

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060622\
 Data File : VY009153.D
 Acq On : 06 Jun 2022 17:25
 Operator : KP/MD
 Sample : N3189-03
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20220423-AMENDED-COMPOSITE-C

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: VY009153.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	102	rBV	58238	101682	15.21%	2.222%
2	2.515	107	114	119	rBV6	9956	23037	3.45%	0.503%
3	2.558	119	121	144	rVB	44489	106694	15.96%	2.331%
4	3.942	338	348	353	rBV	24629	62630	9.37%	1.368%
5	4.027	353	362	378	rVV	144177	404327	60.49%	8.834%
6	4.186	378	388	401	rVV	68940	189187	28.31%	4.134%
7	4.698	463	472	482	rBV3	6225	19178	2.87%	0.419%
8	5.747	633	644	653	rBV4	3986	12804	1.92%	0.280%
9	6.978	836	846	861	rBV2	17700	55954	8.37%	1.223%
10	7.716	957	967	971	rBV	45697	105791	15.83%	2.311%
11	7.783	971	978	991	rVB	149995	338373	50.63%	7.393%
12	8.136	1022	1036	1048	rBV3	106130	276548	41.38%	6.042%
13	8.685	1117	1126	1136	rBV	235017	463946	69.41%	10.137%
14	8.880	1151	1158	1165	rBV2	11772	24356	3.64%	0.532%
15	10.173	1363	1370	1384	rBV	393377	668380	100.00%	14.604%
16	10.929	1487	1494	1502	rVB4	8750	16227	2.43%	0.355%
17	11.489	1578	1586	1596	rBV	366237	587328	87.87%	12.833%
18	12.203	1697	1703	1712	rBV7	4490	10650	1.59%	0.233%
19	12.331	1714	1724	1730	rBV3	17697	32096	4.80%	0.701%
20	12.477	1741	1748	1756	rBV	281271	439054	65.69%	9.593%
21	12.727	1782	1789	1796	rBV9	2685	9048	1.35%	0.198%
22	12.812	1796	1803	1804	rVV7	3855	7131	1.07%	0.156%
23	12.837	1804	1807	1812	rVB2	5931	9138	1.37%	0.200%
24	13.276	1870	1879	1883	rBV8	6182	14843	2.22%	0.324%
25	13.422	1897	1903	1910	rBV	353951	537930	80.48%	11.754%
26	13.526	1916	1920	1927	rVB4	7035	10448	1.56%	0.228%
27	13.745	1951	1956	1960	rBV8	3309	6872	1.03%	0.150%
28	13.959	1987	1991	1997	rVB3	7070	11902	1.78%	0.260%
29	14.404	2058	2064	2071	rBV8	5535	12199	1.83%	0.267%
30	15.318	2210	2214	2221	rBV7	3974	7472	1.12%	0.163%
31	15.605	2256	2261	2269	rVB10	4794	11517	1.72%	0.252%

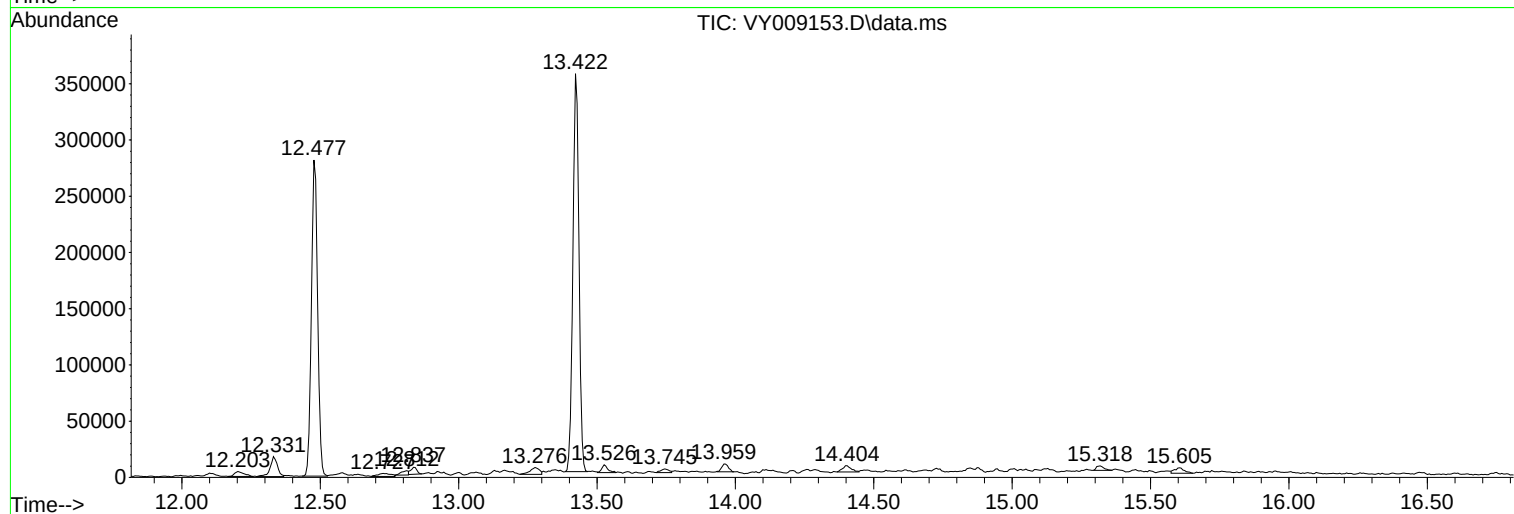
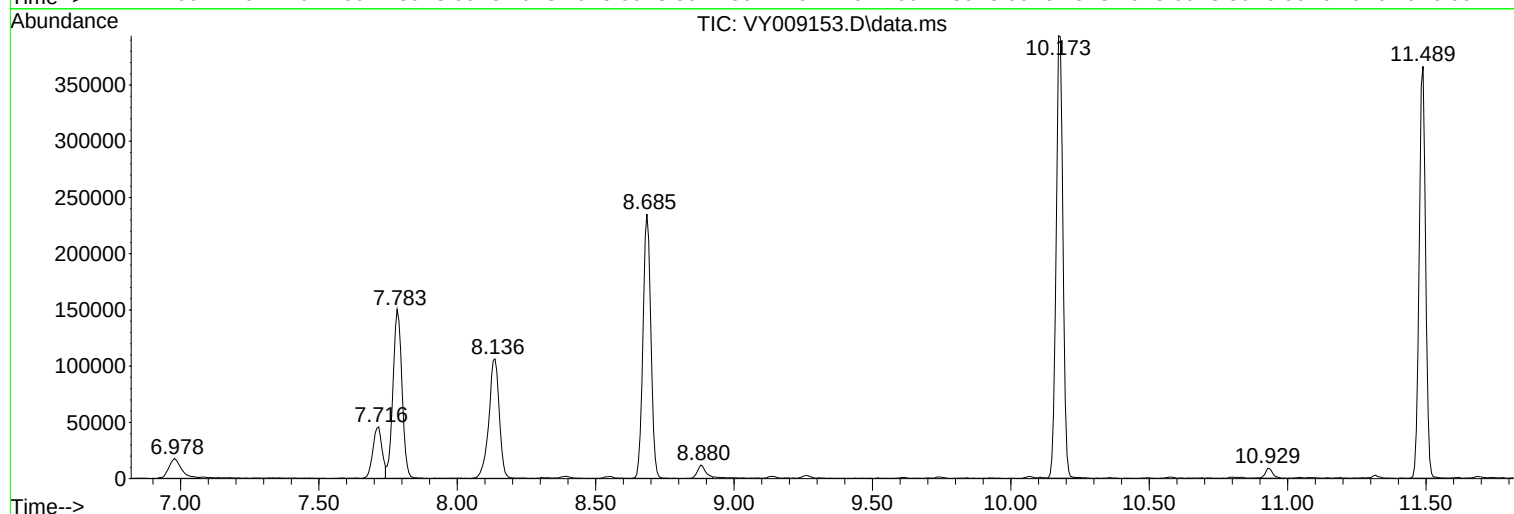
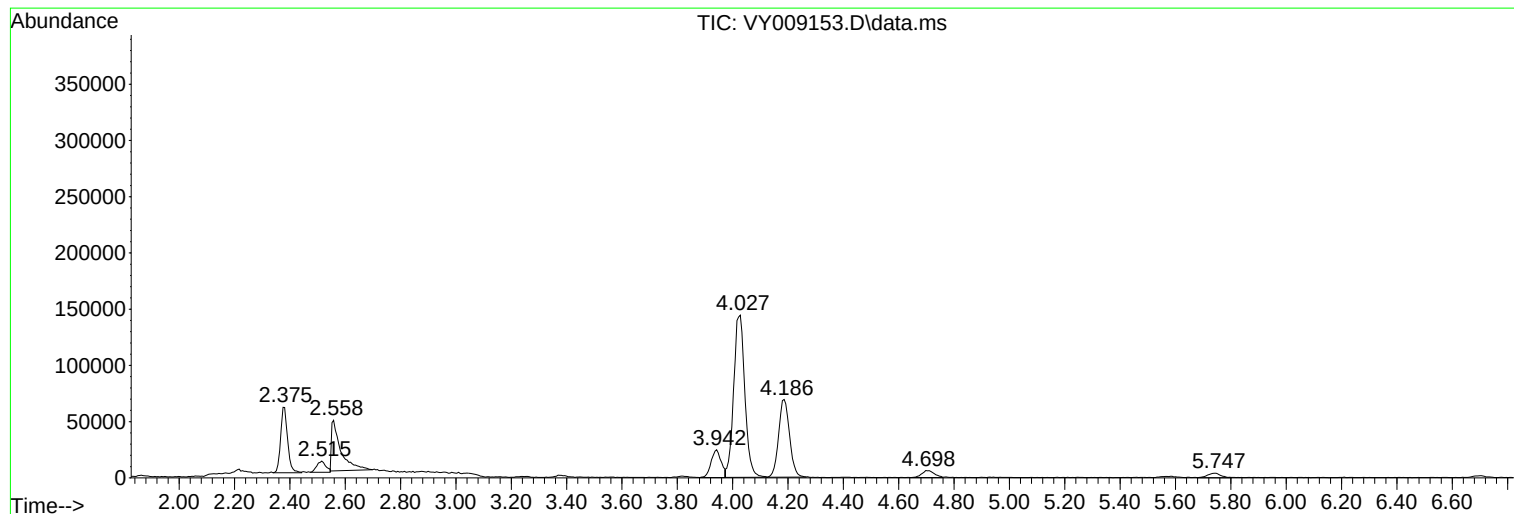
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052022S.M
Quant Title : SW846 8260

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



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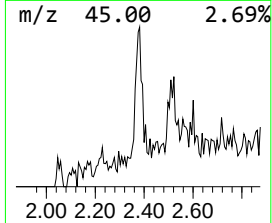
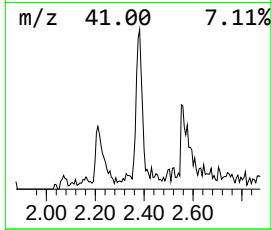
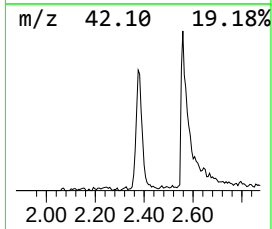
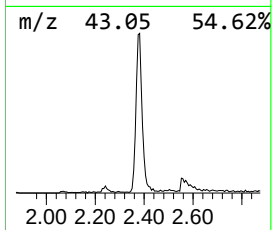
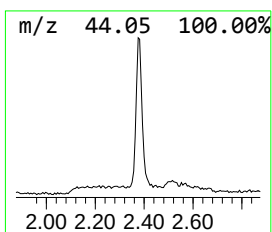
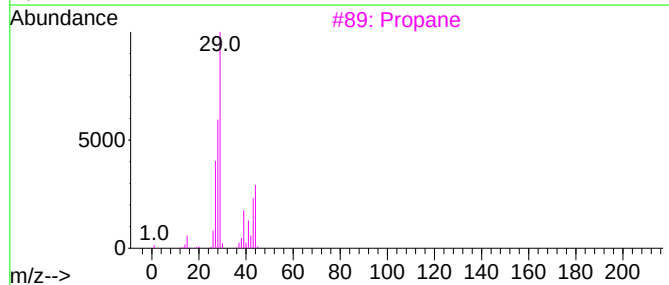
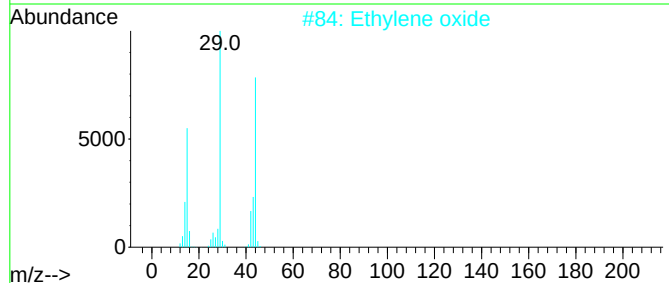
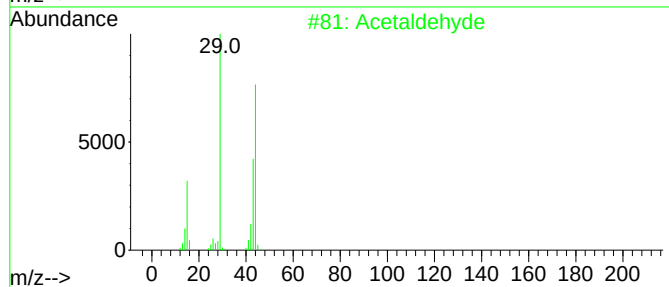
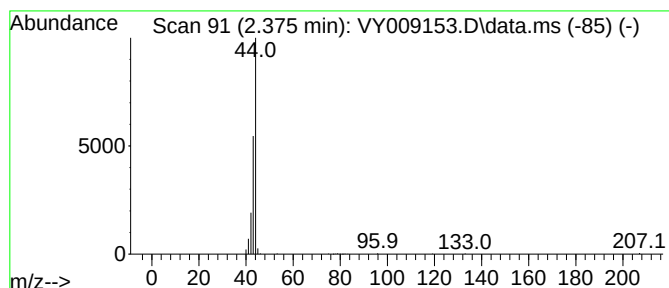
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052022S.M
Quant Title : SW846 8260

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	15.03 ug/l	101682	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			L-Alanine, methyl ester	103	C4H9NO2	010065-72-2	4
5			Acetic acid, 2-(methylaminoethyl...)	117	C5H11NO2	026921-43-7	4



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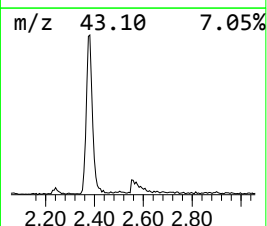
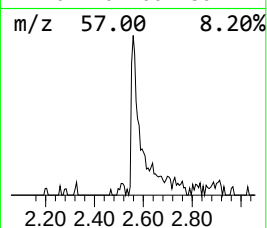
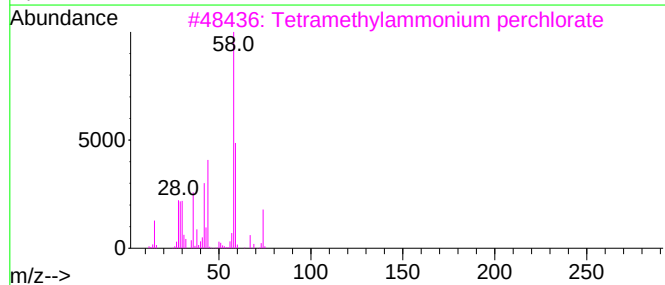
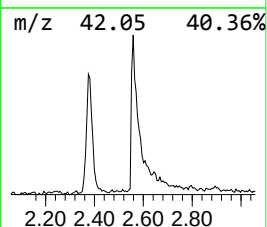
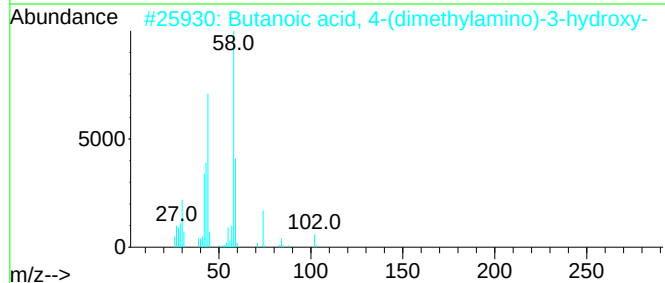
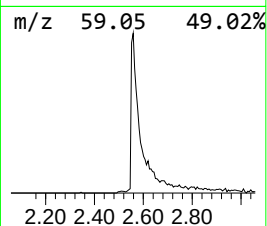
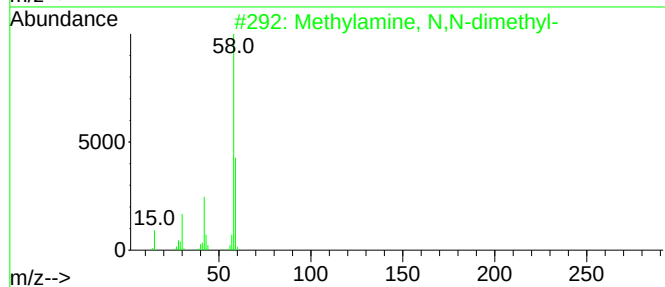
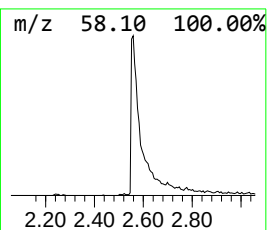
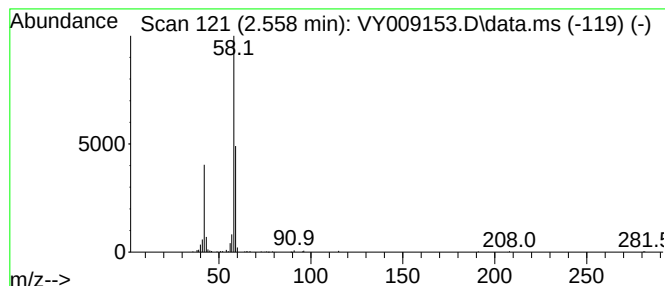
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.558	15.77 ug/l	106694	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	90
2			Butanoic acid, 4-(dimethylamino)...	147	C6H13NO3	003688-46-8	43
3			Tetramethylammonium perchlorate	173	C4H12ClNO4	002537-36-2	43
4			Oxirane, 2,3-diethyl-	100	C6H12O	004468-66-0	43
5			2-Propanamine, 2-methyl-	73	C4H11N	000075-64-9	25



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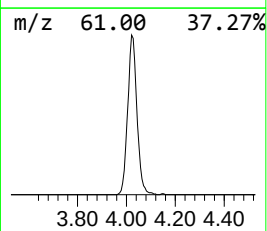
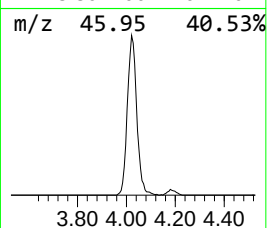
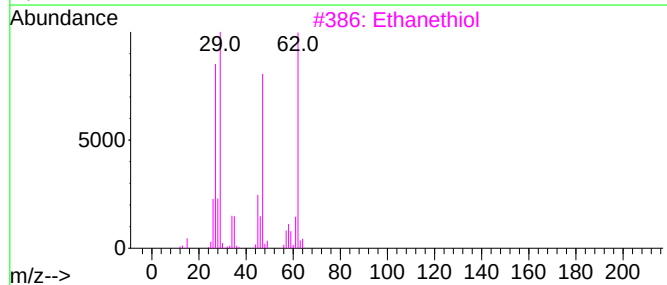
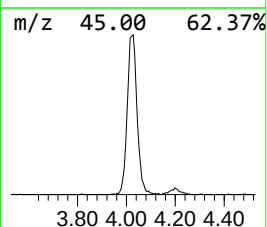
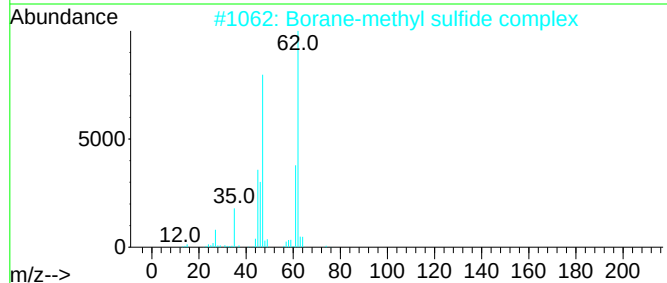
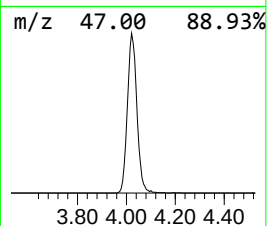
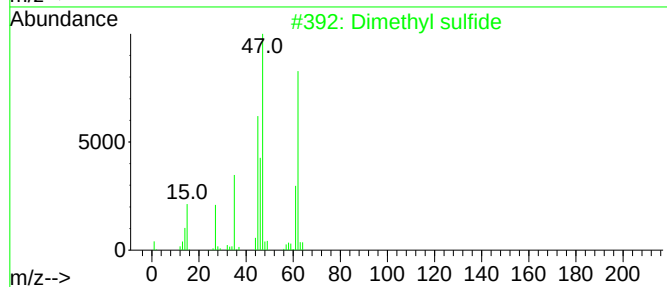
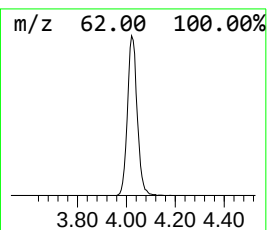
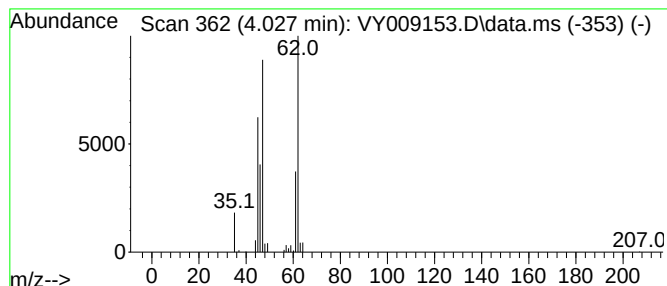
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Quant Title : SW846 8260

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.
4.027	59.75 ug/l	404327	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	80
4			Sulfonium, dimethyl-, cyanonitro...	146	C4H6N2O2S	058992-18-0	25
5			Acetic acid, mercapto-, methyl e...	106	C3H6O2S	002365-48-2	22



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.375	15.0	ug/l	101682	1	7.783	338373	50.0
Methylamine, N,...	2.558	15.8	ug/l	106694	1	7.783	338373	50.0
Dimethyl sulfide	4.027	59.8	ug/l	404327	1	7.783	338373	50.0