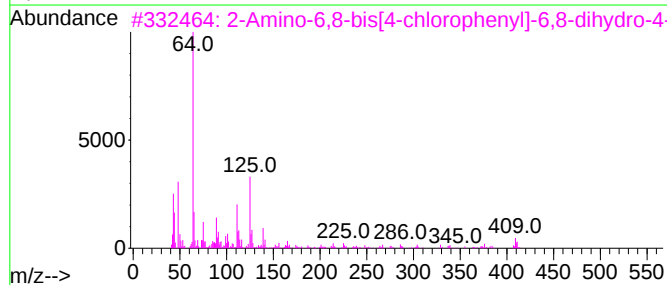
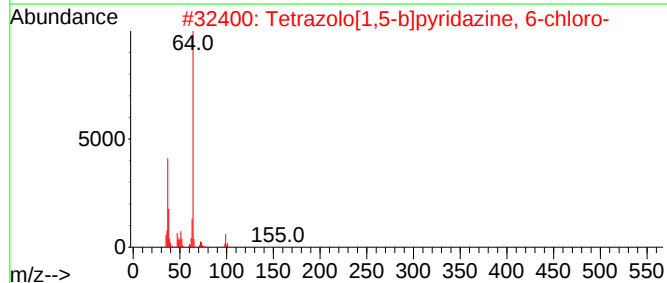
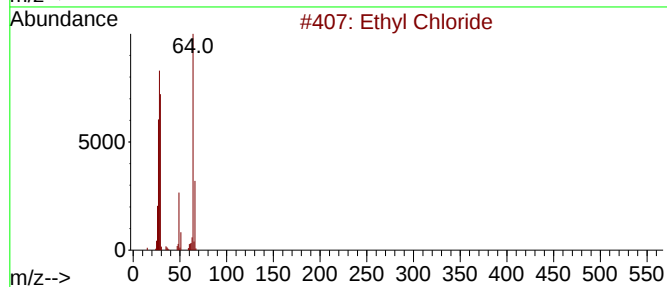
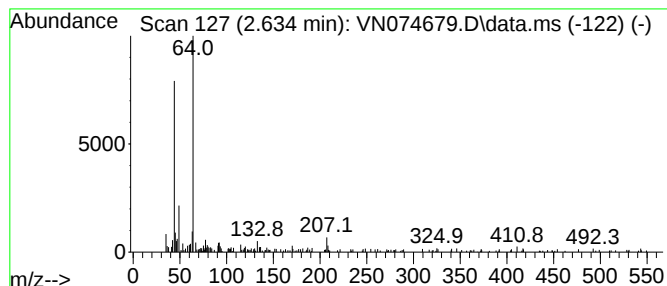
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Peak Number 2 Tetrazolo[1,5-b]pyridazine,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.634	6.87 ug/l	241600	Pentafluorobenzene	7.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Chloride	64	C2H5Cl	000075-00-3	64
2			Tetrazolo[1,5-b]pyridazine, 6-ch...	155	C4H2ClN5	021413-15-0	52
3			2-Amino-6,8-bis[4-chlorophenyl]-...	473	C20H13Cl2N5O3S	049647-41-8	33
4			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	9
5			Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	9



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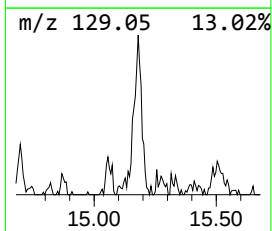
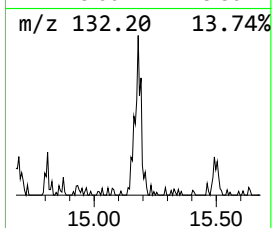
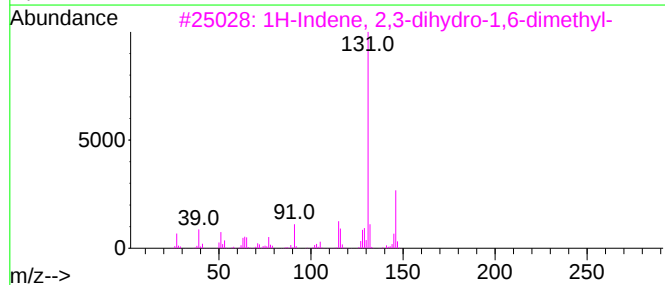
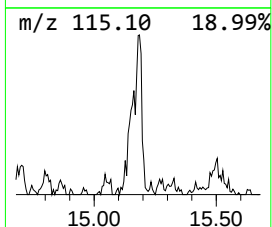
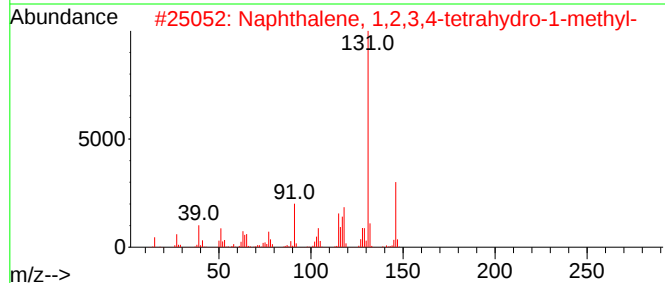
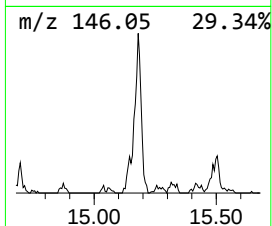
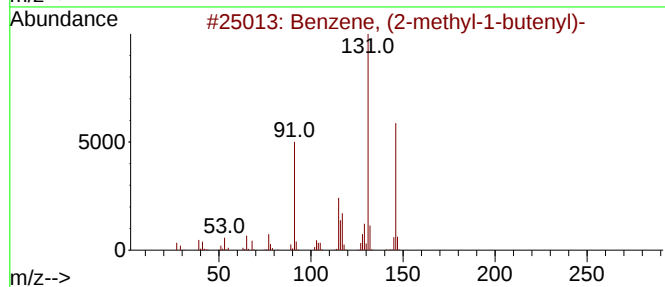
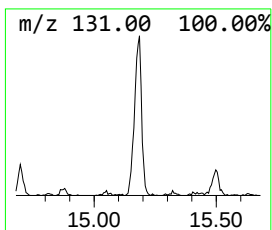
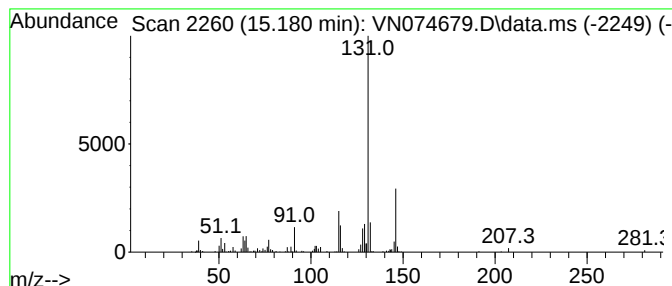
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Peak Number 3 Benzene, (2-methyl-1-butenyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	7.88 ug/l	553292	1,4-Dichlorobenzene-d4	13.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	94
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	91
3			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	91
4			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	91
5			Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.152	28.6	ug/l	1003660	1	7.933	1757400	50.0
Tetrazolo[1,5-b...	2.634	6.9	ug/l	241600	1	7.933	1757400	50.0
Benzene, (2-met...	15.180	7.9	ug/l	553292	4	13.551	3511620	50.0