

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060622\
 Data File : VY009141.D
 Acq On : 06 Jun 2022 12:44
 Operator : KP/MD
 Sample : N3143-03RE
 Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20220425-AMENDED-COMP-ERE

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_Y\methods\82Y052022S.M
 Title : SW846 8260

Signal : TIC: VY009141.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.217	60	65	73	rVB3	7361	13521	1.89%	0.256%
2	2.382	87	92	99	rBV	26286	41896	5.84%	0.792%
3	2.516	106	114	116	rBV5	9232	18720	2.61%	0.354%
4	2.546	116	119	129	rVV	152262	253035	35.30%	4.786%
5	3.942	336	348	354	rBV	39877	105810	14.76%	2.001%
6	4.028	354	362	379	rVV	230160	601124	83.86%	11.371%
7	4.192	379	389	402	rVB	65895	179875	25.09%	3.402%
8	4.704	462	473	484	rBV6	6143	20410	2.85%	0.386%
9	6.978	833	846	858	rBV2	46817	143420	20.01%	2.713%
10	7.716	958	967	972	rBV2	42519	104472	14.57%	1.976%
11	7.789	972	979	988	rVB	156157	350309	48.87%	6.626%
12	8.137	1022	1036	1046	rBV2	109955	278057	38.79%	5.260%
13	8.319	1056	1066	1073	rBV3	4369	10305	1.44%	0.195%
14	8.685	1118	1126	1135	rBV	253734	496765	69.30%	9.397%
15	8.880	1151	1158	1170	rBV	15059	36017	5.02%	0.681%
16	9.142	1194	1201	1204	rBV2	3723	7371	1.03%	0.139%
17	9.612	1273	1278	1288	rVB5	3750	8140	1.14%	0.154%
18	9.746	1293	1300	1307	rBV3	3781	8234	1.15%	0.156%
19	10.179	1364	1371	1381	rBV	435146	716810	100.00%	13.559%
20	10.935	1490	1495	1504	rVB4	7880	15081	2.10%	0.285%
21	11.319	1551	1558	1565	rVB5	5459	10661	1.49%	0.202%
22	11.490	1579	1586	1597	rBV	395399	629000	87.75%	11.898%
23	12.105	1681	1687	1694	rVB4	5139	10439	1.46%	0.197%
24	12.203	1698	1703	1706	rBV6	5511	10139	1.41%	0.192%
25	12.477	1741	1748	1756	rBV	287703	469145	65.45%	8.874%
26	12.642	1769	1775	1783	rVB10	4265	11073	1.54%	0.209%
27	12.733	1783	1790	1792	rBV5	3402	7398	1.03%	0.140%
28	12.813	1796	1803	1804	rBV5	6355	12379	1.73%	0.234%
29	12.843	1804	1808	1816	rVB	12824	22613	3.15%	0.428%
30	13.075	1838	1846	1850	rVV7	4810	10430	1.46%	0.197%
31	13.130	1850	1855	1858	rVV7	4255	7513	1.05%	0.142%
32	13.166	1858	1861	1868	rVB7	5624	11553	1.61%	0.219%
33	13.282	1872	1880	1888	rVV6	10631	25722	3.59%	0.487%
34	13.422	1896	1903	1910	rBV	352991	566147	78.98%	10.709%
35	13.483	1910	1913	1916	rVV4	5596	8834	1.23%	0.167%
36	13.526	1916	1920	1924	rVV2	8755	11421	1.59%	0.216%

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Title : SW846 8260

37	13.745	1951	1956	1962	rBV7	5634	11780	1.64%	0.223%
38	13.965	1987	1992	1997	rVB2	8287	14226	1.98%	0.269%
39	14.105	2008	2015	2017	rBV6	4202	8360	1.17%	0.158%
40	14.257	2035	2040	2042	rBV5	5025	8408	1.17%	0.159%
41	15.318	2210	2214	2218	rVV2	6139	10075	1.41%	0.191%

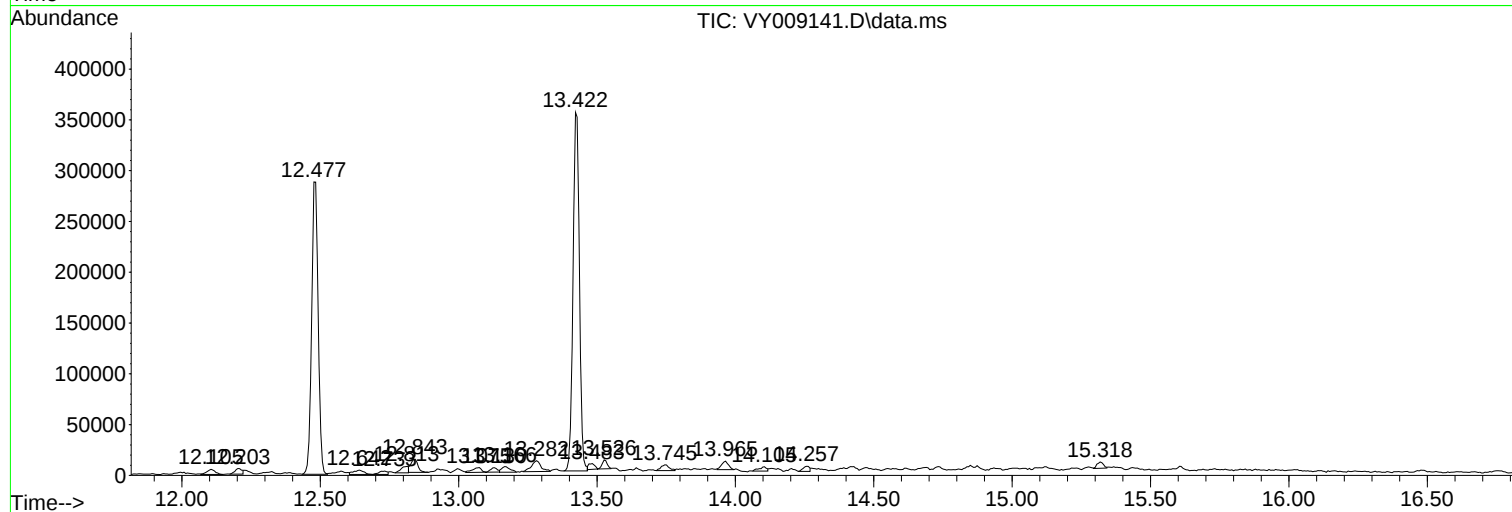
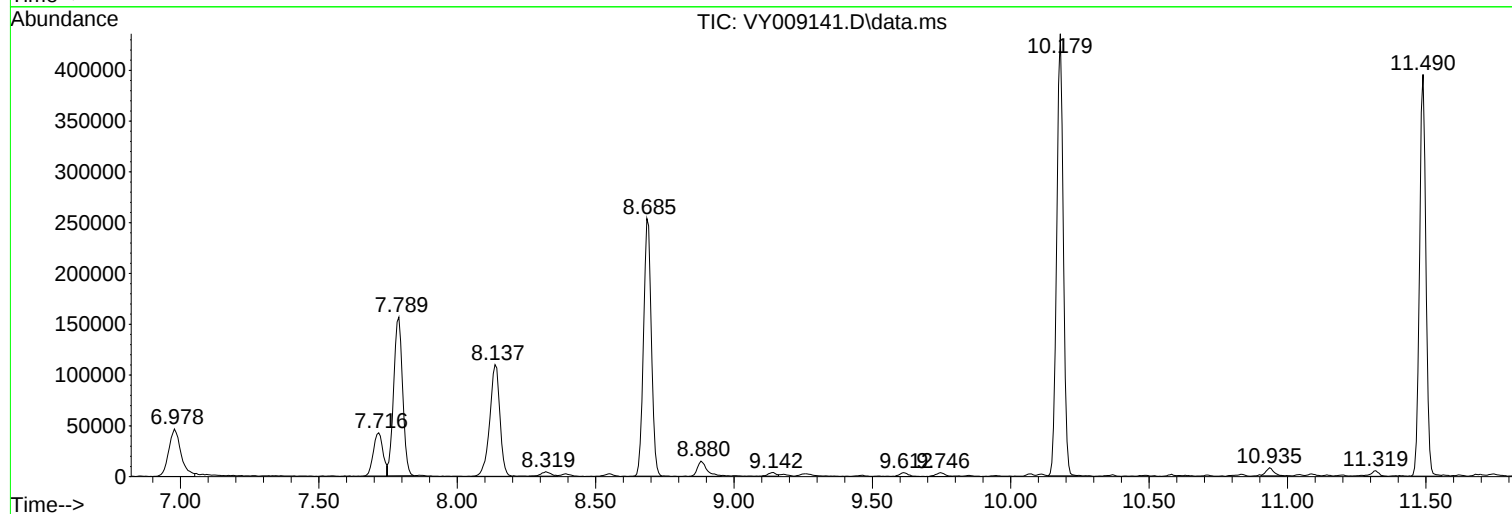
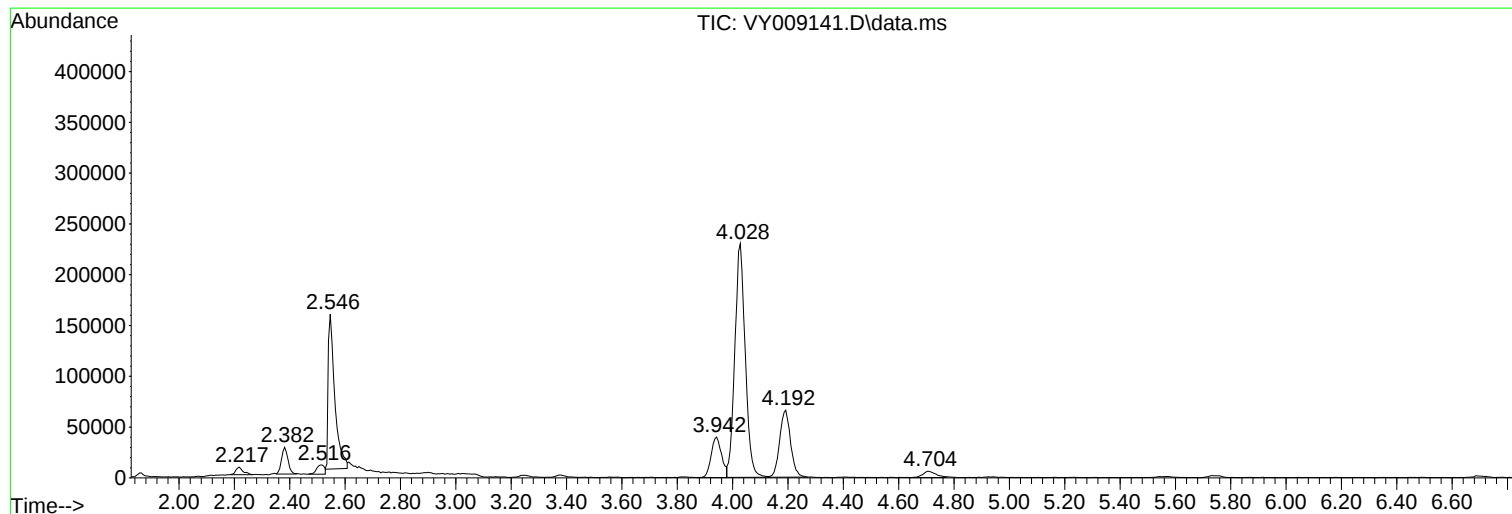
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Quant Title : SW846 8260

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



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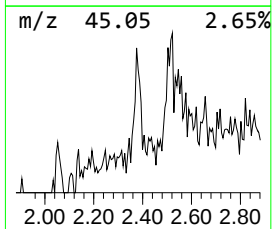
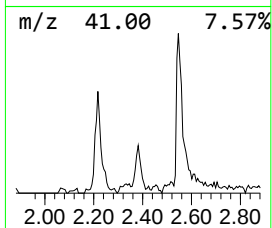
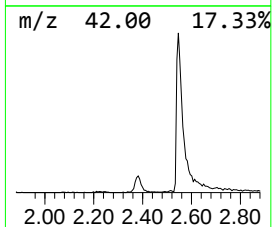
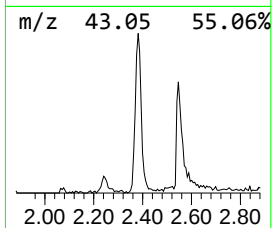
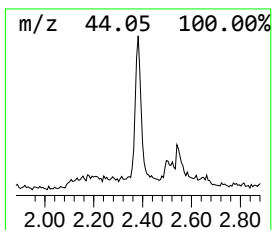
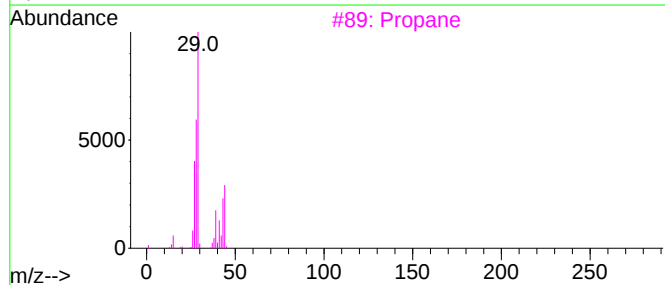
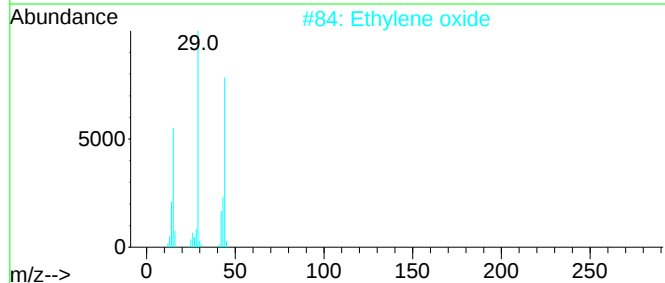
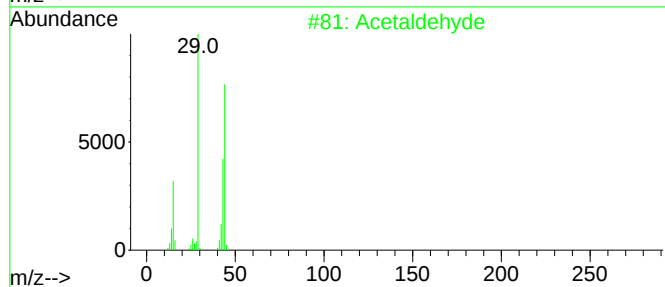
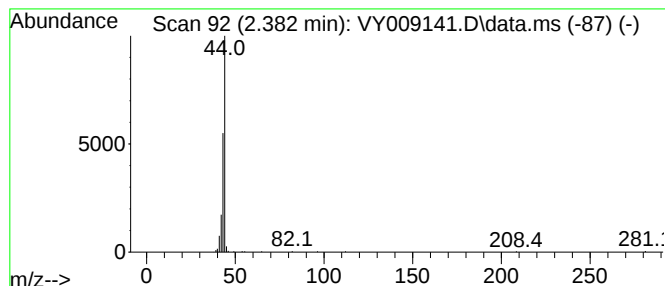
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052022S.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.382	5.98 ug/l	41896	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Ethylene oxide	44	C2H4O	000075-21-8	9
3			Propane	44	C3H8	000074-98-6	4
4			Acetic acid, [(aminocarbonyl)ami...	132	C3H4N2O4	000585-05-7	4
5			L-Alanine, methyl ester	103	C4H9NO2	010065-72-2	4



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MSVOA_Y
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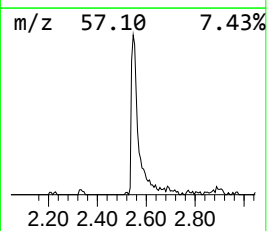
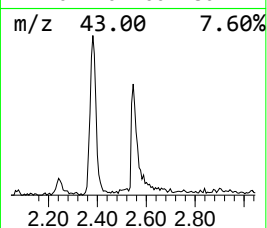
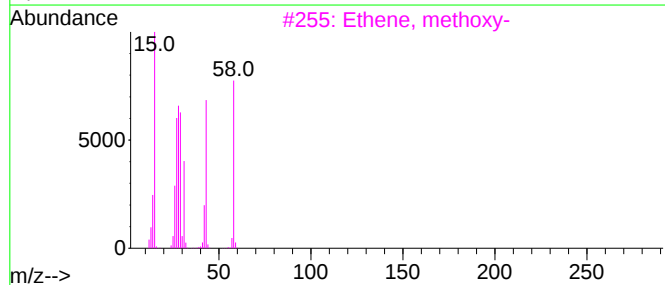
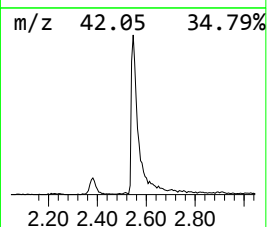
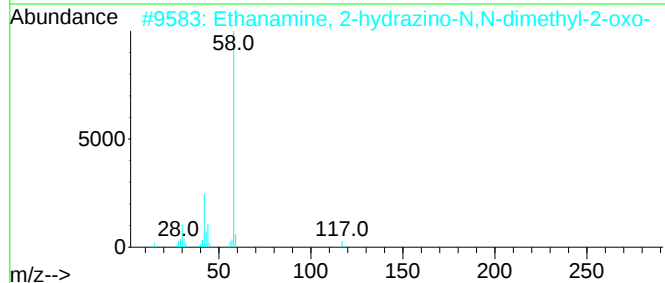
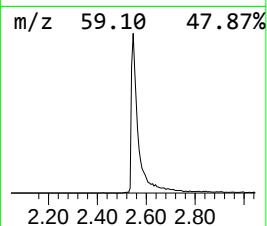
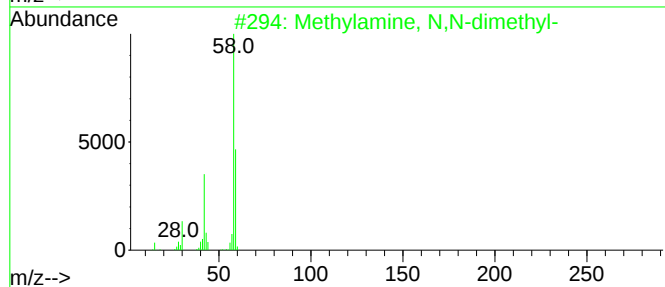
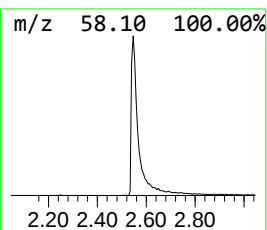
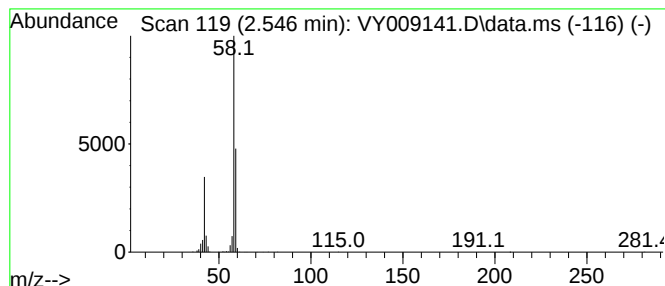
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052022S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Methylamine, N,N-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.546	36.12 ug/l	253035	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	91
2			Ethanamine, 2-hydrazino-N,N-dime...	117	C4H11N3O	000055-85-6	9
3			Ethene, methoxy-	58	C3H6O	000107-25-5	7
4			Propylamine	59	C3H9N	000107-10-8	5
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	5



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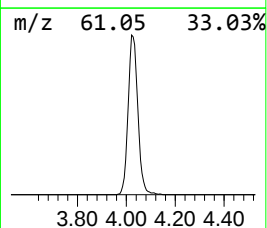
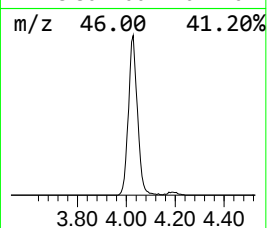
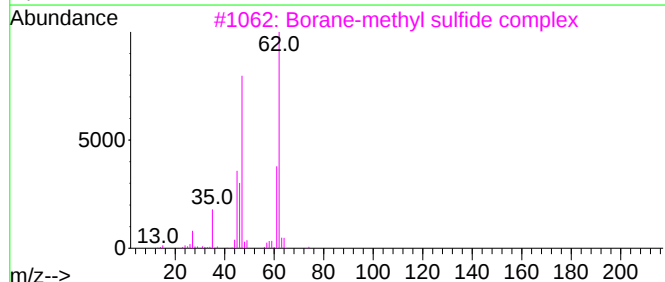
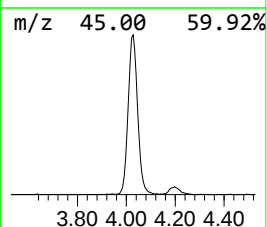
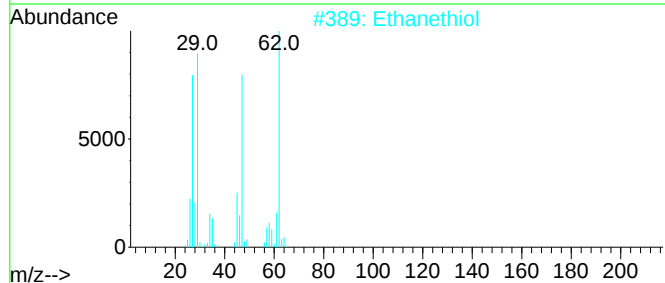
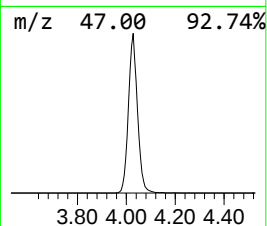
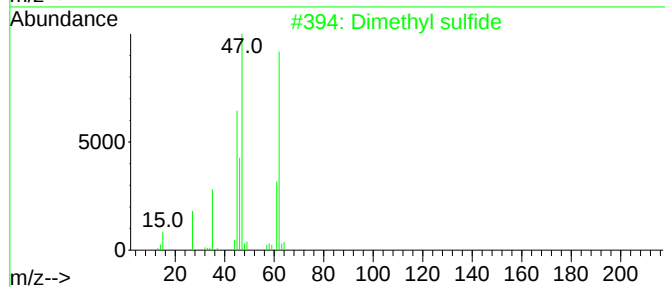
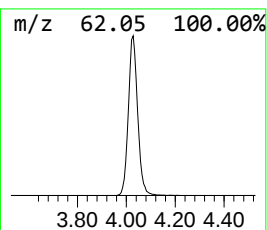
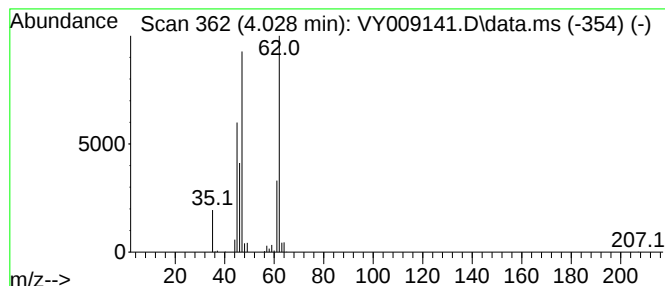
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Peak Number 3 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.028	85.80 ug/l	601124	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	95
2			Ethanethiol	62	C2H6S	000075-08-1	86
3			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	86
4			Ethene, chloro-	62	C2H3Cl	000075-01-4	9
5			Boric acid	62	BH3O3	010043-35-3	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.382	6.0	ug/l	41896	1	7.789	350309	50.0
Methylamine, N,...	2.546	36.1	ug/l	253035	1	7.789	350309	50.0
Dimethyl sulfide	4.028	85.8	ug/l	601124	1	7.789	350309	50.0