

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074540.D
 Acq On : 17 Sep 2022 04:08
 Operator : JC\MD
 Sample : N4549-12
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-56

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: VN074540.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	60	rBV	226806	423428	22.42%	3.647%
2	2.634	122	127	131	rBV2	51952	94234	4.99%	0.812%
3	2.687	132	136	139	rBV2	50858	88910	4.71%	0.766%
4	5.240	558	570	579	rBV4	15302	54247	2.87%	0.467%
5	7.234	899	909	924	rBV2	78867	234913	12.44%	2.023%
6	7.951	1021	1031	1036	rBV	259462	617417	32.70%	5.318%
7	8.016	1036	1042	1050	rVB	386487	886954	46.97%	7.640%
8	8.369	1093	1102	1114	rBV	304290	699880	37.06%	6.029%
9	8.545	1124	1132	1145	rVB3	20143	57528	3.05%	0.496%
10	8.904	1184	1193	1204	rBV	662372	1361942	72.12%	11.731%
11	9.816	1343	1348	1357	rVB5	18847	40914	2.17%	0.352%
12	9.951	1357	1371	1379	rBV3	43029	103181	5.46%	0.889%
13	10.133	1397	1402	1410	rVB4	20400	40351	2.14%	0.348%
14	10.380	1436	1444	1458	rBV	1053337	1888398	100.00%	16.266%
15	10.580	1469	1478	1484	rVB4	36816	66671	3.53%	0.574%
16	10.657	1484	1491	1498	rVB3	28978	54712	2.90%	0.471%
17	11.686	1657	1666	1674	rBV	1036977	1792741	94.93%	15.442%
18	12.674	1824	1834	1842	rBV	815171	1359157	71.97%	11.707%
19	13.616	1985	1994	2004	rBV	975275	1639372	86.81%	14.121%
20	14.086	2068	2074	2080	rBV6	12010	20653	1.09%	0.178%
21	14.268	2100	2105	2111	rBV3	19679	33541	1.78%	0.289%
22	14.410	2124	2129	2132	rBV5	13995	23252	1.23%	0.200%
23	14.480	2135	2141	2148	rVB3	13729	27100	1.44%	0.233%

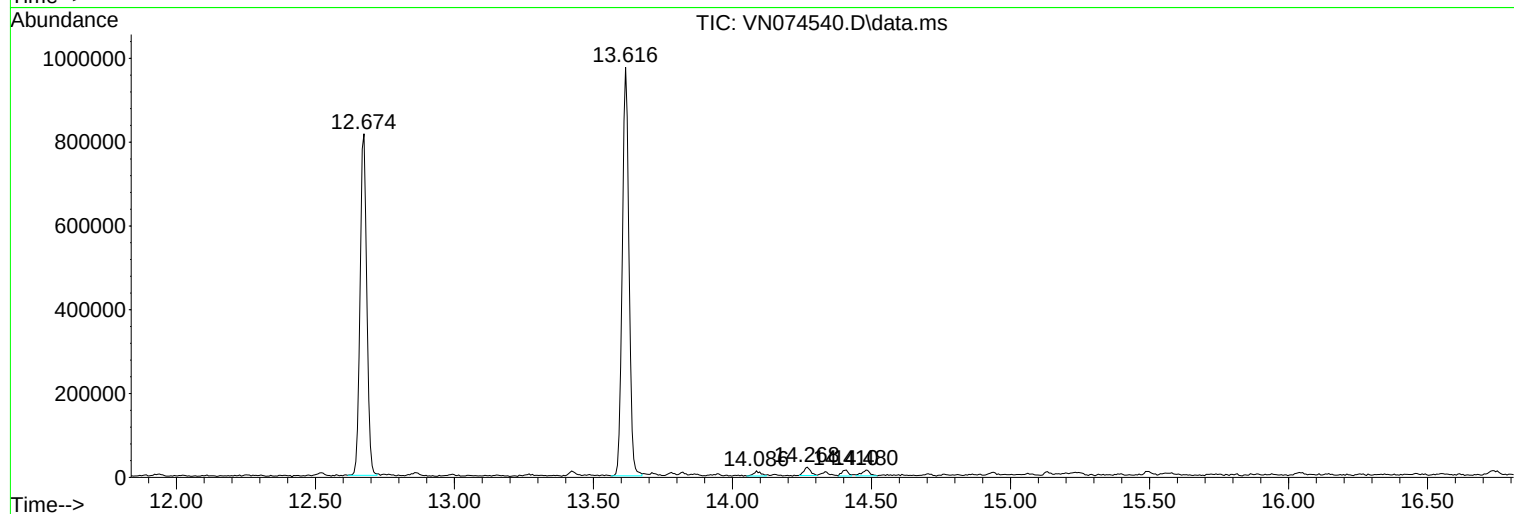
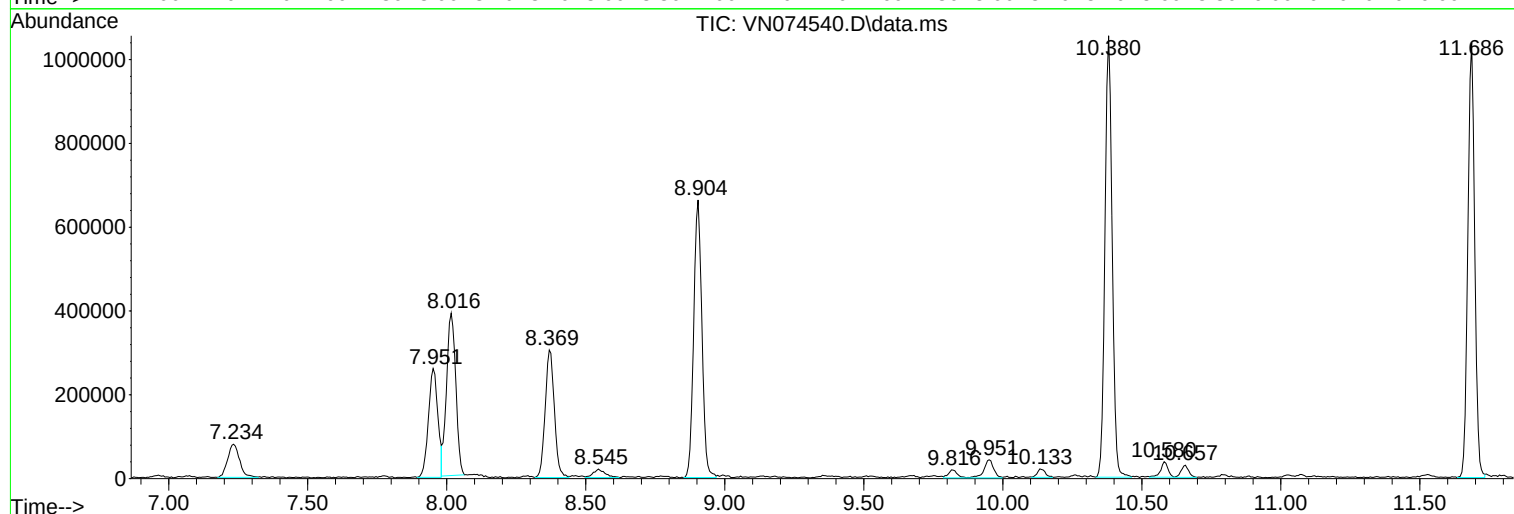
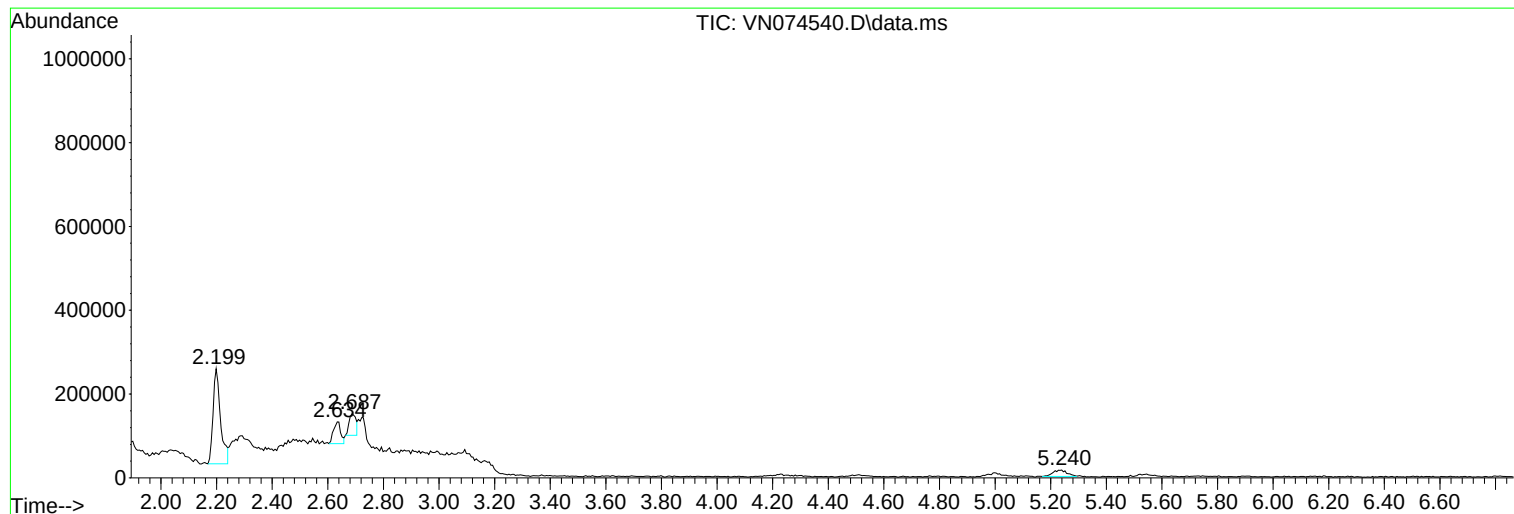
Sum of corrected areas: 11609496

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Instrument :
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ClientSampleId :
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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



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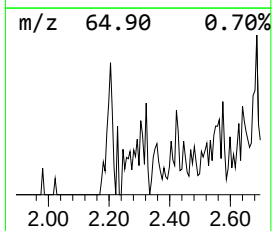
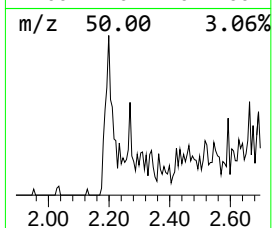
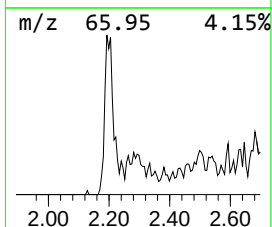
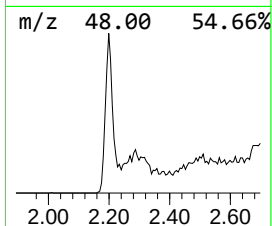
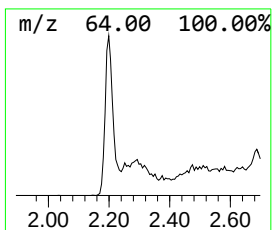
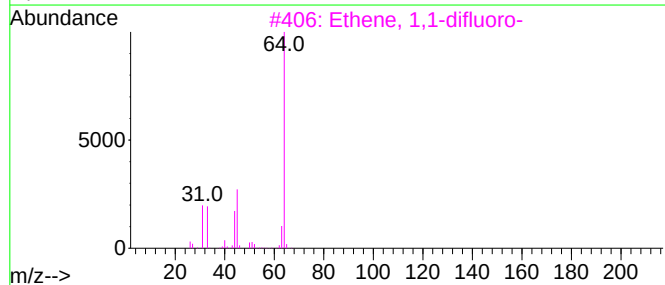
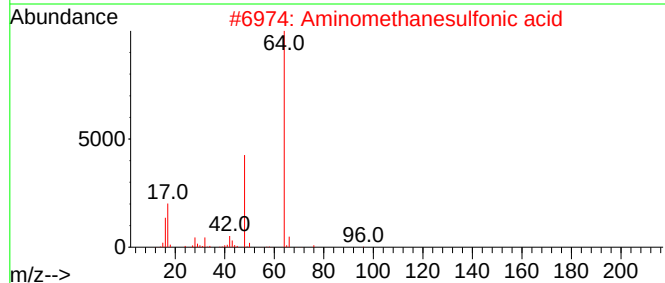
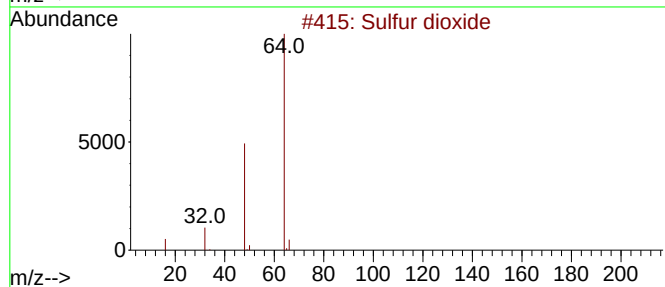
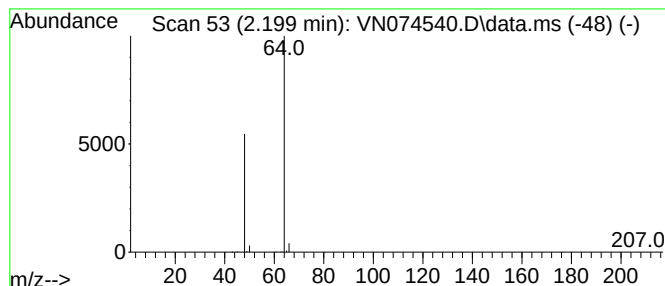
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	23.87 ug/l	423428	Pentafluorobenzene	8.016

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	9
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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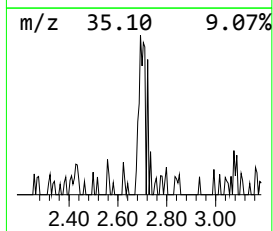
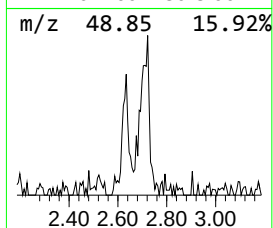
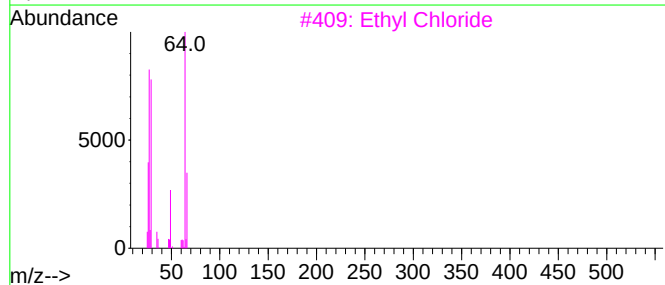
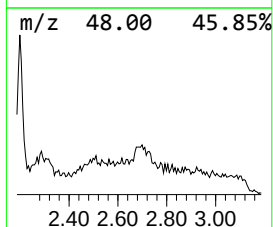
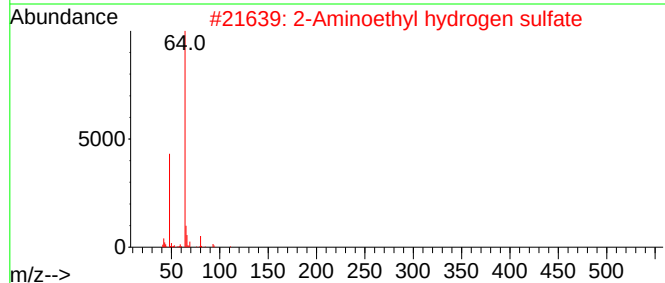
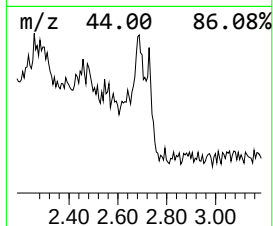
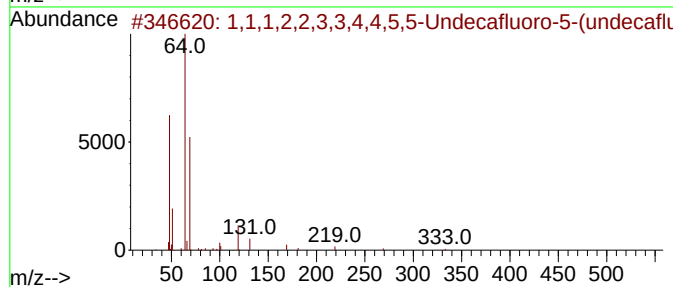
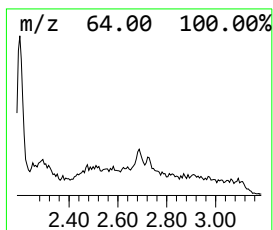
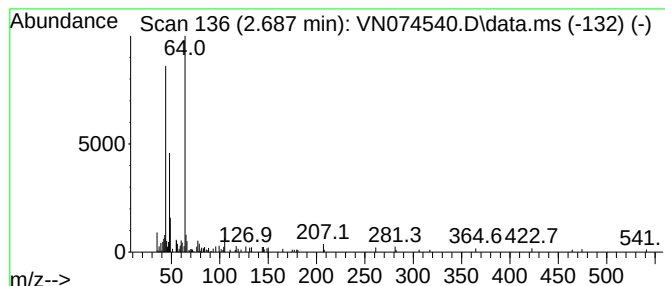
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Aminoethyl hydrogen sulfate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.687	5.01 ug/l	88910	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,2,2,3,3,4,4,5,5-Undecafluoro-5-(undecafluoroethyl)thiophosphorothioic trioxide	602	C10F22O2S	1000486-78-5	74		
2	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	59		
3	Ethyl Chloride	64	C2H5Cl	000075-00-3	53		
4	N,N'-Nonamethylenebis[3-amino-2-methylpropanesulfonic acid]	466	C15H34N2O6S4	035871-58-0	50		
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	45		



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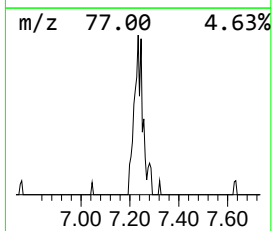
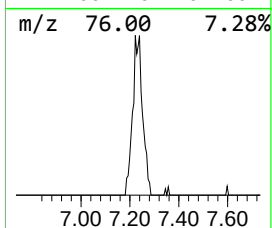
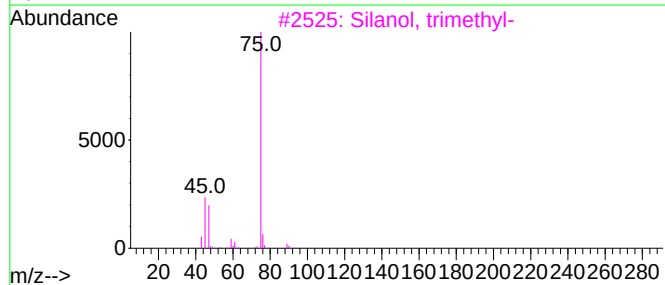
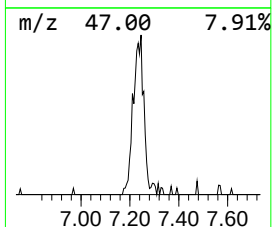
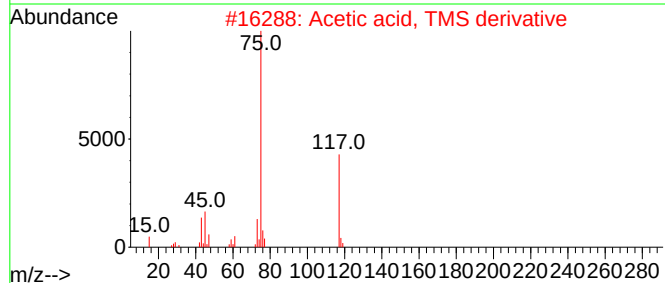
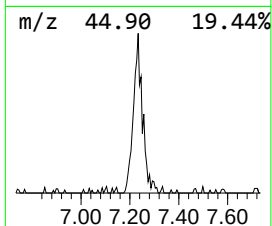
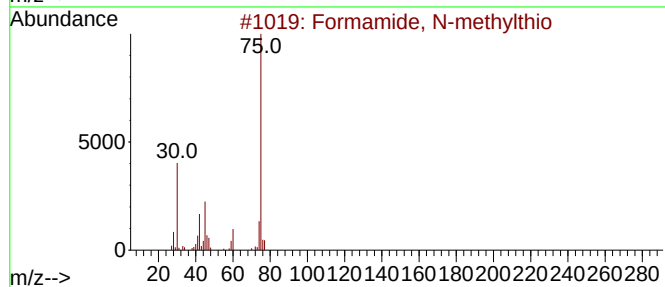
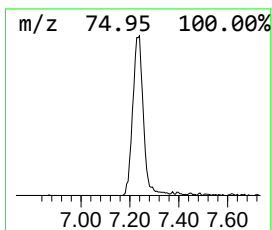
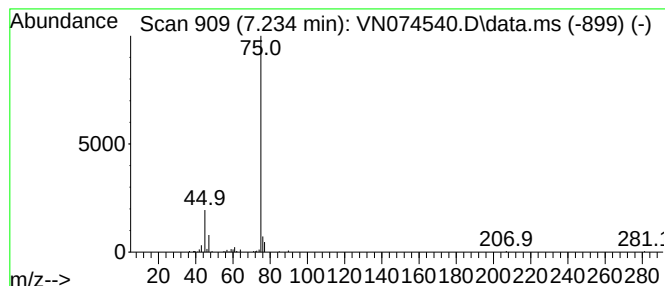
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Peak Number 4 Formamide, N-methylthio Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.234	13.24 ug/l	234913	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formamide, N-methylthio	75	C2H5NS	018952-41-5	78
2			Acetic acid, TMS derivative	132	C5H12O2Si	002754-27-0	74
3			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	72
4			Ethanol, 2-(trimethylsilyl)-	118	C5H14OSi	002916-68-9	50
5			Propanoic acid, TMS derivative	146	C6H14O2Si	016844-98-7	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	23.9	ug/l	423428	1	8.016	886954	50.0
2-Aminoethyl hy...	2.687	5.0	ug/l	88910	1	8.016	886954	50.0
Formamide, N-me...	7.234	13.2	ug/l	234913	1	8.016	886954	50.0