

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072621\
 Data File : VY005451.D
 Acq On : 26 Jul 2021 17:45
 Operator : SY/MD
 Sample : M3176-01
 Misc : 6.04G/5ML/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 18-B7-TP-(9.5-12)

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\82Y072221S.M
 Title : SW846 8260

Signal : TIC: VY005451.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.967	342	352	359	rBV2	7359	20030	1.59%	0.230%
2	4.729	466	477	494	rBV3	13094	45625	3.63%	0.525%
3	7.728	959	969	974	rBV	148562	359833	28.62%	4.137%
4	7.795	974	980	993	rVB	247219	562182	44.72%	6.464%
5	8.149	1027	1038	1050	rBV	167954	364907	29.03%	4.195%
6	8.697	1119	1128	1139	rBV	405908	789291	62.78%	9.075%
7	9.191	1197	1209	1214	rBV4	5461	13814	1.10%	0.159%
8	9.966	1326	1336	1345	rBV7	3679	13176	1.05%	0.151%
9	10.185	1364	1372	1387	rBV	696307	1176538	93.59%	13.527%
10	10.721	1455	1460	1468	rVV5	9371	15371	1.22%	0.177%
11	11.038	1504	1512	1516	rBV3	9977	16042	1.28%	0.184%
12	11.093	1516	1521	1527	rVB2	17558	27766	2.21%	0.319%
13	11.295	1544	1554	1564	rVB4	11444	33733	2.68%	0.388%
14	11.380	1564	1568	1574	rBV2	8675	14785	1.18%	0.170%
15	11.496	1579	1587	1596	rBV	613047	1015942	80.81%	11.681%
16	11.709	1612	1622	1624	rBV5	13745	34352	2.73%	0.395%
17	11.740	1625	1627	1632	rVB2	12714	17820	1.42%	0.205%
18	12.008	1664	1671	1678	rBV6	24183	66872	5.32%	0.769%
19	12.124	1686	1690	1694	rVB2	18683	26346	2.10%	0.303%
20	12.209	1699	1704	1706	rVV4	21827	36489	2.90%	0.420%
21	12.239	1706	1709	1715	rVB5	23077	47275	3.76%	0.544%
22	12.337	1720	1725	1729	rBV3	22715	37801	3.01%	0.435%
23	12.489	1742	1750	1758	rVB2	711595	1257156	100.00%	14.454%
24	12.648	1770	1776	1784	rVB4	44446	96763	7.70%	1.113%
25	12.733	1784	1790	1794	rBV7	20647	49548	3.94%	0.570%
26	12.813	1796	1803	1809	rBV5	62373	132539	10.54%	1.524%
27	12.953	1822	1826	1829	rBV6	18447	29110	2.32%	0.335%
28	13.044	1837	1841	1849	rVB2	47946	89234	7.10%	1.026%
29	13.123	1849	1854	1859	rBV	32679	60268	4.79%	0.693%
30	13.300	1878	1883	1884	rVV3	14955	25208	2.01%	0.290%
31	13.319	1884	1886	1890	rVV3	25671	34966	2.78%	0.402%
32	13.367	1891	1894	1897	rVB3	16117	20066	1.60%	0.231%
33	13.428	1898	1904	1913	rVV	588029	886707	70.53%	10.195%
34	13.569	1923	1927	1929	rBV4	9940	14734	1.17%	0.169%
35	13.623	1933	1936	1941	rVV3	18120	33155	2.64%	0.381%
36	13.666	1941	1943	1951	rVB3	14179	23410	1.86%	0.269%

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	13.751	1952	1957	1962	rBV3	69578	114374	9.10%	1.315%
38	13.916	1981	1984	1988	rVV2	15506	19658	1.56%	0.226%
39	13.971	1988	1993	1998	rVB2	53289	87994	7.00%	1.012%
40	14.081	2006	2011	2016	rBV3	30365	50260	4.00%	0.578%
41	14.135	2016	2020	2028	rVV7	15022	37782	3.01%	0.434%
42	14.215	2028	2033	2036	rVV	13633	28516	2.27%	0.328%
43	14.264	2036	2041	2051	rVV8	25657	102551	8.16%	1.179%
44	14.337	2051	2053	2057	rVV	18628	22059	1.75%	0.254%
45	14.385	2057	2061	2064	rVV3	24353	36573	2.91%	0.420%
46	14.422	2064	2067	2071	rVB4	21595	30786	2.45%	0.354%
47	14.617	2095	2099	2103	rVB	32988	45700	3.64%	0.525%
48	14.678	2103	2109	2115	rBV3	39020	86573	6.89%	0.995%
49	14.733	2115	2118	2124	rVB3	24865	41913	3.33%	0.482%
50	14.952	2149	2154	2157	rBV4	14953	22543	1.79%	0.259%
51	15.050	2166	2170	2176	rBV5	12606	26131	2.08%	0.300%
52	15.141	2181	2185	2191	rVB8	11317	23507	1.87%	0.270%
53	15.239	2192	2201	2207	rBV	125974	237305	18.88%	2.728%
54	15.343	2214	2218	2222	rBV5	8441	14534	1.16%	0.167%
55	15.434	2230	2233	2242	rVB4	15040	26254	2.09%	0.302%
56	15.532	2243	2249	2256	rBV4	7654	22408	1.78%	0.258%
57	15.684	2269	2274	2278	rBV7	6066	13418	1.07%	0.154%
58	15.891	2303	2308	2316	rVB7	4741	13492	1.07%	0.155%
59	16.038	2326	2332	2338	rVB10	8223	15496	1.23%	0.178%
60	16.294	2369	2374	2380	rBV	20395	39244	3.12%	0.451%
61	16.495	2401	2407	2415	rBV	21739	49724	3.96%	0.572%

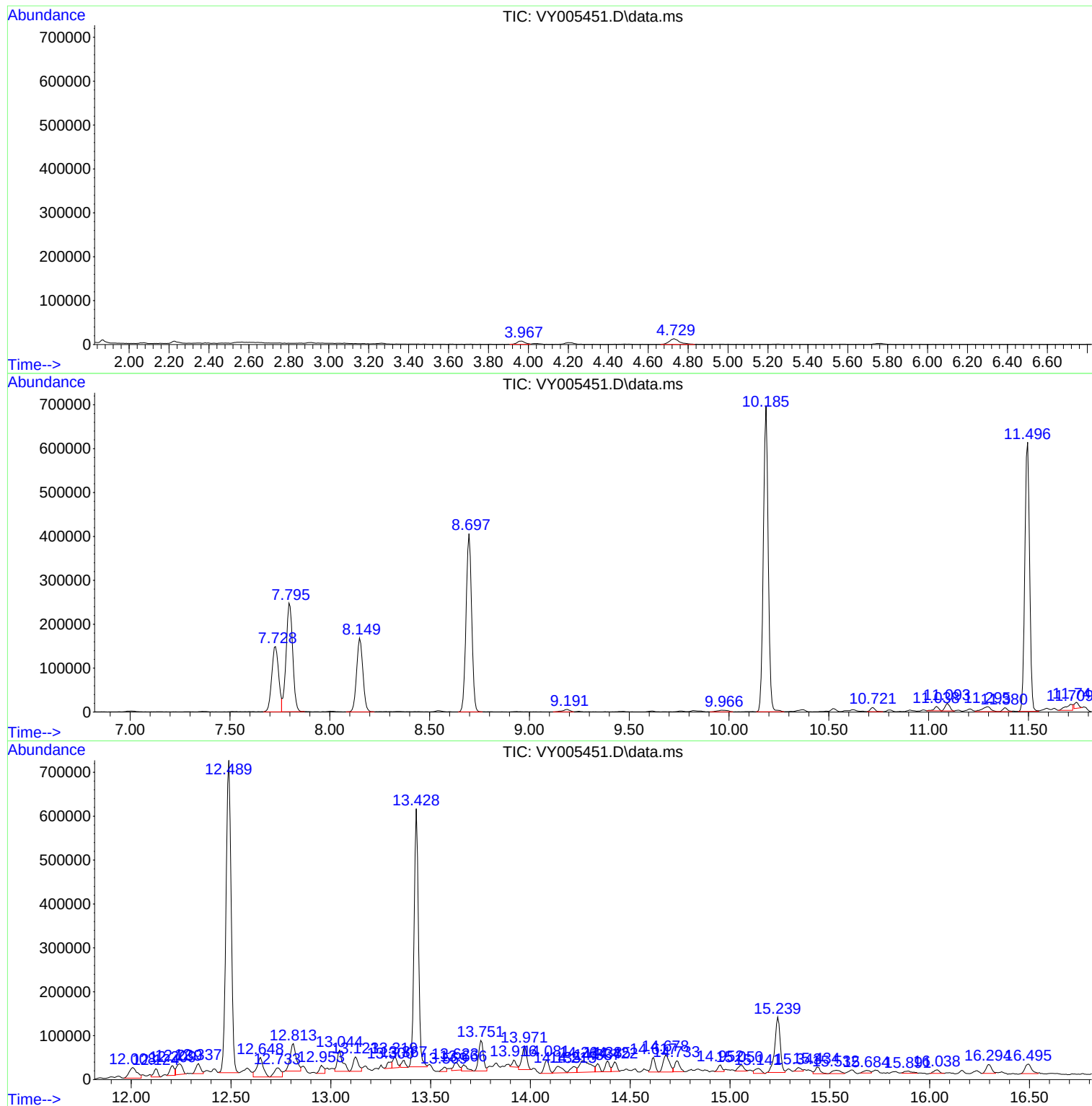
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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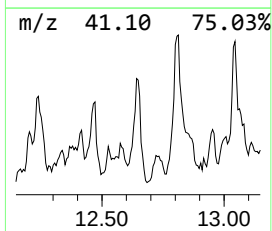
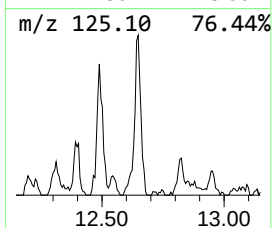
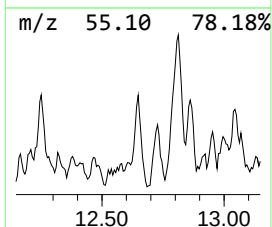
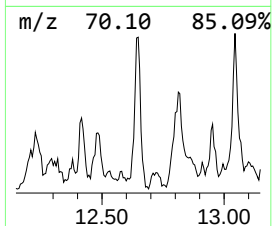
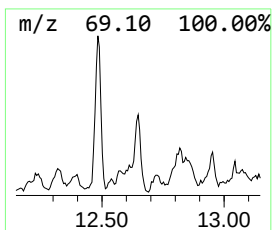
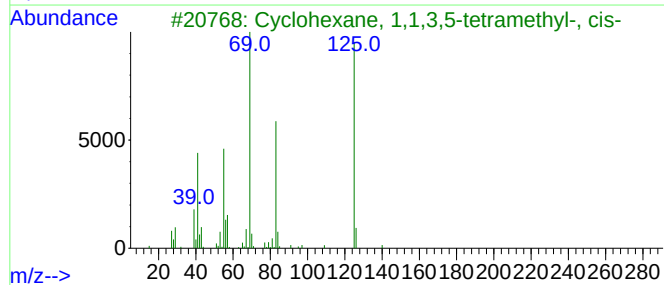
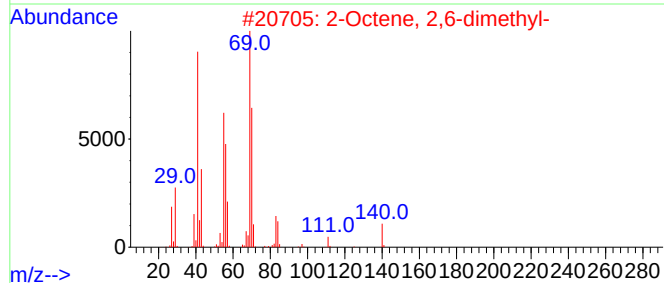
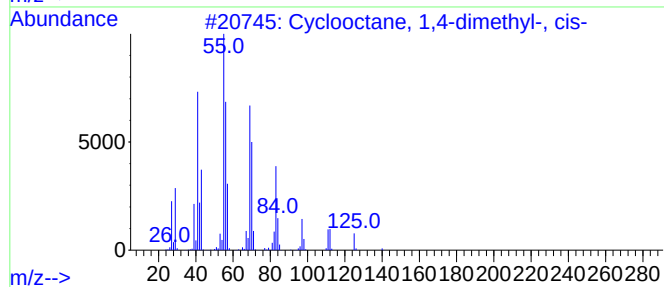
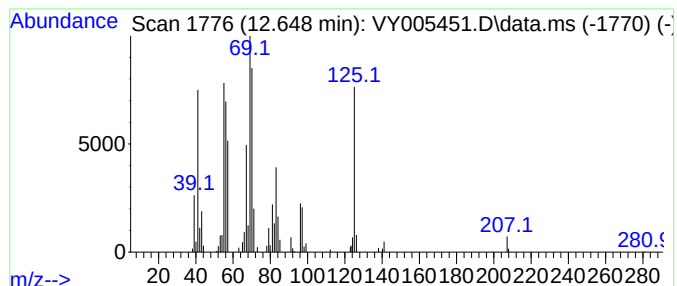
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072221S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown12.648 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.648	5.46 ug/l	96763	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	46
2			2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	43
3			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	43
4			Cyclohexane, 1,1'-(1-methylethyl...	208	C15H28	054934-90-6	38
5			4-Undecene, 2-methyl-, (E)-	168	C12H24	028665-57-8	38



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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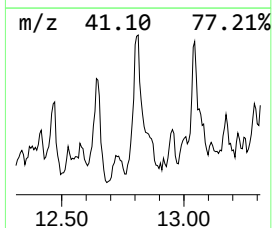
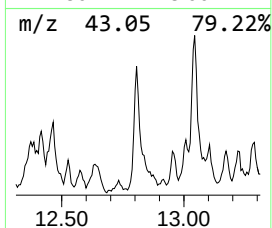
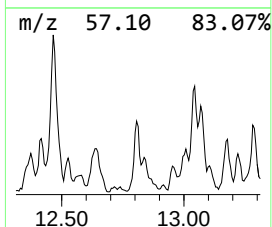
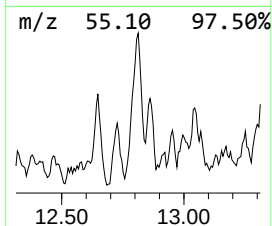
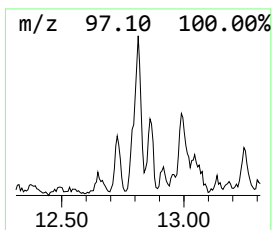
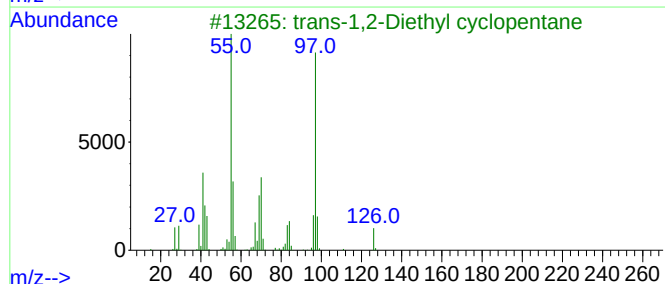
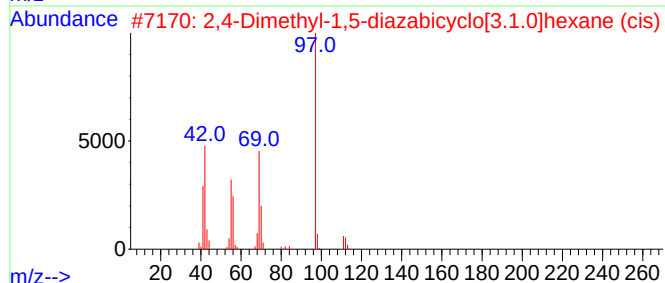
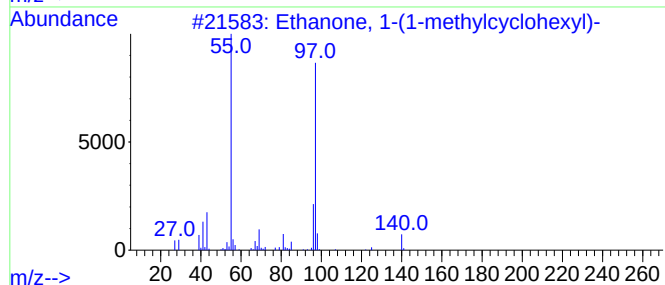
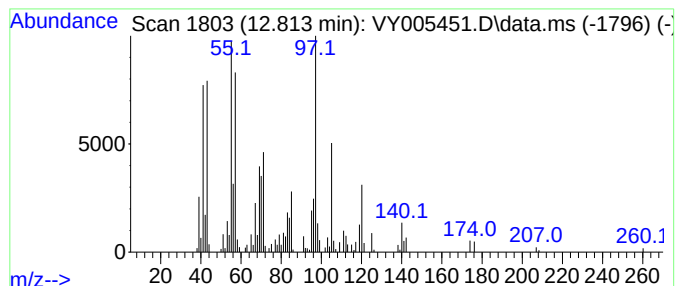
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072221S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.813 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.813	7.47 ug/l	132539	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(1-methylcyclohexyl)-	140	C9H16O	002890-62-2	43
2			2,4-Dimethyl-1,5-diazabicyclo[3.3.0]heptane	112	C6H12N2	100463-01-2	38
3			trans-1,2-Diethyl cyclopentane	126	C9H18	000932-40-1	38
4			Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	35
5			1-(Ethenesulfonyl)dodecane	260	C14H28O2S	030719-66-5	30



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Instrument :
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ClientSampleId :
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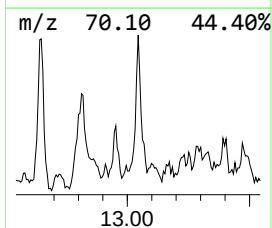
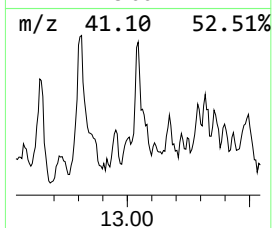
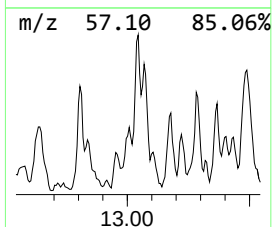
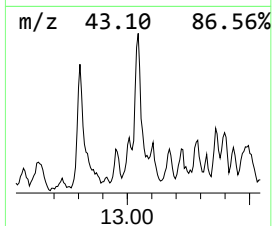
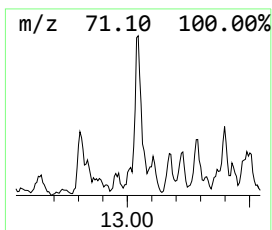
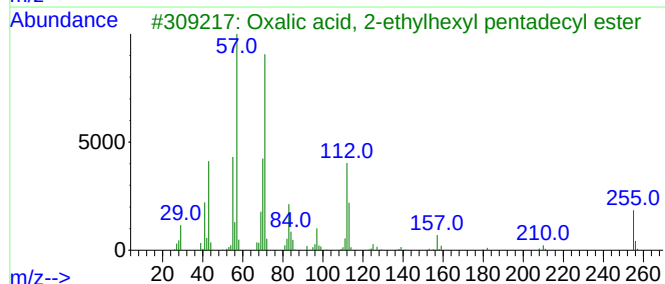
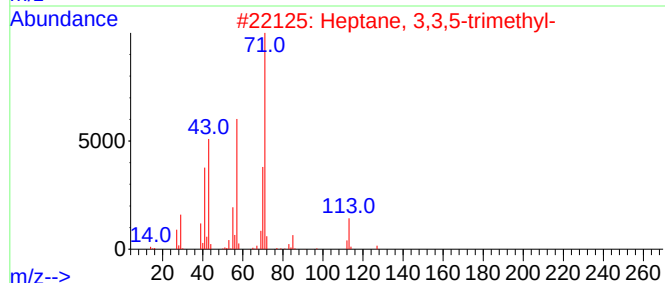
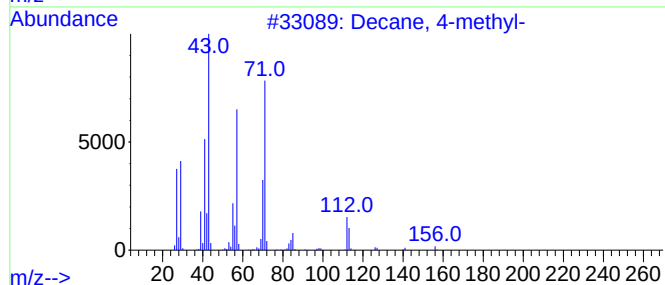
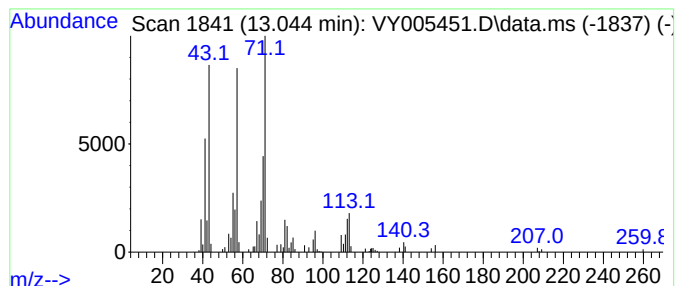
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072221S.M
Quant Title : SW846 8260

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

Peak Number 3 Decane, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.044	5.03 ug/l	89234	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 4-methyl-	156	C11H24	002847-72-5	72
2			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	64
3			Oxalic acid, 2-ethylhexyl pentadecyl ester	412	C25H48O4	1000309-39-8	59
4			Decane, 2,3,4-trimethyl-	184	C13H28	062238-15-7	53
5			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	53



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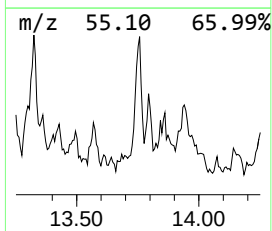
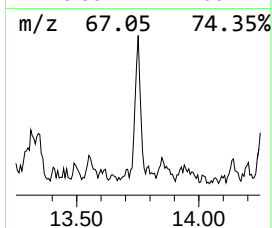
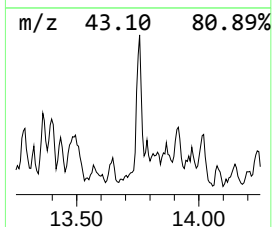
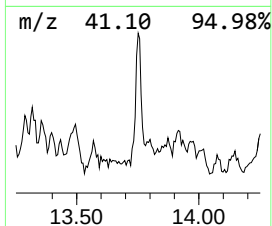
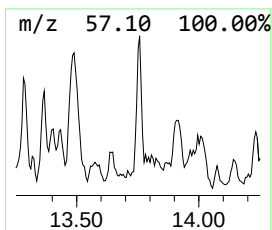
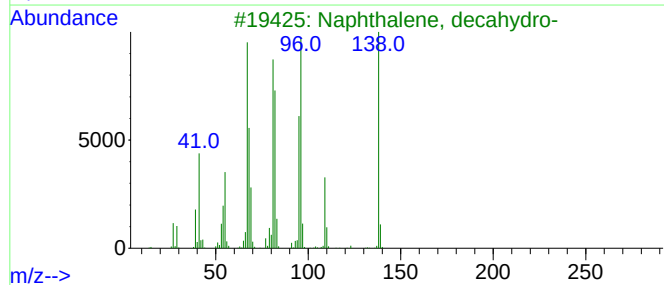
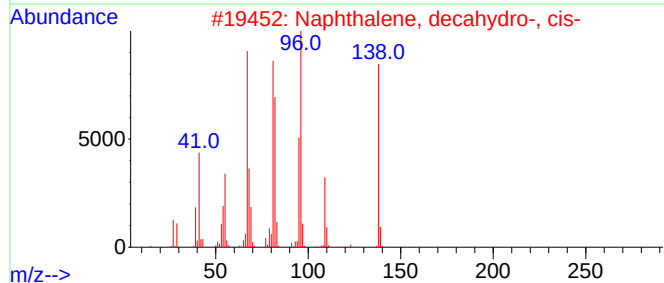
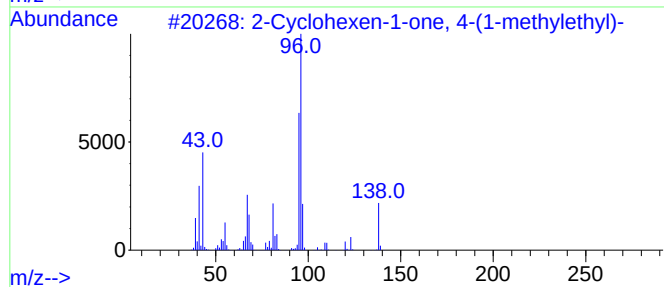
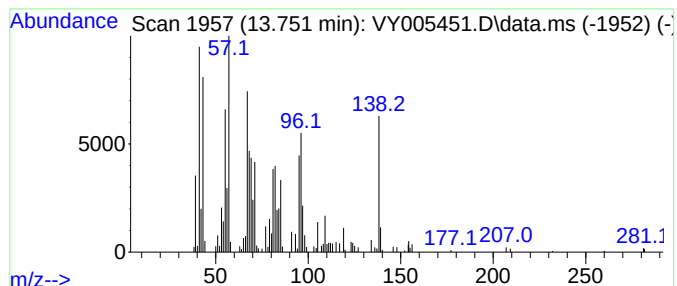
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072221S.M
Quant Title : SW846 8260

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

Peak Number 4 2-Cyclohexen-1-one, 4-(1-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	6.45 ug/l	114374	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one, 4-(1-methyle...	138	C9H14O	000500-02-7	58
2			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	58
3			Naphthalene, decahydro-	138	C10H18	000091-17-8	58
4			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	52
5			Spiro[4.4]nonan-2-one	138	C9H14O	034177-18-9	46



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ClientSampleId :
18-B7-TP-(9.5-12)

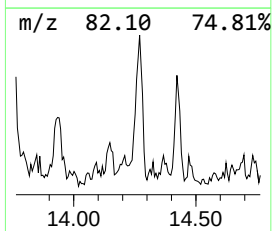
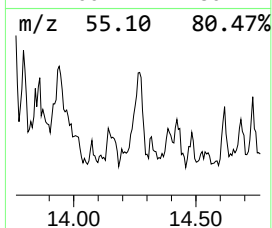
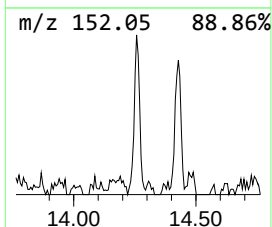
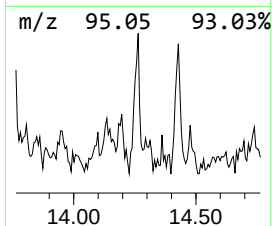
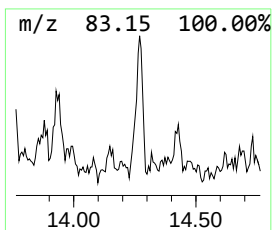
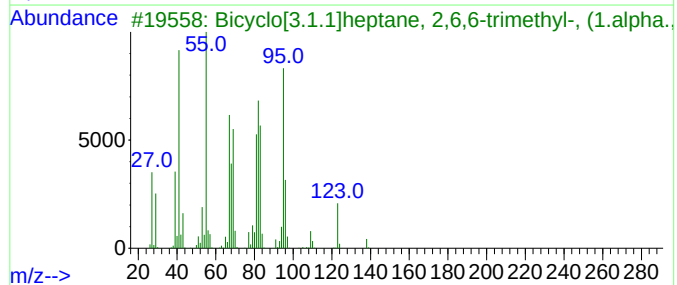
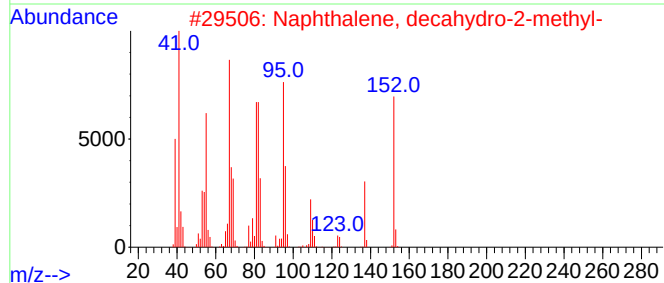
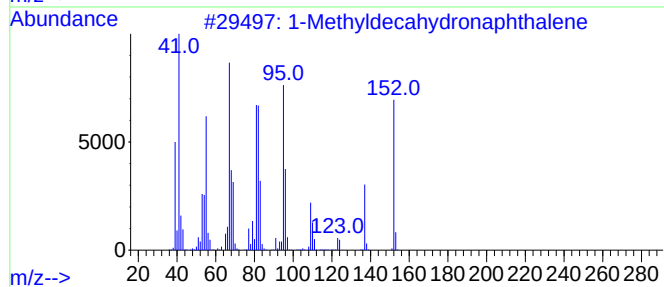
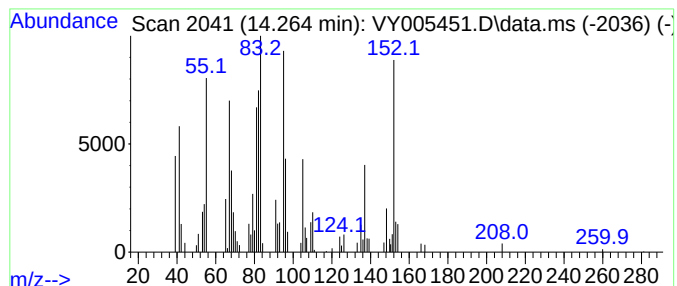
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Quant Title : SW846 8260

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

Peak Number 5 1-Methyldecahydronaphthalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.264	5.78 ug/l	102551	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	90
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	90
3			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	006876-13-7	55
4			(-)-trans-Pinane	138	C10H18	033626-25-4	55
5			Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-04-9	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072621\
Data File : VY005451.D
Acq On : 26 Jul 2021 17:45
Operator : SY/MD
Sample : M3176-01
Misc : 6.04G/5ML/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
18-B7-TP-(9.5-12)

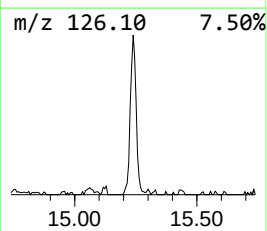
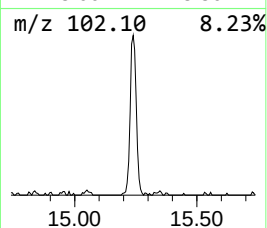
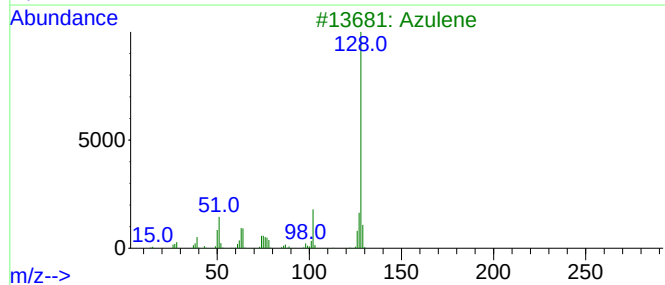
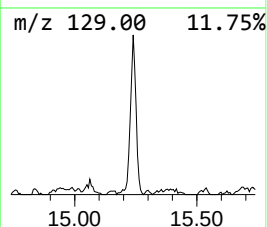
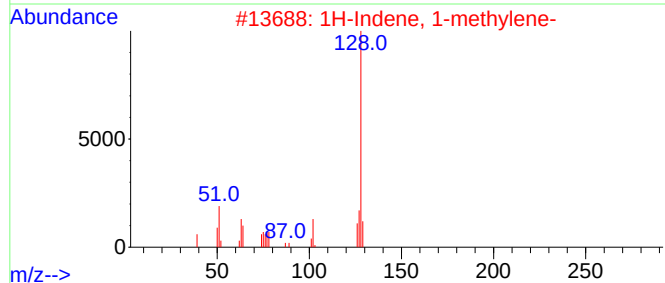
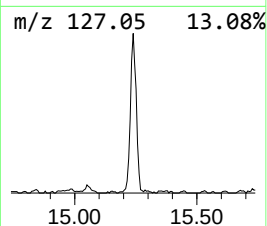
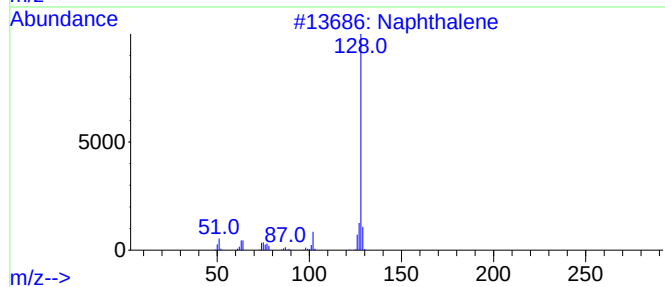
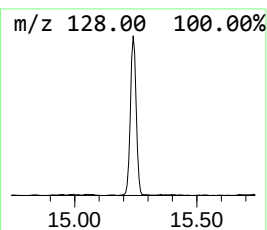
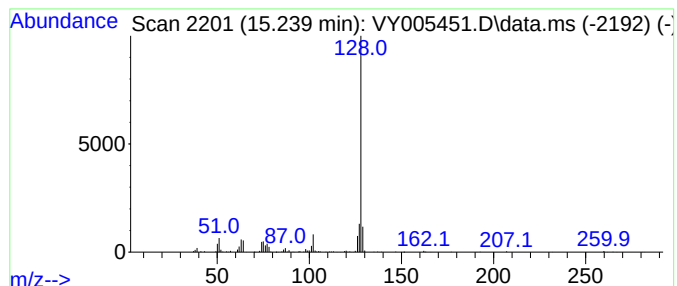
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072221S.M
Quant Title : SW846 8260

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

Peak Number 6 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.239	13.38 ug/l	237305	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	93
3			Azulene	128	C10H8	000275-51-4	91
4			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072621\
Data File : VY005451.D
Acq On : 26 Jul 2021 17:45
Operator : SY/MD
Sample : M3176-01
Misc : 6.04G/5ML/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
18-B7-TP-(9.5-12)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072221S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown12.813	12.813	7.5	ug/l	132539	4	13.428	886707	50.0
Decane, 4-methyl-	13.044	5.0	ug/l	89234	4	13.428	886707	50.0
2-Cyclohexen-1-...	13.751	6.5	ug/l	114374	4	13.428	886707	50.0
1-Methyldecahyd...	14.264	5.8	ug/l	102551	4	13.428	886707	50.0
Azulene	15.239	13.4	ug/l	237305	4	13.428	886707	50.0