

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD073021\
 Data File : VD069940.D
 Acq On : 30 Jul 2021 16:54
 Operator : VA/SY
 Sample : M3241-02
 Misc : 5.00G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 20210592-AMENDED-COM-6

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_D\Method\82D072221S.M
 Title : SW846 8260

Signal : TIC: VD069940.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.156	370	380	384	rBV2	21301	47849	1.40%	0.222%
2	4.238	387	394	406	rVB2	60353	168382	4.91%	0.781%
3	4.409	413	423	436	rBV	71355	214892	6.27%	0.997%
4	4.962	504	517	530	rBV3	70511	227140	6.63%	1.053%
5	5.985	683	691	693	rBV3	20196	38415	1.12%	0.178%
6	7.197	890	897	904	rBV5	12578	35870	1.05%	0.166%
7	7.914	1009	1019	1024	rBV	434610	1036176	30.23%	4.805%
8	7.979	1024	1030	1040	rVB	729231	1644658	47.97%	7.627%
9	8.326	1080	1089	1102	rVB	455009	1069729	31.20%	4.961%
10	8.861	1172	1180	1198	rBV	1189440	2400541	70.02%	11.133%
11	9.908	1350	1358	1365	rBV6	20097	46185	1.35%	0.214%
12	10.338	1423	1431	1446	rBV	1921730	3428183	100.00%	15.898%
13	11.638	1644	1652	1661	rBV	1570491	2744303	80.05%	12.727%
14	11.826	1679	1684	1689	rBV6	18231	41337	1.21%	0.192%
15	11.891	1689	1695	1701	rVV3	27809	58772	1.71%	0.273%
16	12.144	1731	1738	1746	rBV8	46439	135470	3.95%	0.628%
17	12.261	1749	1758	1763	rVB4	63316	132418	3.86%	0.614%
18	12.373	1763	1777	1785	rBV7	92711	345487	10.08%	1.602%
19	12.467	1785	1793	1796	rBV8	41045	99914	2.91%	0.463%
20	12.626	1812	1820	1827	rVB	1230301	2083104	60.76%	9.661%
21	12.714	1827	1835	1840	rBV10	42293	125547	3.66%	0.582%
22	12.791	1840	1848	1855	rVB7	88531	249939	7.29%	1.159%
23	12.873	1855	1862	1868	rBV6	63965	195333	5.70%	0.906%
24	12.949	1868	1875	1889	rVB10	88481	353667	10.32%	1.640%
25	13.091	1891	1899	1903	rBV5	47350	108159	3.15%	0.502%
26	13.132	1903	1906	1910	rVV4	29032	42971	1.25%	0.199%
27	13.202	1915	1918	1926	rVB3	96041	168826	4.92%	0.783%
28	13.273	1926	1930	1931	rBV3	31641	38500	1.12%	0.179%
29	13.308	1932	1936	1940	rVV2	48036	73644	2.15%	0.342%
30	13.426	1951	1956	1959	rBV	119950	187258	5.46%	0.868%
31	13.491	1965	1967	1972	rVB5	34027	39826	1.16%	0.185%
32	13.567	1973	1980	1985	rVV	1319158	2219260	64.74%	10.292%
33	13.614	1985	1988	1997	rVB2	139674	293433	8.56%	1.361%
34	13.708	2001	2004	2008	rVB4	44915	59302	1.73%	0.275%
35	13.779	2014	2016	2021	rVB5	37265	43214	1.26%	0.200%
36	13.891	2029	2035	2039	rBV6	96749	176165	5.14%	0.817%

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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	14.091	2061	2069	2073	rBV5	65278	165045	4.81%	0.765%
38	14.143	2073	2078	2085	rVB	299311	494979	14.44%	2.296%
39	14.208	2085	2089	2093	rBV7	35354	54714	1.60%	0.254%
40	14.279	2096	2101	2107	rVB9	44270	85371	2.49%	0.396%
41	14.396	2116	2121	2124	rBV5	69811	132591	3.87%	0.615%
42	14.514	2137	2141	2144	rBV6	37190	65726	1.92%	0.305%
43	15.085	2234	2238	2245	rVB9	22127	34967	1.02%	0.162%
44	15.355	2280	2284	2291	rBV8	35386	55486	1.62%	0.257%
45	15.767	2348	2354	2360	rVB8	29428	64799	1.89%	0.301%
46	16.326	2447	2449	2455	rVB6	23321	35404	1.03%	0.164%

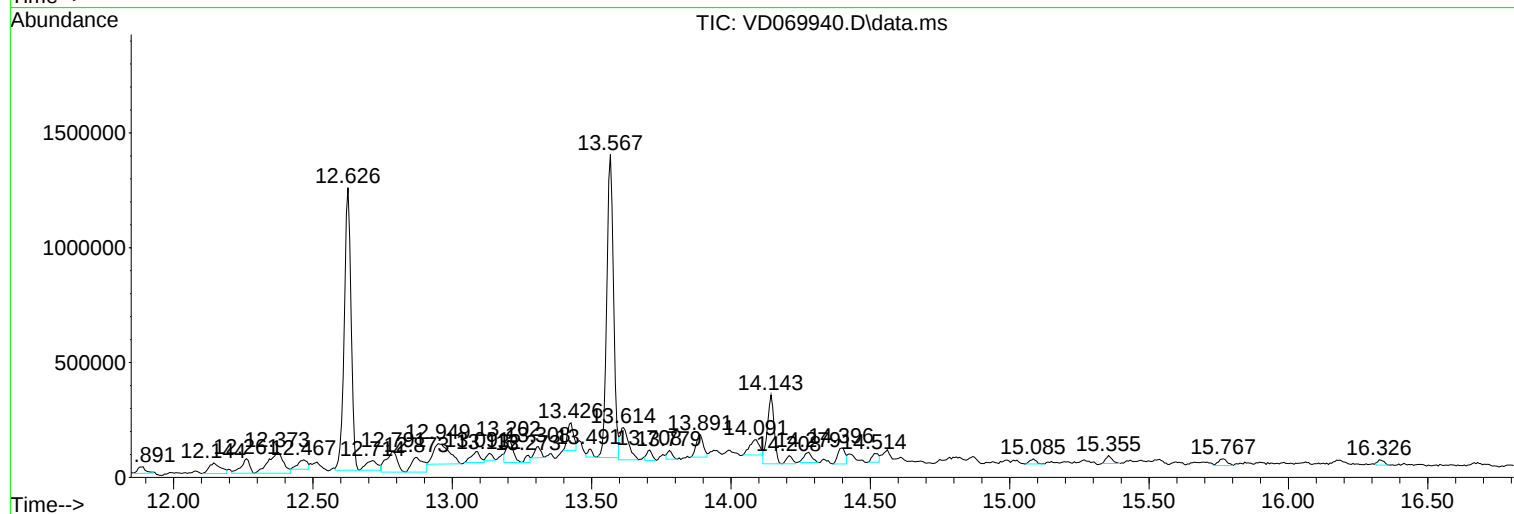
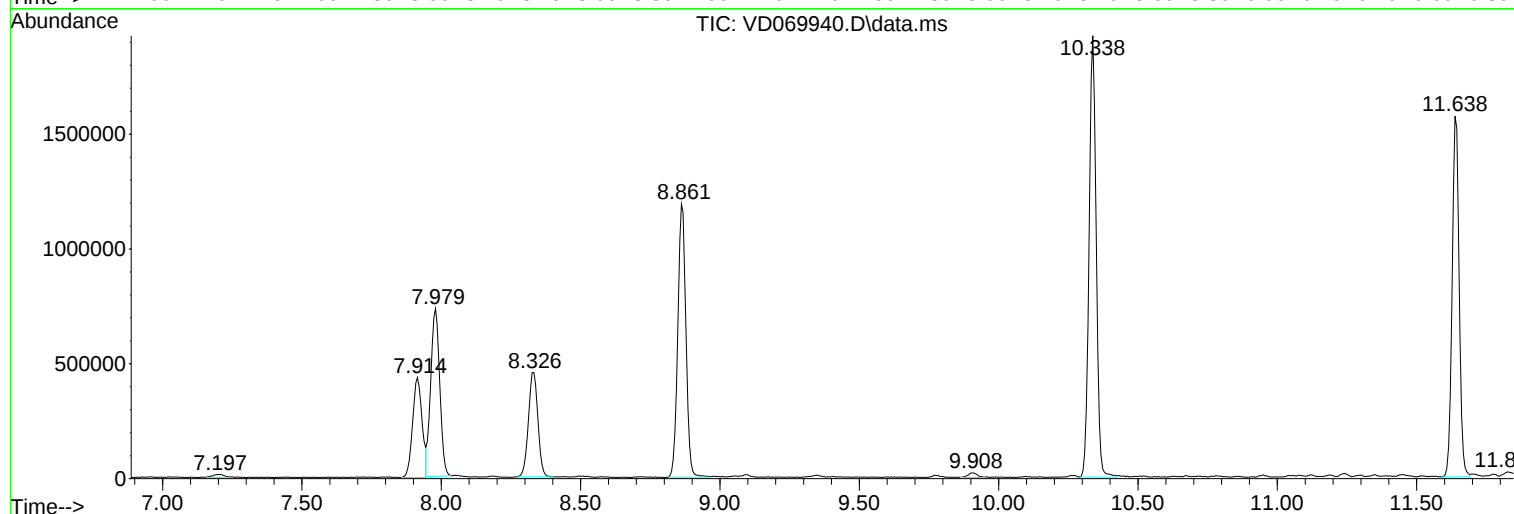
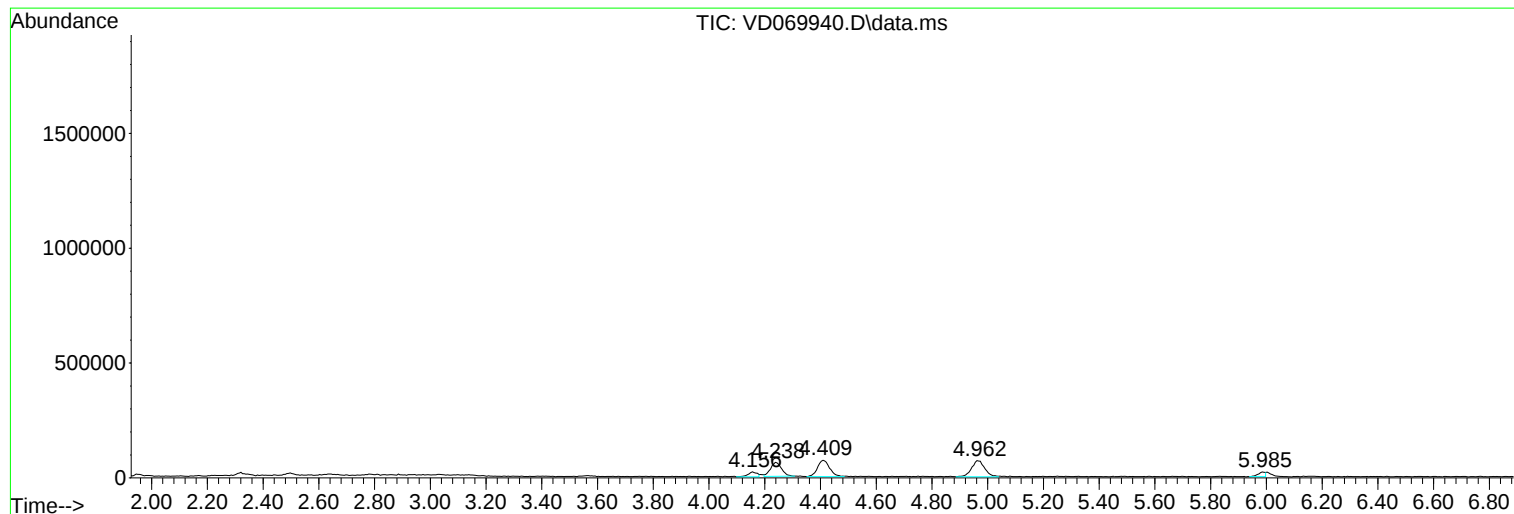
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D072221S.M
Quant Title : SW846 8260

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



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20210592-AMENDED-COM-6

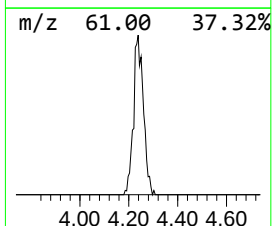
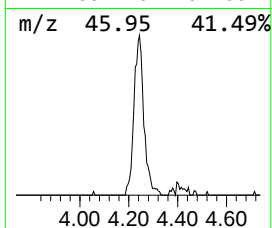
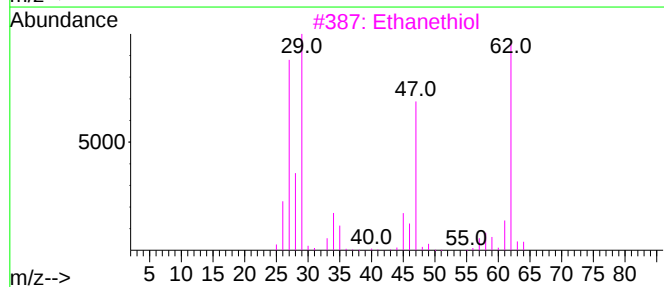
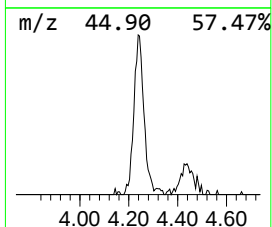
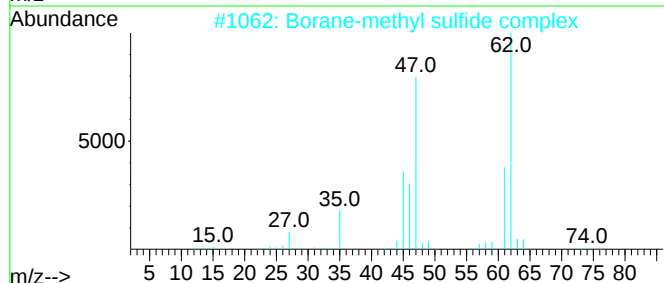
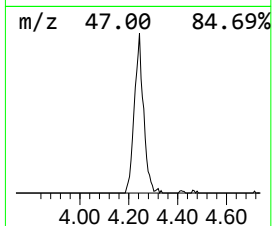
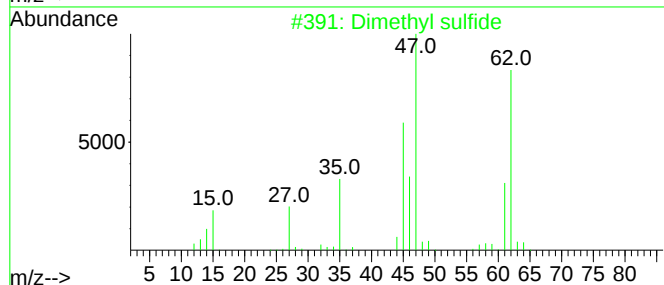
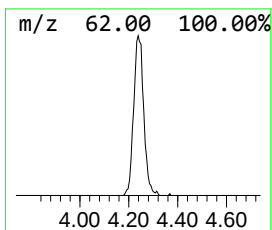
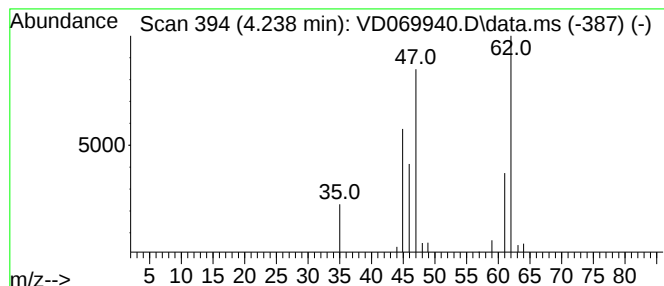
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D072221S.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl sulfide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.238	5.12 ug/l	168382	Pentafluorobenzene	7.979

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	86
3			Ethanethiol	62	C2H6S	000075-08-1	64
4			Boric acid	62	BH3O3	010043-35-3	5
5			Ethene, chloro-	62	C2H3Cl	000075-01-4	5



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Instrument :
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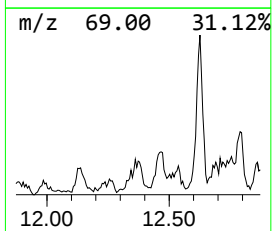
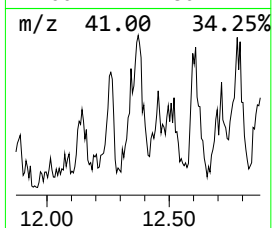
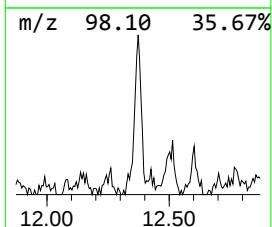
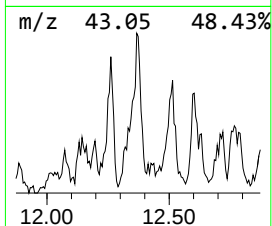
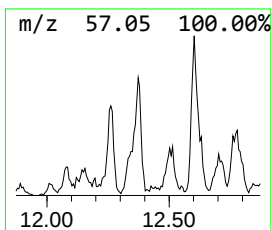
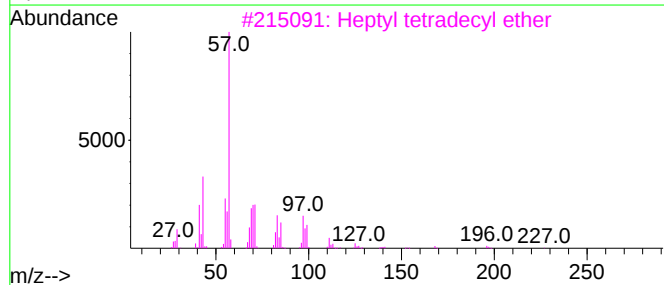
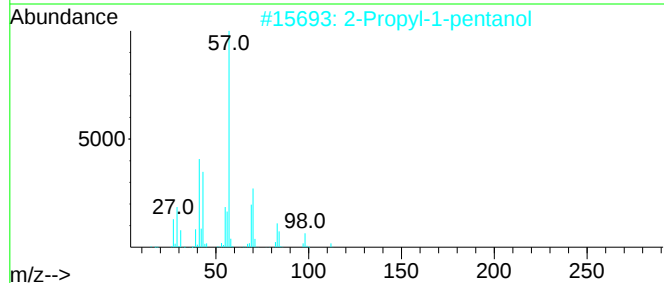
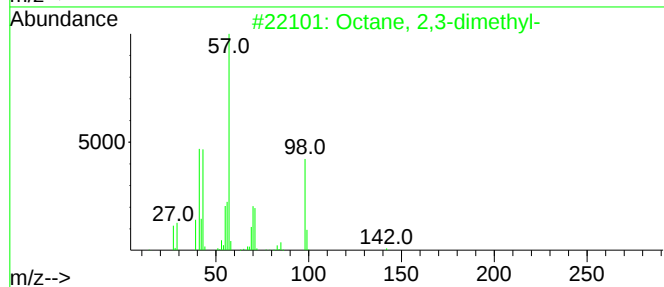
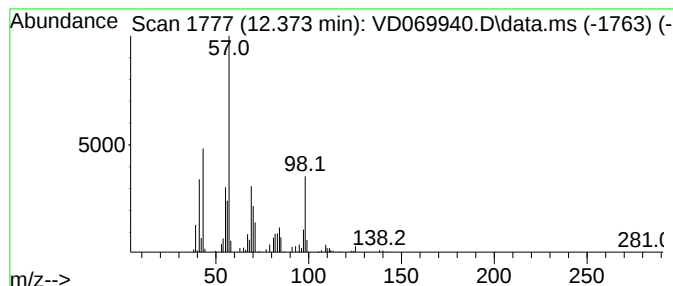
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D072221S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown12.373 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.373	6.29 ug/l	345487	Chlorobenzene-d5	11.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,3-dimethyl-		142	C10H22	007146-60-3	43	
2	2-Propyl-1-pentanol		130	C8H18O	058175-57-8	43	
3	Heptyl tetradecyl ether		312	C21H44O	1000406-39-3	35	
4	2-Methyl-1-undecanol		186	C12H26O	010522-26-6	35	
5	Heptyl octadecyl ether		368	C25H52O	1000406-39-5	27	



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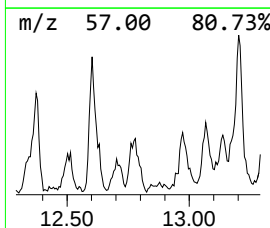
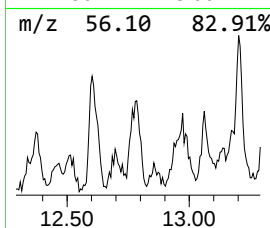
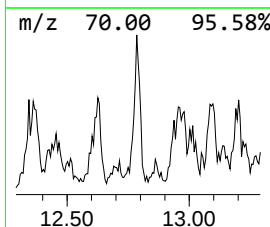
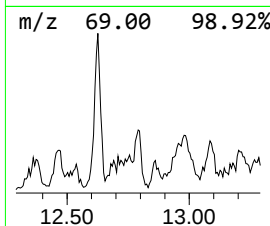
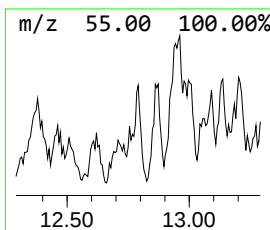
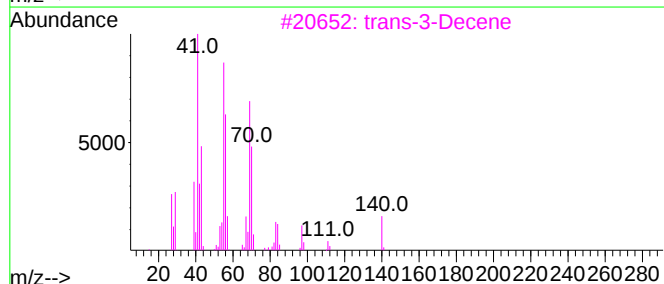
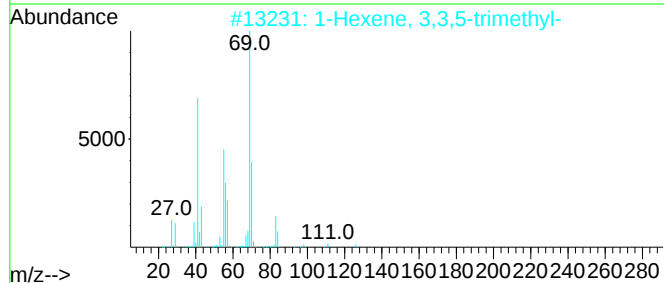
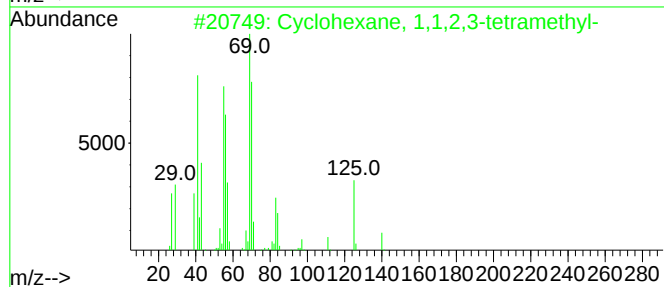
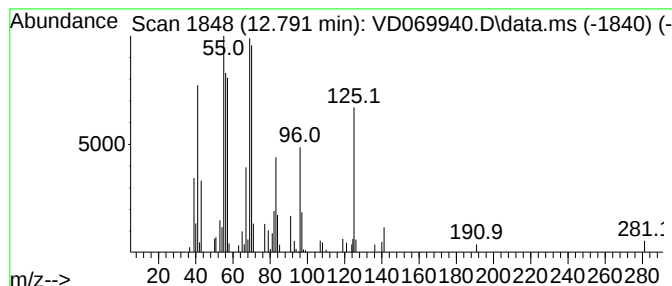
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Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, 1,1,2,3-tetram... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.791	5.63 ug/l	249939	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	50
2			1-Hexene, 3,3,5-trimethyl-	126	C9H18	013427-43-5	43
3			trans-3-Decene	140	C10H20	019150-21-1	43
4			3-Octene, 2,6-dimethyl-	140	C10H20	006874-28-8	43
5			3-Undecene, 10-methyl-	168	C12H24	1000061-84-5	43



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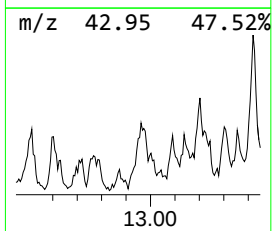
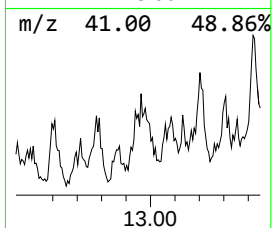
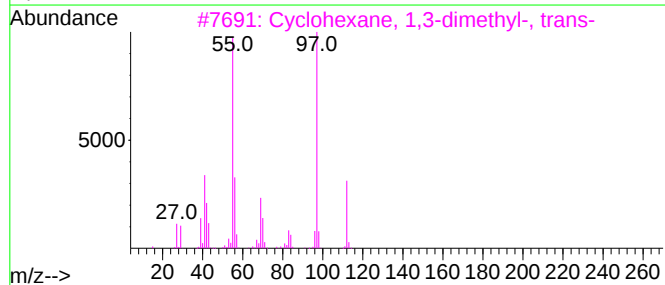
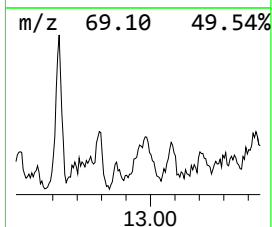
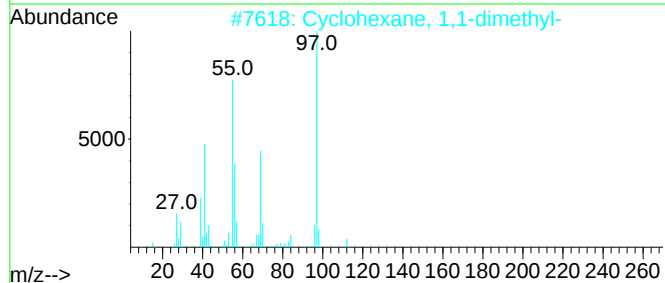
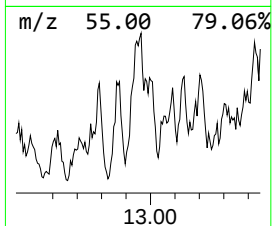
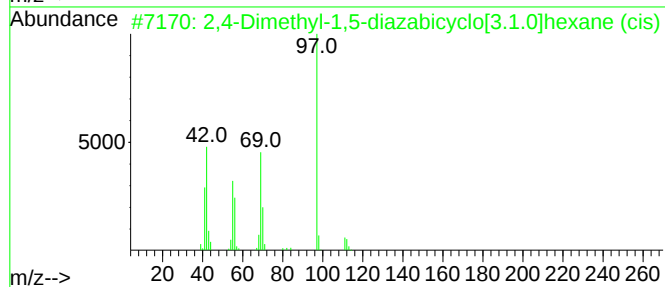
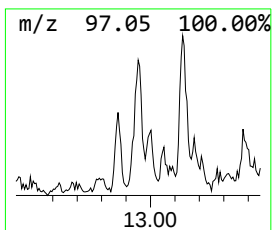
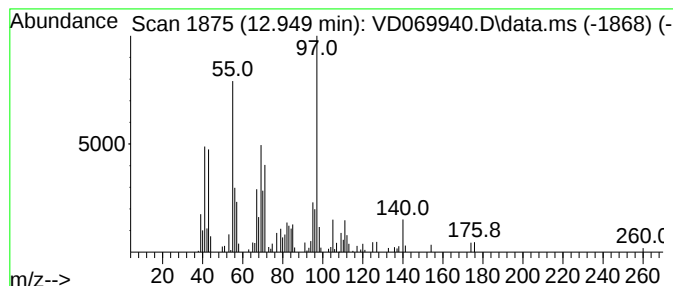
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown12.949 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.949	7.97 ug/l	353667	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dimethyl-1,5-diazabicyclo[3.3.1]nonane	112	C6H12N2	100463-01-2	43
2			Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	43
3			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	43
4			Ethanone, 1-(3,4-dihydro-6-methoxyphenyl)-	140	C8H12O2	028450-02-4	38
5			Oxazole, 4,5-dimethyl-	97	C5H7NO	020662-83-3	38



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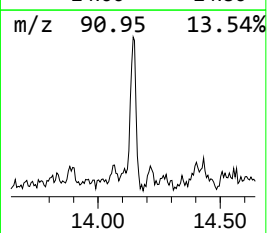
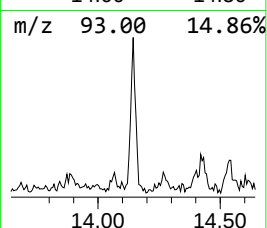
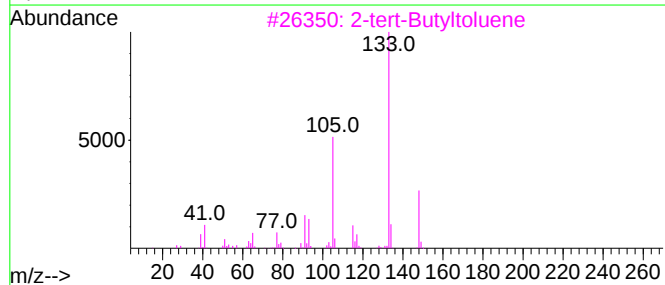
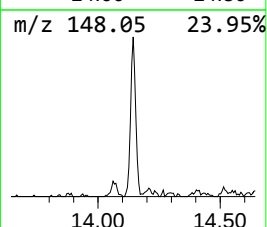
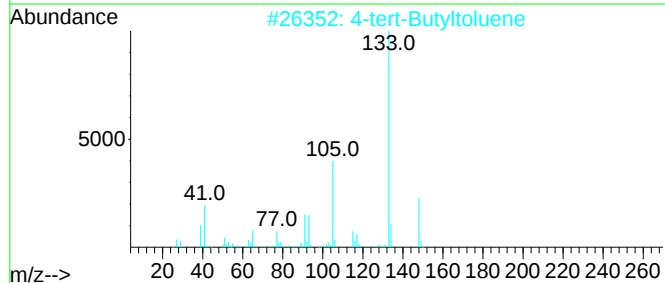
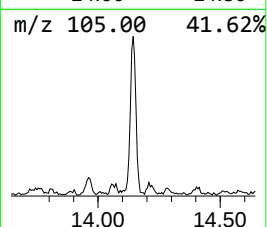
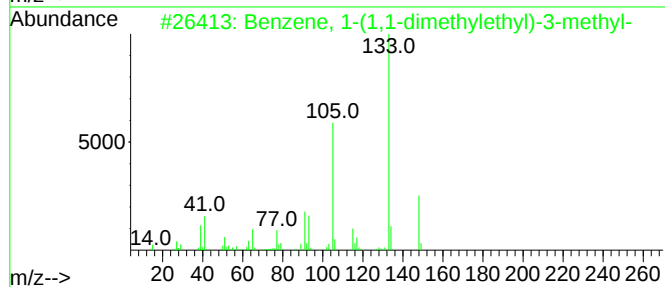
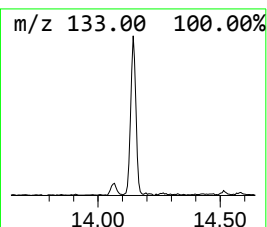
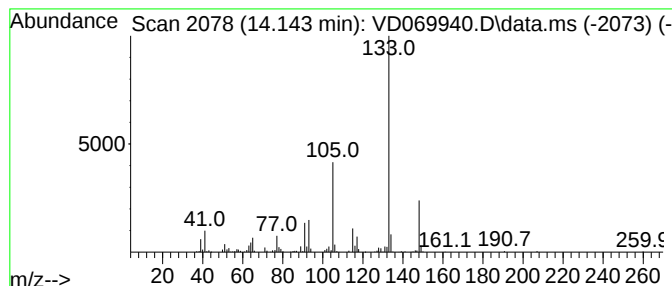
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D072221S.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-(1,1-dimethyleth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.144	11.15 ug/l	494979	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-(1,1-dimethylethyl)-3...	148	C11H16	001075-38-3	97
2			4-tert-Butyltoluene	148	C11H16	000098-51-1	95
3			2-tert-Butyltoluene	148	C11H16	001074-92-6	95
4			Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	81
5			3,4-Dimethylcumene	148	C11H16	1000370-34-1	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD073021\
Data File : VD069940.D
Acq On : 30 Jul 2021 16:54
Operator : VA/SY
Sample : M3241-02
Misc : 5.00G/5.00ml/MSVOA_D/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
20210592-AMENDED-COM-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D072221S.M
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
Dimethyl sulfide	4.238	5.1	ug/l	168382	1	7.979	1644660	50.0
unknown12.373	12.373	6.3	ug/l	345487	3	11.638	2744300	50.0
Cyclohexane, 1,...	12.791	5.6	ug/l	249939	4	13.567	2219260	50.0
unknown12.949	12.949	8.0	ug/l	353667	4	13.567	2219260	50.0
Benzene, 1-(1,1...	14.144	11.2	ug/l	494979	4	13.567	2219260	50.0