

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060222\
 Data File : VY009125.D
 Acq On : 02 Jun 2022 14:18
 Operator : KP/MD
 Sample : N3099-03
 Misc : 3.35g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20220426-AMENDED-COMPOSITE-F

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: VY009125.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.241	59	69	77	rBV2	59956	108996	14.81%	1.762%
2	2.381	87	92	97	rBV	18473	28996	3.94%	0.469%
3	2.509	107	113	118	rBV6	12650	30215	4.10%	0.489%
4	2.552	118	120	137	rVB	54746	111303	15.12%	1.800%
5	2.790	154	159	164	rVB2	8775	14962	2.03%	0.242%
6	2.894	169	176	186	rBV	48807	111055	15.09%	1.796%
7	3.064	202	204	212	rVB5	4404	7446	1.01%	0.120%
8	3.174	216	222	227	rVV5	4372	9097	1.24%	0.147%
9	3.241	227	233	243	rVB3	7280	18037	2.45%	0.292%
10	3.863	328	335	341	rBV2	8624	22553	3.06%	0.365%
11	3.942	341	348	354	rVV	32416	86757	11.79%	1.403%
12	4.021	354	361	378	rVV	143888	379613	51.57%	6.138%
13	4.186	378	388	406	rVB2	51929	144028	19.57%	2.329%
14	4.698	460	472	481	rBV4	12349	52894	7.19%	0.855%
15	5.235	547	560	573	rBV2	11236	37965	5.16%	0.614%
16	5.741	631	643	653	rVB5	5090	15483	2.10%	0.250%
17	6.009	676	687	702	rVB2	36239	114666	15.58%	1.854%
18	6.789	806	815	828	rVB4	11848	36362	4.94%	0.588%
19	6.978	834	846	857	rBV	77008	220677	29.98%	3.568%
20	7.710	956	966	972	rBV	43542	109640	14.89%	1.773%
21	7.783	972	978	987	rVV	170534	393675	53.48%	6.365%
22	7.868	987	992	1000	rVV4	6053	15169	2.06%	0.245%
23	7.996	1004	1013	1017	rVV4	5049	12184	1.66%	0.197%
24	8.045	1017	1021	1028	rVV3	7275	17921	2.43%	0.290%
25	8.136	1028	1036	1046	rVV	100729	227793	30.95%	3.683%
26	8.271	1047	1058	1065	rVV5	9634	28741	3.90%	0.465%
27	8.344	1065	1070	1075	rVV5	7704	18021	2.45%	0.291%
28	8.411	1075	1081	1092	rVB4	15150	36917	5.02%	0.597%
29	8.685	1116	1126	1140	rBV	246510	484417	65.81%	7.833%
30	8.880	1150	1158	1161	rBV4	5060	9727	1.32%	0.157%
31	8.935	1161	1167	1175	rVB4	15498	33022	4.49%	0.534%
32	9.179	1194	1207	1214	rBV3	37099	100982	13.72%	1.633%
33	9.362	1232	1237	1244	rVB4	4389	8495	1.15%	0.137%
34	9.459	1247	1253	1261	rVB3	5893	11583	1.57%	0.187%
35	9.600	1270	1276	1283	rVB5	7687	14677	1.99%	0.237%
36	9.941	1324	1332	1338	rBV7	4000	9869	1.34%	0.160%

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37	10.179	1363	1371	1382	rBV	428989	736115	100.00%	11.902%
38	10.343	1392	1398	1407	rVB5	9569	26577	3.61%	0.430%
39	10.520	1421	1427	1433	rVB3	17945	30980	4.21%	0.501%
40	10.612	1433	1442	1449	rBV5	7979	17446	2.37%	0.282%
41	10.715	1455	1459	1464	rVB4	7802	13728	1.86%	0.222%
42	10.935	1489	1495	1502	rBV6	5773	13718	1.86%	0.222%
43	11.008	1502	1507	1508	rVV4	4574	7717	1.05%	0.125%
44	11.038	1508	1512	1516	rVV2	9797	15883	2.16%	0.257%
45	11.087	1516	1520	1525	rVB3	8263	13773	1.87%	0.223%
46	11.490	1578	1586	1595	rBV	380524	627289	85.22%	10.143%
47	11.581	1595	1601	1604	rBV	6682	9987	1.36%	0.161%
48	11.733	1622	1626	1639	rVB7	5930	14356	1.95%	0.232%
49	12.203	1698	1703	1713	rVB6	8386	16302	2.21%	0.264%
50	12.331	1718	1724	1729	rVB2	10325	16136	2.19%	0.261%
51	12.483	1741	1749	1755	rBV	282399	451313	61.31%	7.297%
52	12.843	1798	1808	1815	rVB	285345	431723	58.65%	6.981%
53	12.965	1825	1828	1836	rVB4	5510	10183	1.38%	0.165%
54	13.245	1868	1874	1882	rBV3	23180	47535	6.46%	0.769%
55	13.422	1896	1903	1909	rBV	353417	555378	75.45%	8.980%
56	13.751	1951	1957	1962	rBV9	3960	9984	1.36%	0.161%
57	13.965	1987	1992	1996	rVB2	5945	9216	1.25%	0.149%
58	14.081	2006	2011	2013	rBV3	6622	10456	1.42%	0.169%
59	14.404	2058	2064	2070	rBV5	8212	14951	2.03%	0.242%

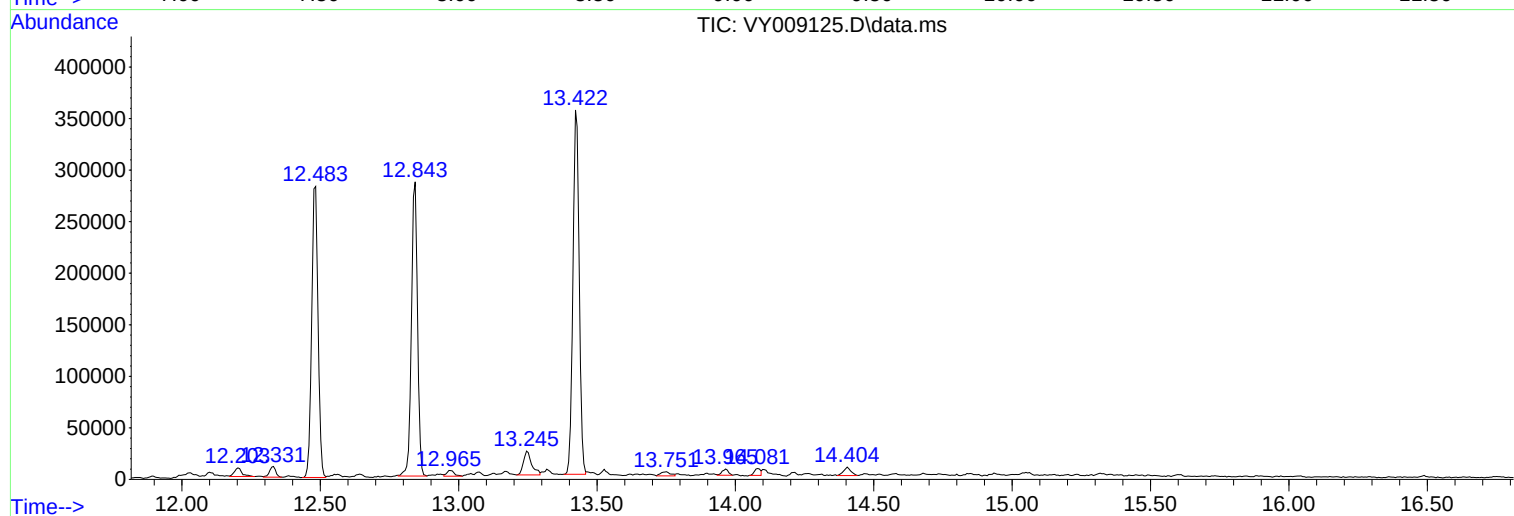
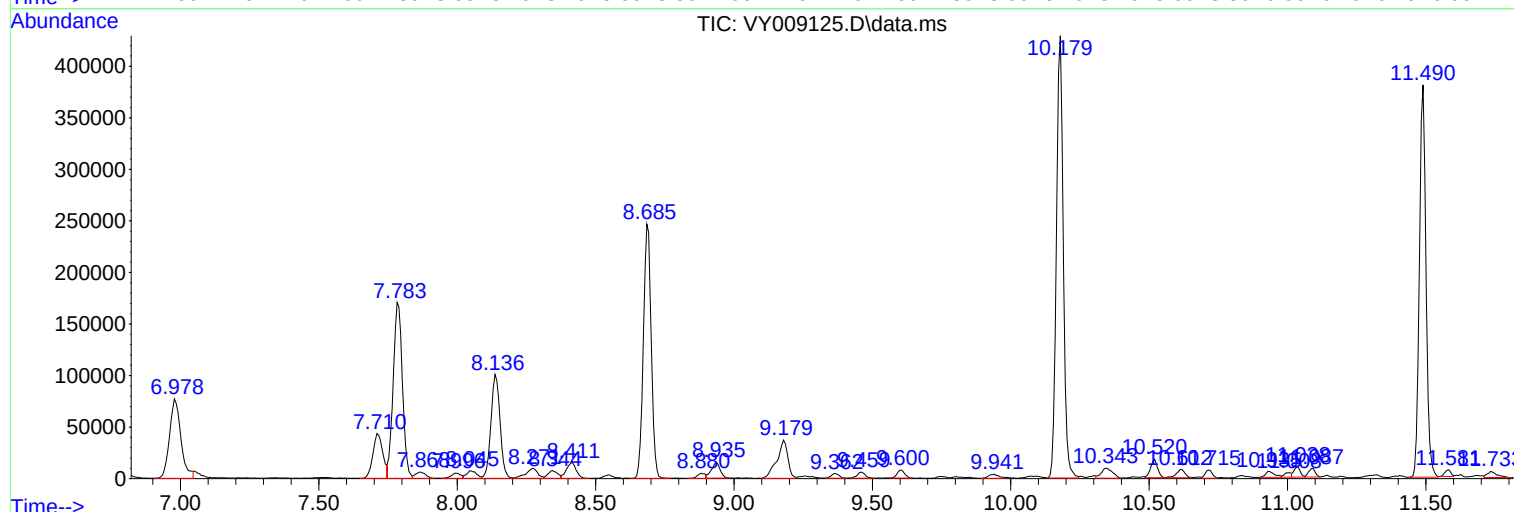
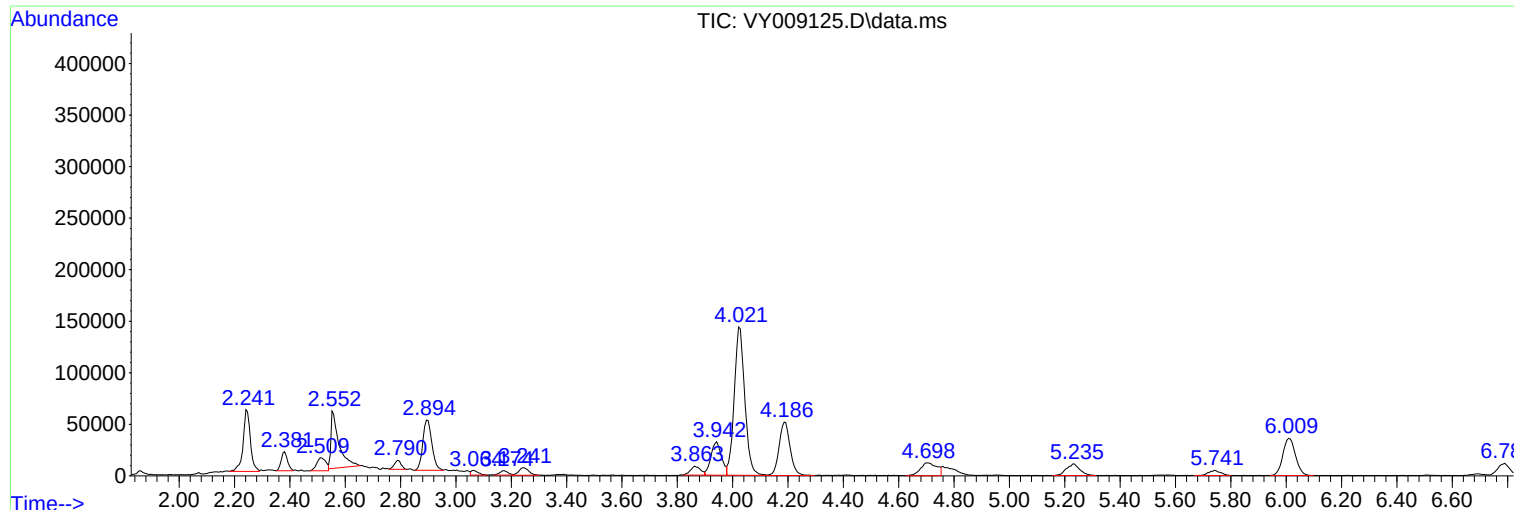
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Quant Title : SW846 8260

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



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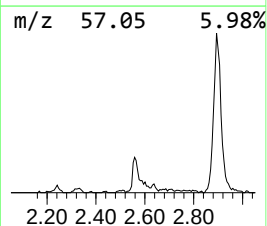
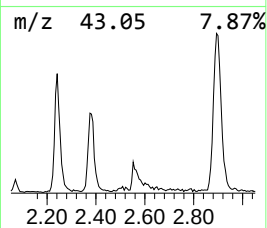
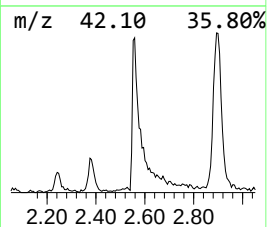
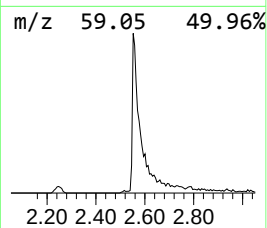
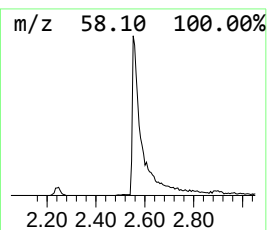
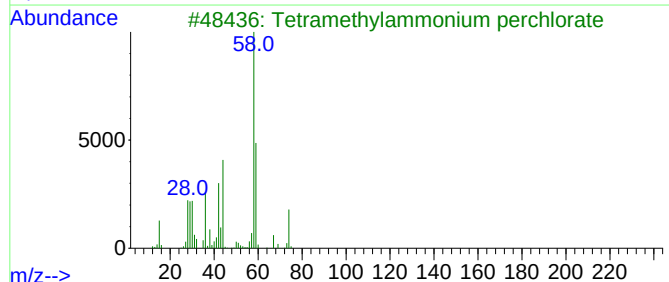
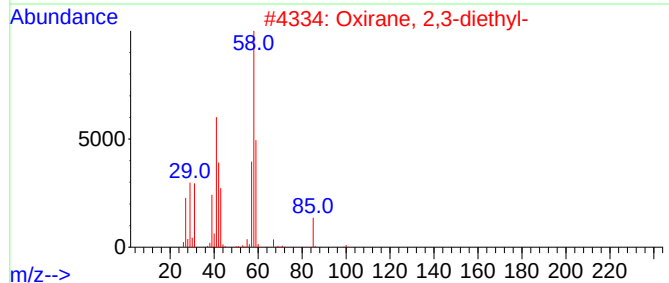
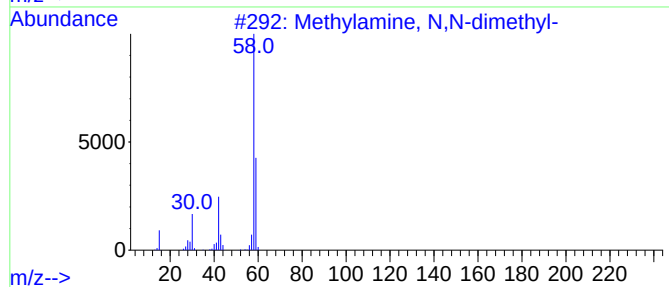
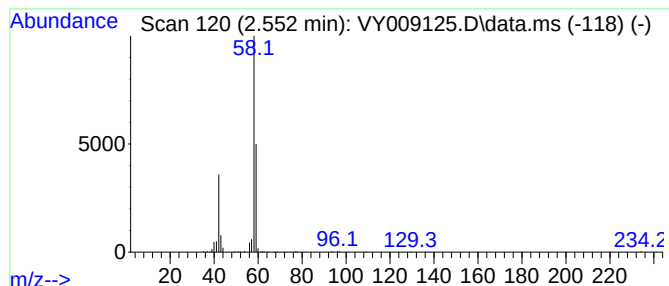
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052022S.M
Quant Title : SW846 8260

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

Peak Number 1 Methylamine, N,N-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.552	14.14 ug/l	111303	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	86
2			Oxirane, 2,3-diethyl-	100	C6H12O	004468-66-0	43
3			Tetramethylammonium perchlorate	173	C4H12ClNO4	002537-36-2	43
4			Sulfur trioxide trimethylamine c...	139	C3H9NO3S	003162-58-1	40
5			Butanoic acid, 4-(dimethylamino)...	147	C6H13NO3	003688-46-8	9



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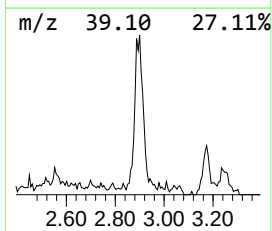
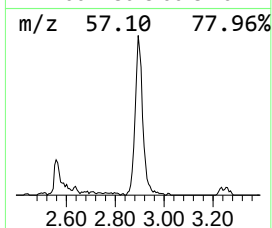
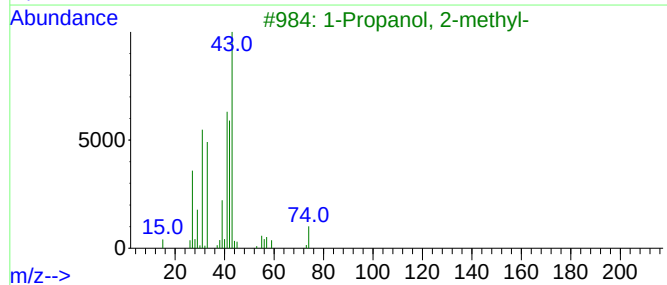
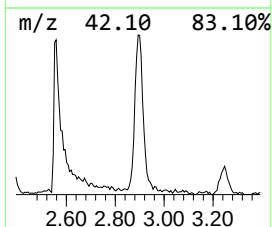
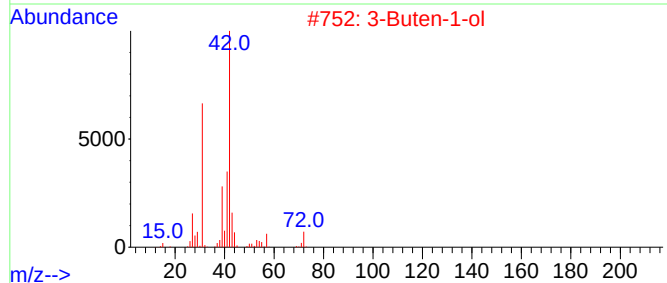
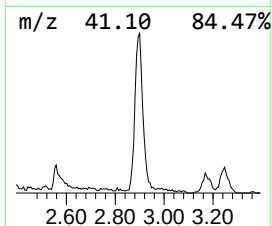
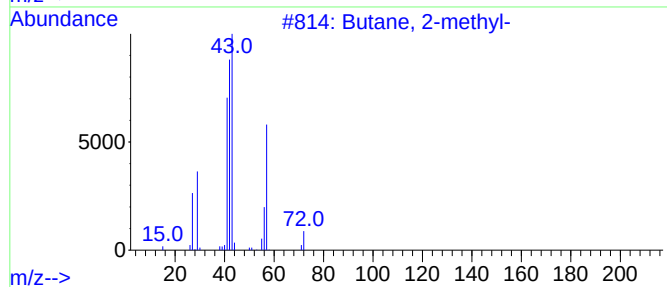
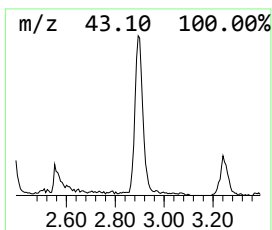
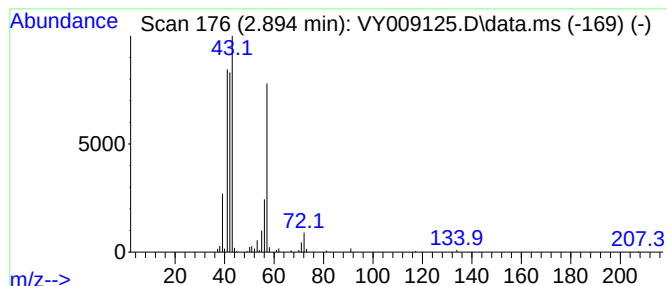
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052022S.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.894	14.10 ug/l	111055	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			3-Buten-1-ol	72	C4H8O	000627-27-0	43
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	36
4			Pentane	72	C5H12	000109-66-0	28
5			1-Butene	56	C4H8	000106-98-9	10



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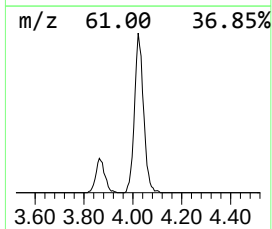
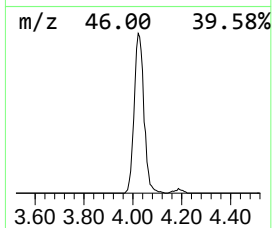
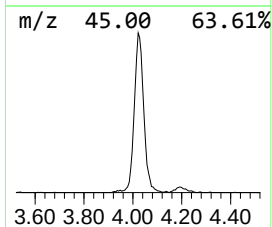
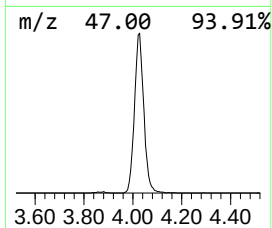
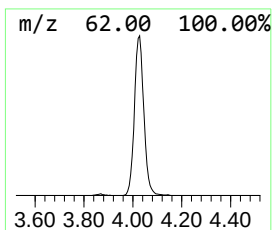
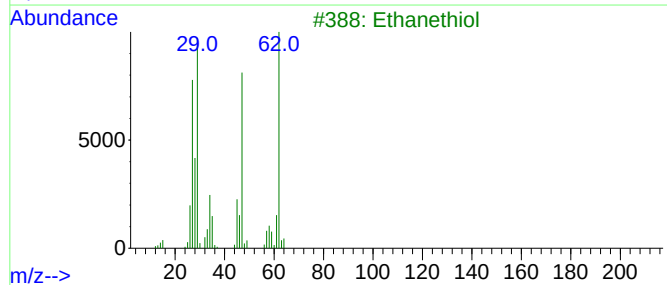
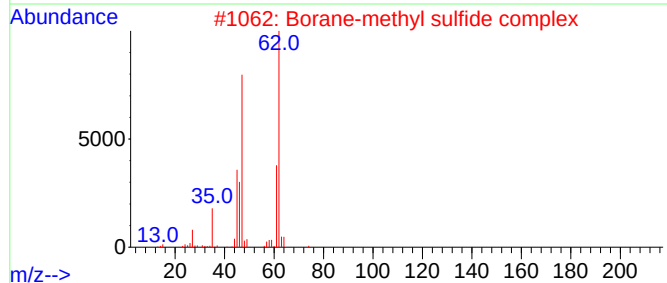
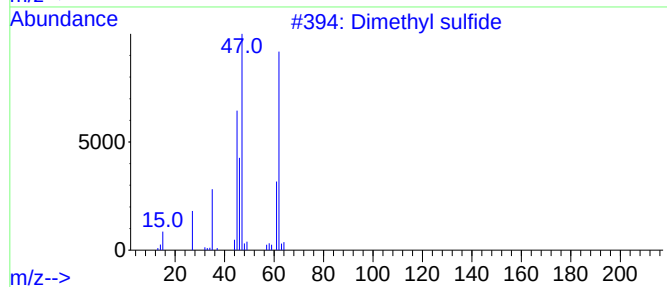
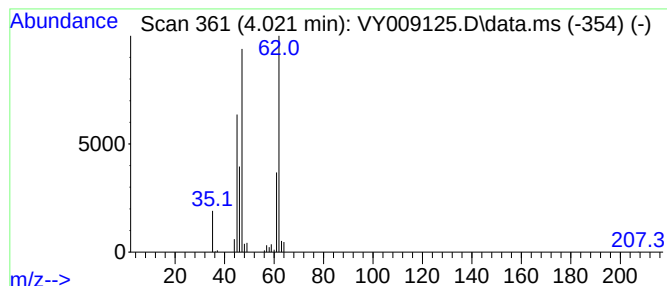
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052022S.M
Quant Title : SW846 8260

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

Peak Number 3 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.021	48.21 ug/l	379613	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	95
2			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90
3			Ethanethiol	62	C2H6S	000075-08-1	80
4			Ethene, chloro-	62	C2H3Cl	000075-01-4	9
5			Propane, 2-fluoro-	62	C3H7F	000420-26-8	9



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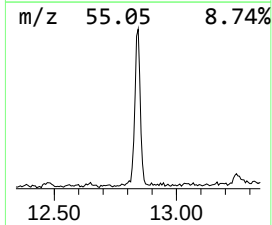
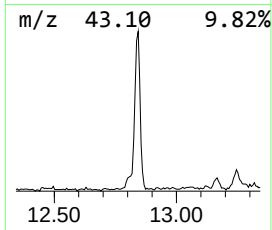
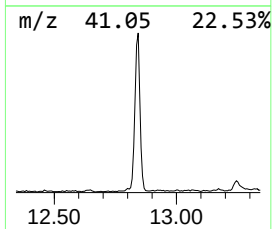
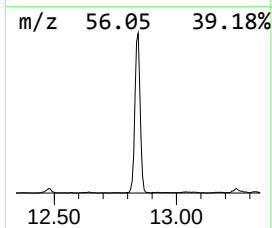
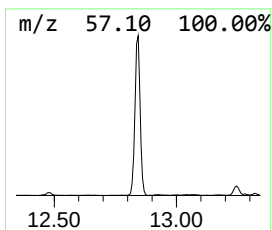
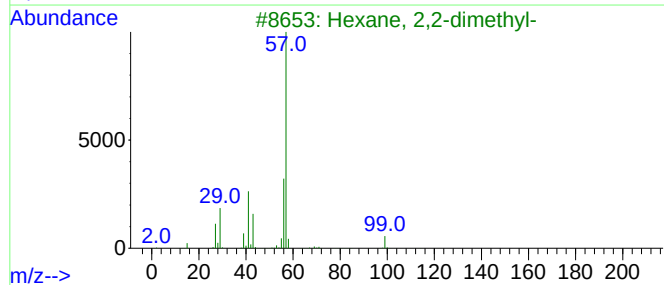
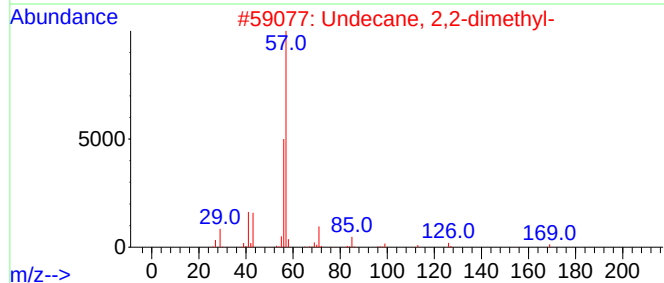
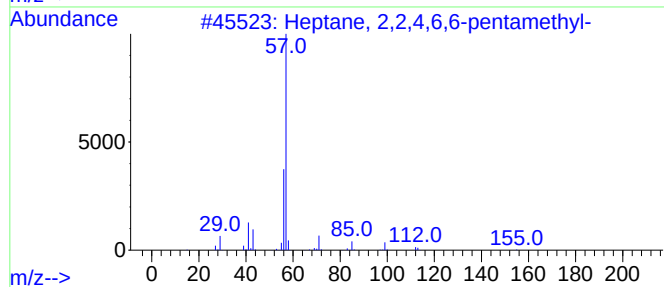
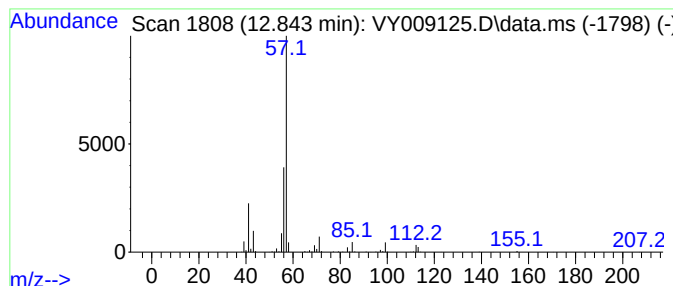
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Quant Title : SW846 8260

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

Peak Number 5 Heptane, 2,2,4,6,6-pentamet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.843	38.87 ug/l	431723	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	83
2			Undecane, 2,2-dimethyl-	184	C13H28	017312-64-0	78
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
4			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
5			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	64



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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
Methylamine, N,...	2.552	14.1	ug/l	111303	1	7.789	393675	50.0
Butane, 2-methyl-	2.894	14.1	ug/l	111055	1	7.789	393675	50.0
Dimethyl sulfide	4.021	48.2	ug/l	379613	1	7.789	393675	50.0
Heptane, 2,2,4,...	12.843	38.9	ug/l	431723	4	13.428	555378	50.0