

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060622\
 Data File : VY009155.D
 Acq On : 06 Jun 2022 18:12
 Operator : KP/MD
 Sample : N3170-03
 Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20220422-AMENDED-COMPOSITE-B

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: VY009155.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.375	85	91	100	rBV	50166	86123	13.05%	1.812%
2	2.521	106	115	117	rBV6	10520	27274	4.13%	0.574%
3	2.546	117	119	143	rVB	107255	217822	33.02%	4.583%
4	3.387	247	257	266	rVB4	2662	7724	1.17%	0.163%
5	3.936	336	347	354	rBV	51885	139210	21.10%	2.929%
6	4.021	354	361	379	rVV	98217	267144	40.49%	5.621%
7	4.186	379	388	401	rVB3	22734	66383	10.06%	1.397%
8	4.704	463	473	490	rBV3	7122	23936	3.63%	0.504%
9	5.734	632	642	650	rBV4	2494	7589	1.15%	0.160%
10	6.978	835	846	870	rBV2	41041	134339	20.36%	2.826%
11	7.710	957	966	972	rBV	49278	119520	18.12%	2.515%
12	7.783	972	978	991	rVB	149679	329640	49.96%	6.935%
13	8.130	1022	1035	1047	rBV2	127361	394809	59.84%	8.307%
14	8.685	1116	1126	1138	rBV	244668	467153	70.81%	9.829%
15	8.880	1151	1158	1170	rBV2	12611	26980	4.09%	0.568%
16	9.136	1194	1200	1206	rBV3	3568	7242	1.10%	0.152%
17	10.179	1363	1371	1379	rBV	387825	659745	100.00%	13.881%
18	10.575	1429	1436	1443	rBV2	7342	13231	2.01%	0.278%
19	10.935	1489	1495	1504	rVB3	10877	21933	3.32%	0.461%
20	11.319	1552	1558	1563	rVB	10839	18133	2.75%	0.382%
21	11.489	1578	1586	1595	rBV	352545	576090	87.32%	12.121%
22	12.105	1681	1687	1695	rBV6	6162	15332	2.32%	0.323%
23	12.203	1698	1703	1706	rVV4	4684	9142	1.39%	0.192%
24	12.331	1719	1724	1728	rBV4	4927	7848	1.19%	0.165%
25	12.477	1740	1748	1759	rVB2	275148	442704	67.10%	9.314%
26	12.642	1769	1775	1783	rVB6	3883	8367	1.27%	0.176%
27	12.812	1796	1803	1804	rVV3	6240	12298	1.86%	0.259%
28	12.837	1804	1807	1814	rVB	11470	19369	2.94%	0.408%
29	13.160	1857	1860	1867	rVB4	7147	12667	1.92%	0.267%
30	13.282	1872	1880	1884	rBV8	5842	12418	1.88%	0.261%
31	13.422	1897	1903	1909	rBV	324858	497995	75.48%	10.478%
32	13.483	1909	1913	1917	rVV6	5568	9797	1.48%	0.206%
33	13.526	1917	1920	1924	rVB2	9354	11984	1.82%	0.252%
34	13.751	1950	1957	1961	rBV6	5498	13029	1.97%	0.274%
35	13.958	1988	1991	1998	rVB2	6418	9926	1.50%	0.209%
36	14.099	2006	2014	2019	rBV3	8925	19266	2.92%	0.405%

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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

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37	14.257	2036	2040	2045	rVB9	3480	7039	1.07%	0.148%
38	14.733	2114	2118	2123	rVB7	5542	8580	1.30%	0.181%
39	15.318	2209	2214	2218	rBV	10207	15454	2.34%	0.325%
40	15.964	2316	2320	2327	rVB10	3305	7720	1.17%	0.162%

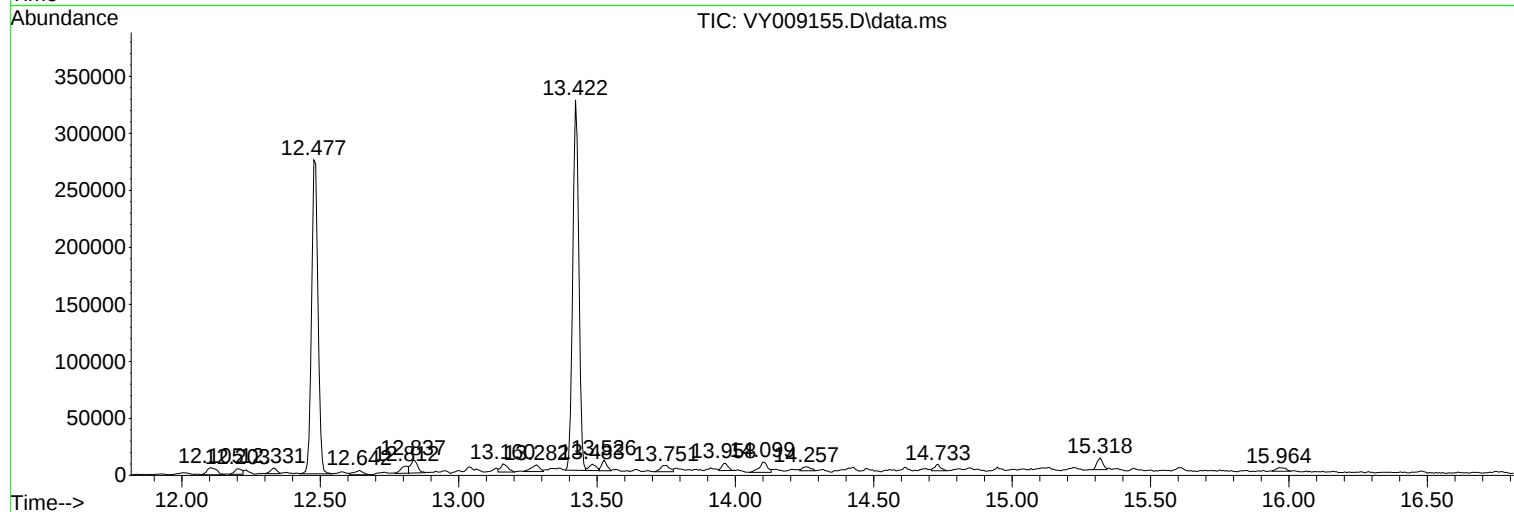
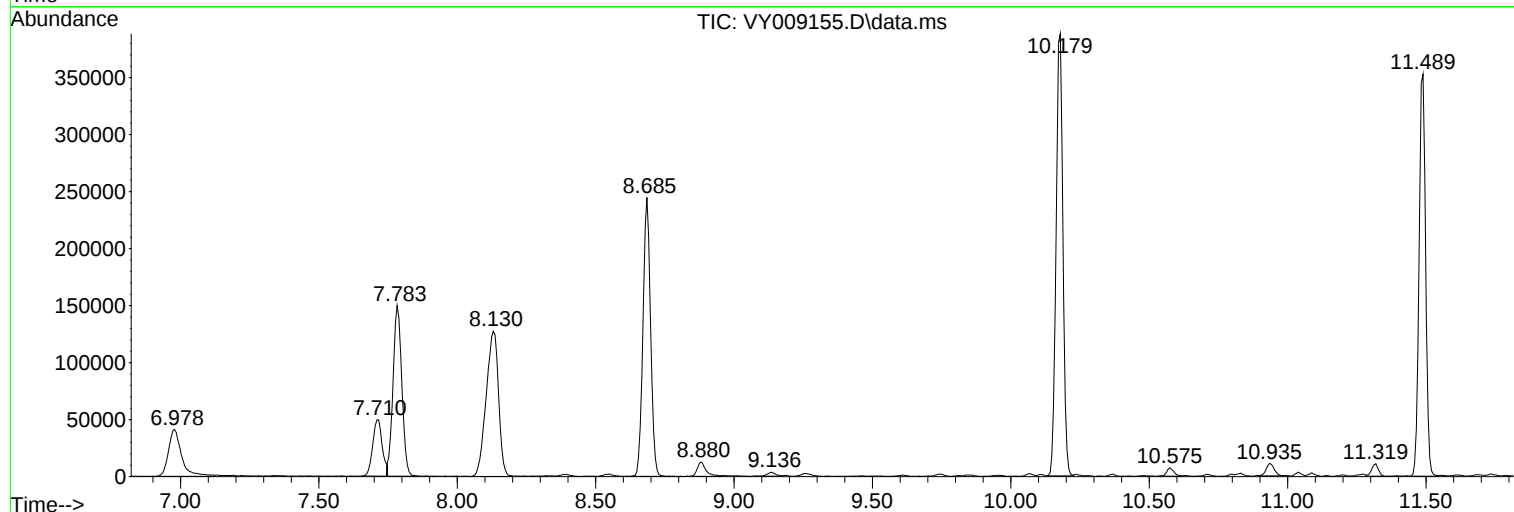
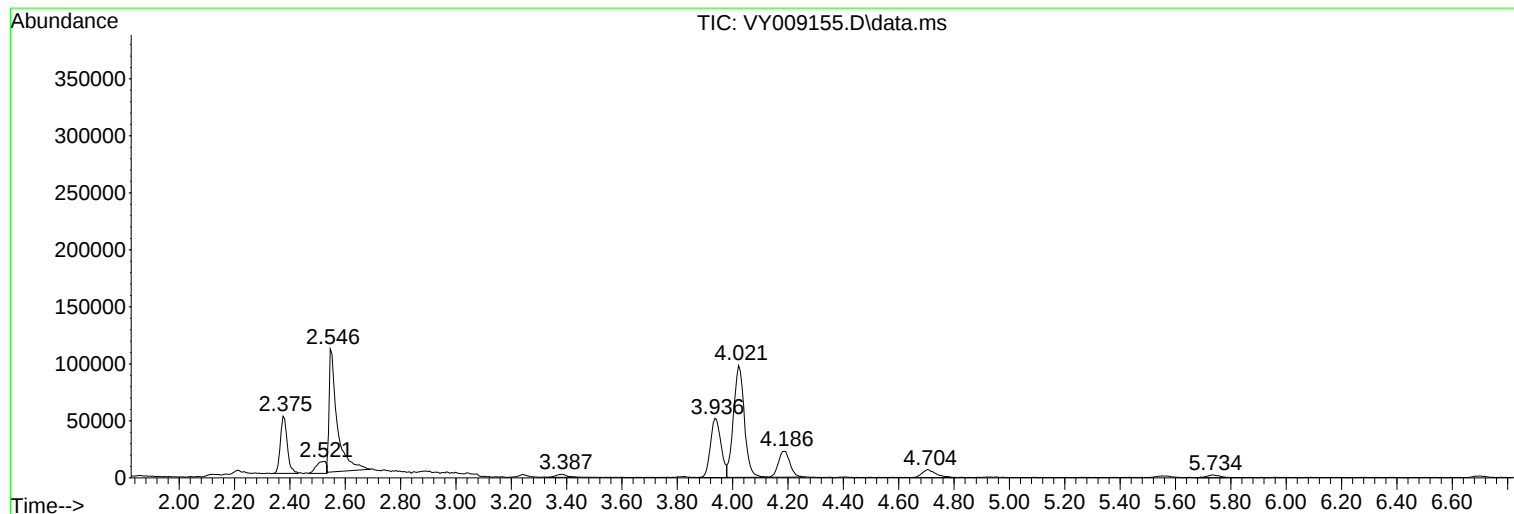
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052022S.M
Quant Title : SW846 8260

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



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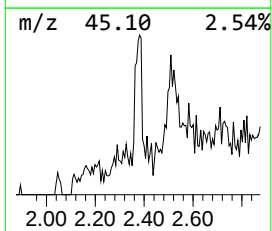
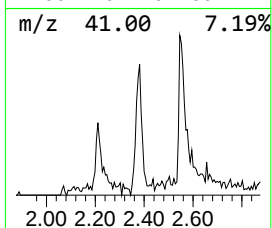
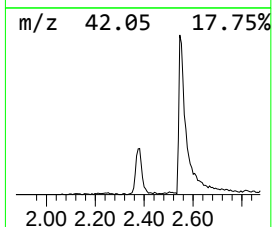
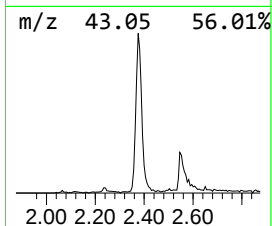
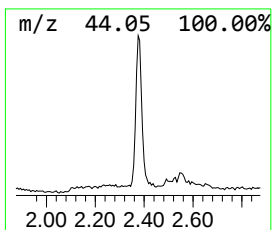
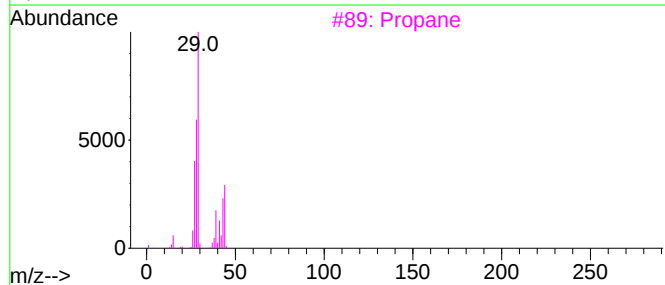
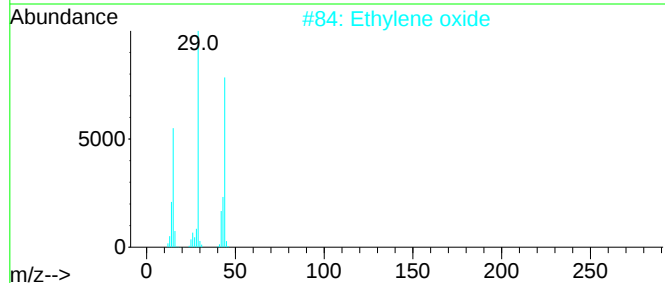
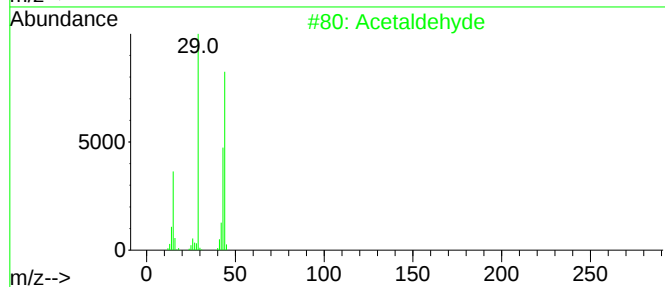
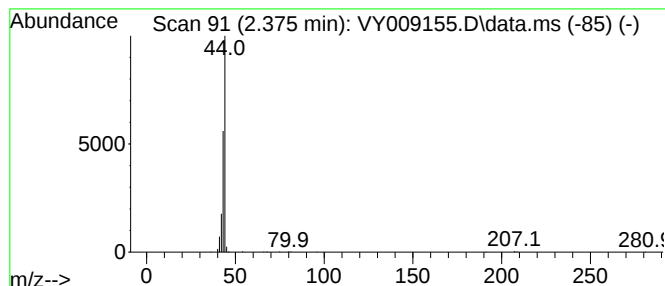
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052022S.M
Quant Title : SW846 8260

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.
2.375	13.06 ug/l	86123	Pentafluorobenzene	7.783

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	5
3			Propane	44	C3H8	000074-98-6	4
4			Acetic acid, 2-(methylaminoethyl...	117	C5H11NO2	026921-43-7	4
5			L-Alanine, methyl ester	103	C4H9NO2	010065-72-2	4



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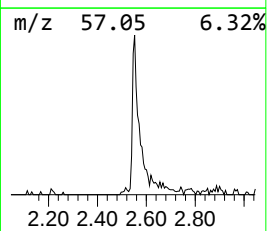
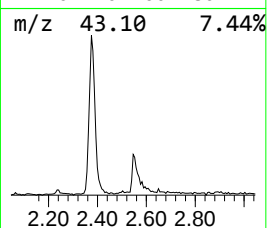
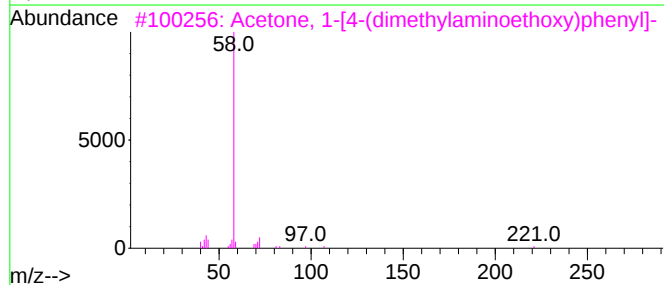
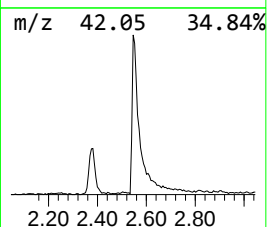
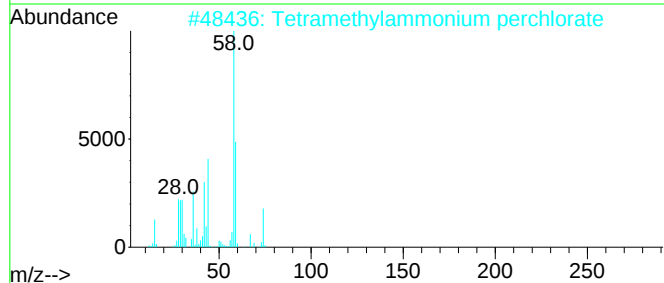
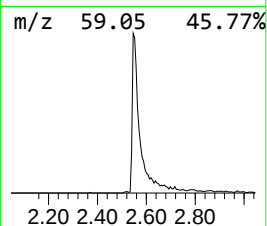
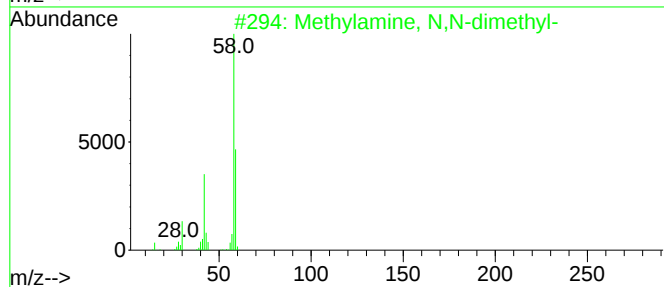
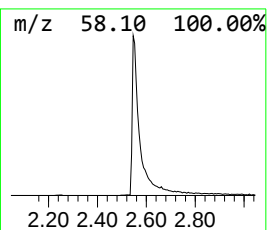
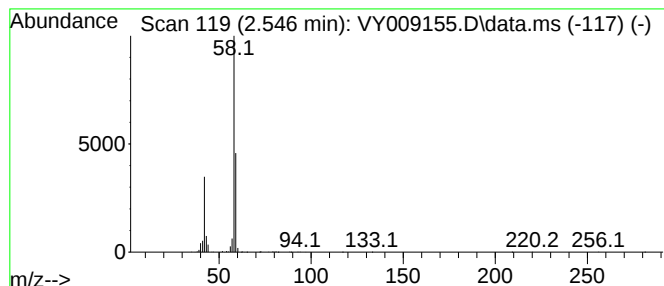
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052022S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.546	33.04 ug/l	217822	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	91
2			Tetramethylammonium perchlorate	173	C4H12ClNO4	002537-36-2	40
3			Acetone, 1-[4-(dimethylaminoetho...	221	C13H19NO2	086608-11-9	9
4			2-Methyl-1,2-propanediamine	88	C4H12N2	000811-93-8	9
5			Ethanamine, 2-hydrazino-N,N-dime...	117	C4H11N3O	000055-85-6	9



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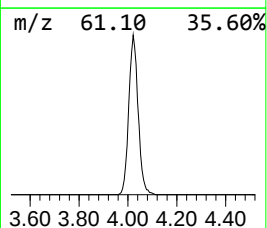
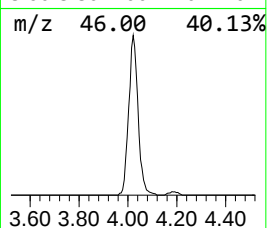
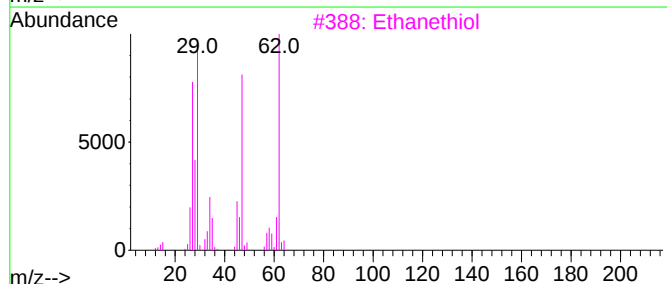
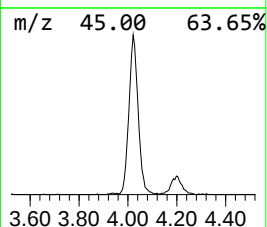
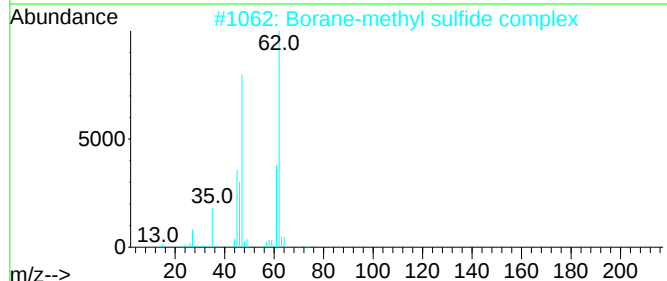
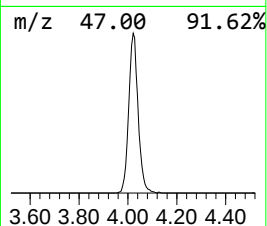
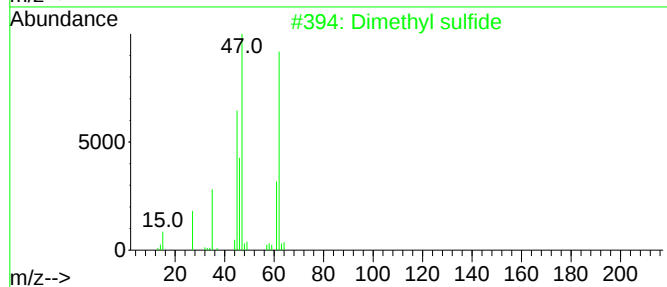
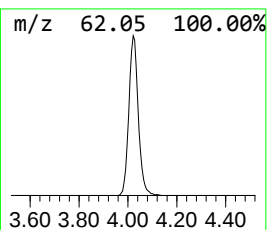
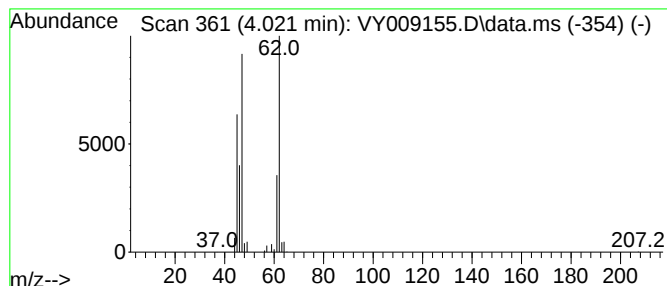
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.021	40.52 ug/l	267144	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90
3			Ethanethiol	62	C2H6S	000075-08-1	72
4			Ethene, chloro-	62	C2H3Cl	000075-01-4	7
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	2.375	13.1	ug/l	86123	1	7.783	329640	50.0
Methylamine, N,...	2.546	33.0	ug/l	217822	1	7.783	329640	50.0
Dimethyl sulfide	4.021	40.5	ug/l	267144	1	7.783	329640	50.0