

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY032323\
 Data File : VY013065.D
 Acq On : 23 Mar 2023 17:12
 Operator : KP/MD
 Sample : 02049-01
 Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 OK-02-032323

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\82Y030223S.M
 Title : SW846 8260

Signal : TIC: VY013065.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.235	66	68	69	rBV	513	352	1.69%	0.196%
2	2.253	69	71	72	rVB2	519	321	1.54%	0.179%
3	2.290	75	77	79	rVB2	624	378	1.81%	0.210%
4	2.351	83	87	88	rBV3	570	679	3.26%	0.378%
5	2.546	118	119	123	rVB3	362	249	1.20%	0.138%
6	3.454	264	268	271	rBV2	182	265	1.27%	0.147%
7	3.942	344	348	351	rVB2	290	371	1.78%	0.206%
8	4.704	469	473	475	rBV3	589	851	4.09%	0.473%
9	5.759	643	646	650	rVB2	290	304	1.46%	0.169%
10	6.515	769	770	774	rBV2	208	260	1.25%	0.145%
11	6.625	785	788	792	rVB	196	253	1.21%	0.141%
12	6.966	839	844	849	rBV3	489	1188	5.70%	0.661%
13	7.399	913	915	920	rVB2	185	242	1.16%	0.135%
14	7.484	924	929	930	rVV3	252	375	1.80%	0.209%
15	7.521	933	935	940	rVB	264	326	1.57%	0.181%
16	7.716	960	967	974	rBV3	3657	8633	41.45%	4.801%
17	7.789	974	979	986	rVB4	5466	10948	52.56%	6.088%
18	8.137	1027	1036	1044	rBV2	4512	10342	49.65%	5.751%
19	8.551	1103	1104	1108	rBV2	164	241	1.16%	0.134%
20	8.685	1119	1126	1133	rVB	8393	16114	77.36%	8.961%
21	8.868	1154	1156	1159	rBV2	167	243	1.17%	0.135%
22	9.459	1251	1253	1257	rBV2	134	235	1.13%	0.131%
23	9.819	1308	1312	1316	rVB2	157	268	1.29%	0.149%
24	10.179	1364	1371	1377	rBV	11938	20829	100.00%	11.584%
25	10.289	1387	1389	1392	rBV2	270	325	1.56%	0.181%
26	10.368	1400	1402	1406	rBV3	289	481	2.31%	0.267%
27	10.551	1429	1432	1436	rVB	265	355	1.70%	0.197%
28	10.904	1486	1490	1492	rBV	242	300	1.44%	0.167%
29	11.197	1536	1538	1541	rBV	192	239	1.15%	0.133%
30	11.307	1553	1556	1559	rVB2	465	373	1.79%	0.207%
31	11.349	1559	1563	1564	rBV2	255	242	1.16%	0.135%
32	11.490	1580	1586	1592	rBV2	12199	20471	98.28%	11.384%
33	11.703	1618	1621	1625	rVB3	501	615	2.95%	0.342%
34	11.898	1651	1653	1657	rBV2	171	247	1.19%	0.137%
35	11.965	1661	1664	1667	rBV4	347	509	2.44%	0.283%
36	11.996	1667	1669	1670	rBV	504	326	1.57%	0.181%

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37	12.026	1673	1674	1676	rBV	446	448	2.15%	0.249%
38	12.087	1682	1684	1687	rVB3	346	289	1.39%	0.161%
39	12.118	1687	1689	1691	rBV	340	286	1.37%	0.159%
40	12.209	1702	1704	1707	rBV2	224	237	1.14%	0.132%

41	12.258	1711	1712	1715	rBV2	273	264	1.27%	0.147%
42	12.288	1715	1717	1720	rVB3	259	269	1.29%	0.150%
43	12.343	1723	1726	1728	rBV2	451	557	2.67%	0.310%
44	12.361	1728	1729	1731	rBV	590	557	2.67%	0.310%
45	12.477	1744	1748	1755	rVB	9130	14109	67.74%	7.846%

46	12.648	1770	1776	1781	rBV5	1598	4162	19.98%	2.315%
47	12.758	1792	1794	1797	rBV2	388	473	2.27%	0.263%
48	12.806	1797	1802	1808	rVB4	2265	3821	18.34%	2.125%
49	12.855	1808	1810	1811	rBV2	288	291	1.40%	0.162%
50	12.892	1814	1816	1817	rBV	430	339	1.63%	0.189%

51	12.941	1820	1824	1825	rBV3	1147	1546	7.42%	0.860%
52	13.044	1838	1841	1843	rBV3	1159	1658	7.96%	0.922%
53	13.117	1848	1853	1859	rVB5	1924	4010	19.25%	2.230%
54	13.319	1882	1886	1889	rBV2	850	1049	5.04%	0.583%
55	13.422	1897	1903	1912	rVB2	11018	18628	89.43%	10.360%

56	13.501	1914	1916	1919	rVB3	745	577	2.77%	0.321%
57	13.550	1922	1924	1926	rBV2	322	298	1.43%	0.166%
58	13.629	1933	1937	1939	rBV4	762	871	4.18%	0.484%
59	13.654	1939	1941	1942	rBV2	503	429	2.06%	0.239%
60	13.751	1952	1957	1961	rBV2	2990	4740	22.76%	2.636%

61	13.873	1971	1977	1978	rBV5	567	1181	5.67%	0.657%
62	13.946	1987	1989	1990	rBV2	415	296	1.42%	0.165%
63	13.971	1991	1993	1995	rVB3	456	356	1.71%	0.198%
64	14.075	2008	2010	2016	rVB3	643	907	4.35%	0.504%
65	14.135	2019	2020	2023	rBV	244	253	1.21%	0.141%

66	14.227	2033	2035	2037	rBV3	458	402	1.93%	0.224%
67	14.294	2043	2046	2047	rBV3	602	700	3.36%	0.389%
68	14.422	2064	2067	2069	rVB2	500	591	2.84%	0.329%
69	14.477	2075	2076	2079	rBV	369	307	1.47%	0.171%
70	14.550	2086	2088	2090	rVB2	385	311	1.49%	0.173%

71	14.581	2090	2093	2094	rBV2	441	460	2.21%	0.256%
72	14.611	2095	2098	2102	rVB3	1126	1535	7.37%	0.854%
73	14.672	2103	2108	2114	rBV4	1138	2004	9.62%	1.114%
74	14.727	2114	2117	2122	rVB4	833	1234	5.92%	0.686%
75	14.794	2126	2128	2130	rBV2	328	304	1.46%	0.169%

76	14.837	2133	2135	2136	rBV	433	362	1.74%	0.201%
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77	14.867	2136	2140	2141	rBV3	440	567	2.72%	0.315%
78	14.995	2158	2161	2165	rBV3	223	289	1.39%	0.161%
79	15.044	2166	2169	2174	rVB2	744	965	4.63%	0.537%
80	15.099	2176	2178	2182	rVV2	328	448	2.15%	0.249%
81	15.154	2184	2187	2190	rVB	352	401	1.93%	0.223%
82	15.239	2195	2201	2206	rBV2	1960	3433	16.48%	1.909%
83	15.318	2210	2214	2216	rBV4	326	418	2.01%	0.232%
84	15.434	2229	2233	2237	rVB3	465	760	3.65%	0.423%
85	15.477	2237	2240	2241	rBV	314	314	1.51%	0.175%
86	15.568	2252	2255	2257	rBV2	312	330	1.58%	0.184%
87	15.635	2264	2266	2267	rBV2	278	237	1.14%	0.132%
88	15.946	2315	2317	2322	rVB4	363	490	2.35%	0.273%
89	15.995	2322	2325	2328	rBV2	298	442	2.12%	0.246%
90	16.038	2328	2332	2334	rBV2	189	320	1.54%	0.178%
91	16.403	2390	2392	2394	rVB2	346	277	1.33%	0.154%
92	16.519	2408	2411	2412	rBV2	273	263	1.26%	0.146%

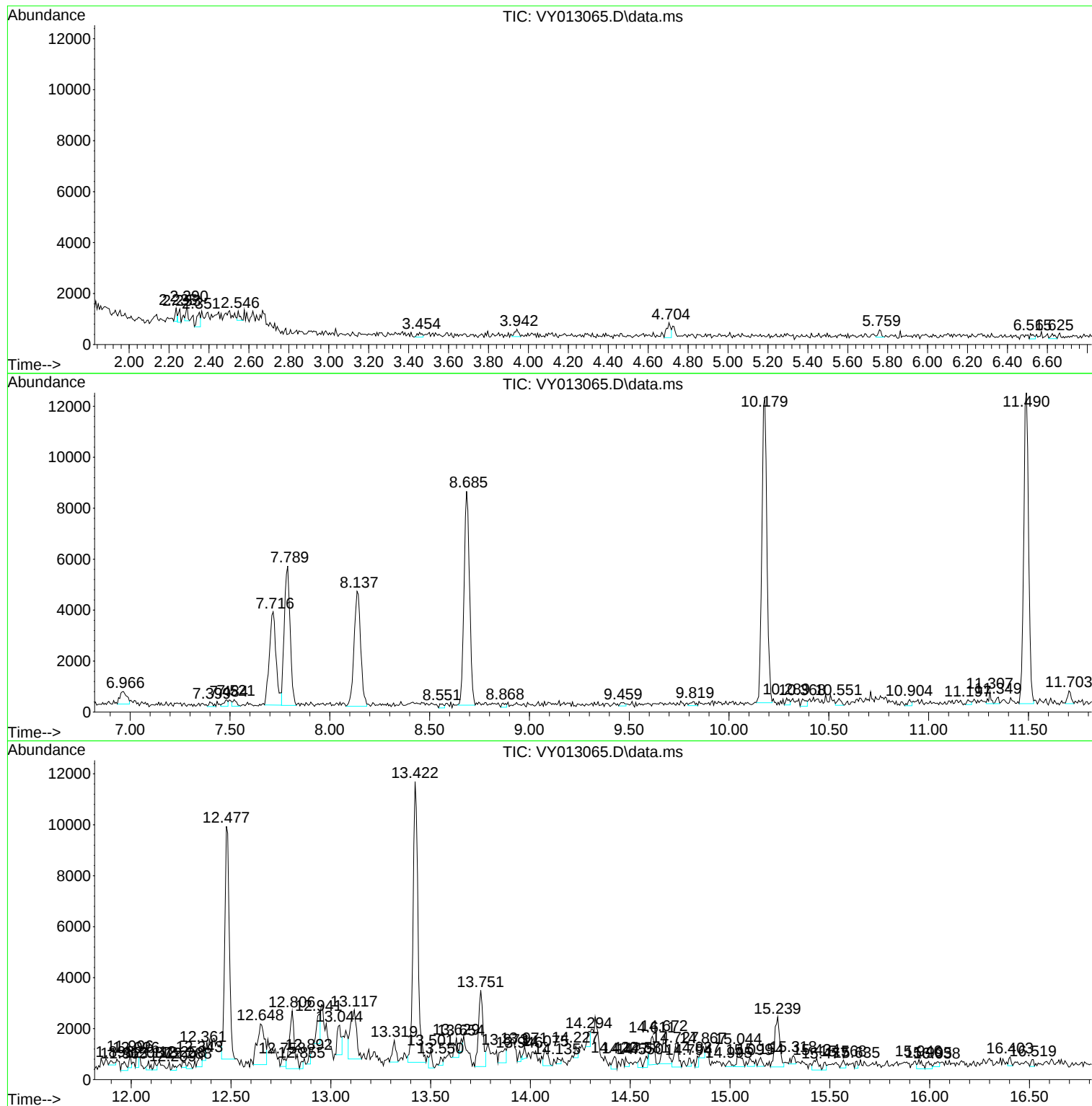
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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



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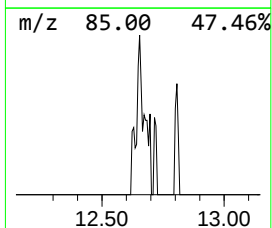
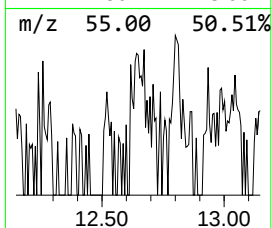
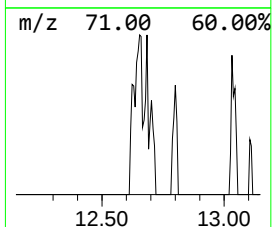
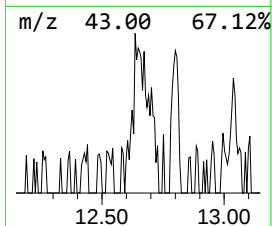
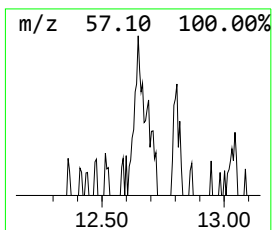
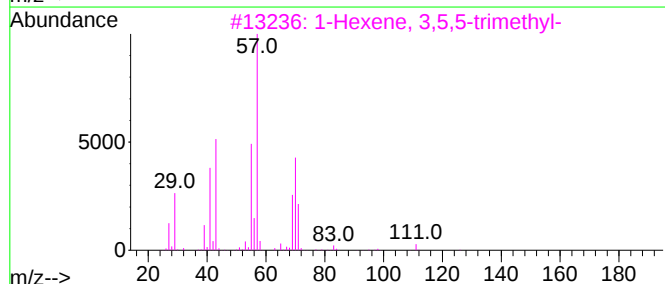
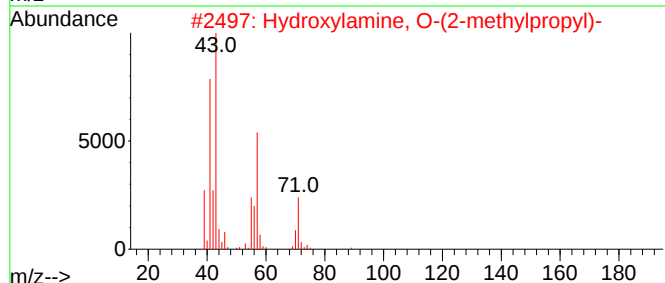
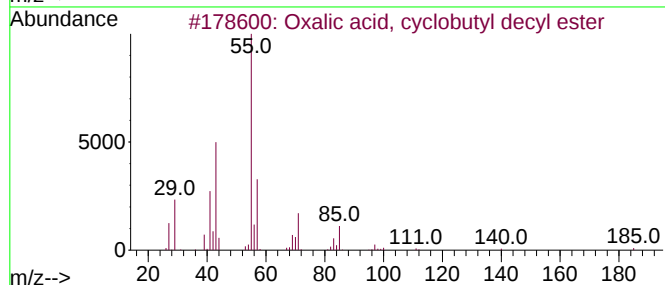
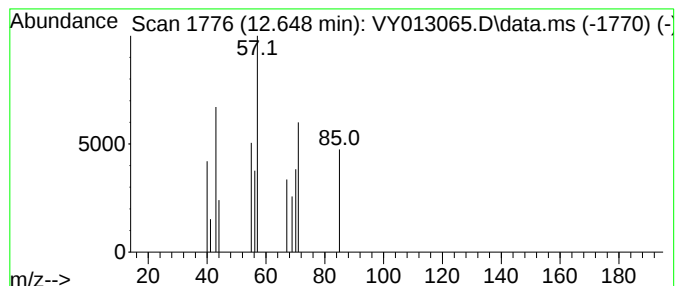
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.648 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.648	11.17 ug/l	4162	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl decyl ester	284	C16H28O4	1000309-70-1	36
2			Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	25
3			1-Hexene, 3,5,5-trimethyl-	126	C9H18	004316-65-8	17
4			1-Hexanol, 3-methyl-	116	C7H16O	013231-81-7	12
5			Vinyl ether	70	C4H6O	000109-93-3	10



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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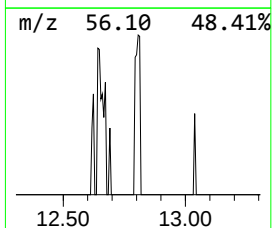
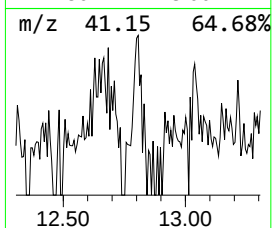
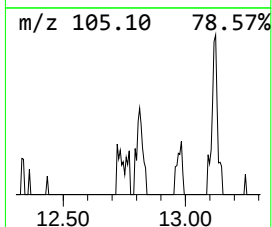
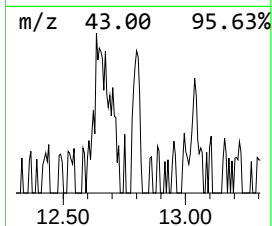
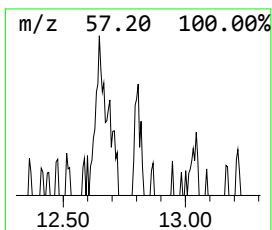
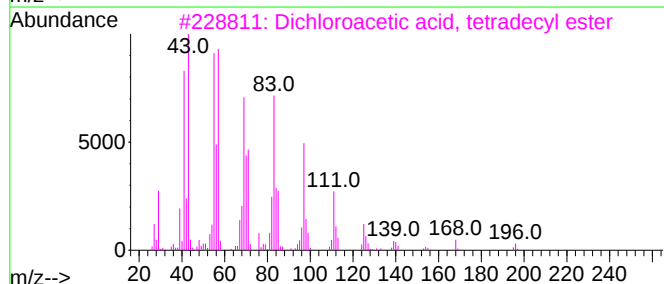
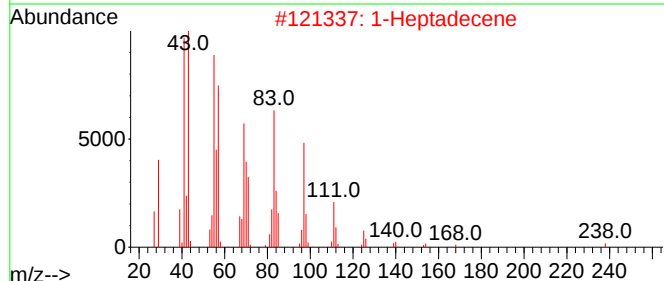
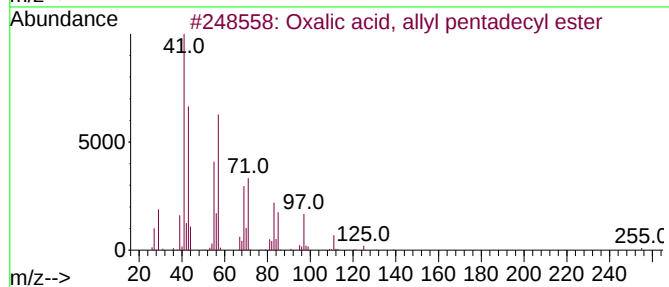
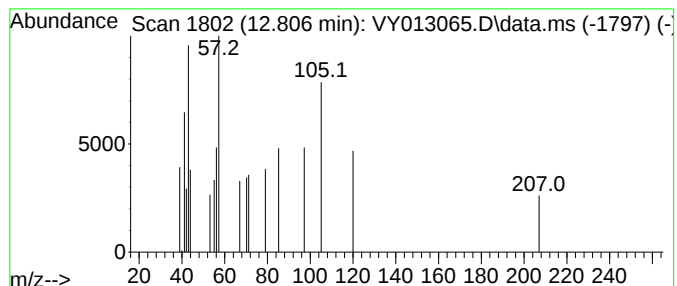
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown12.806 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.806	10.26 ug/l	3821	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	25
2			1-Heptadecene	238	C17H34	006765-39-5	16
3			Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	14
4			Decane, 1-fluoro-	160	C10H21F	000334-56-5	12
5			6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	12



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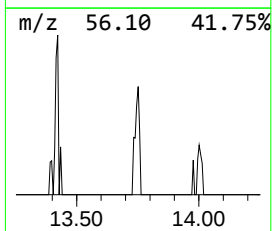
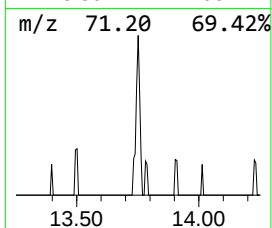
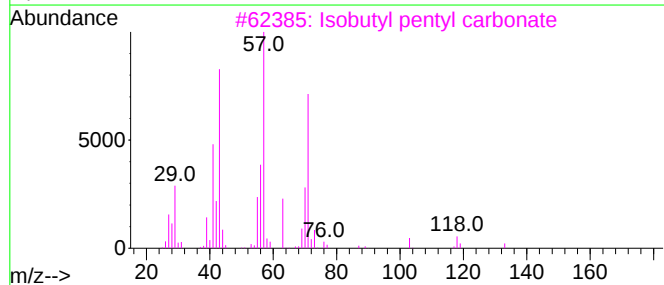
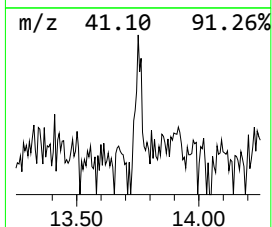
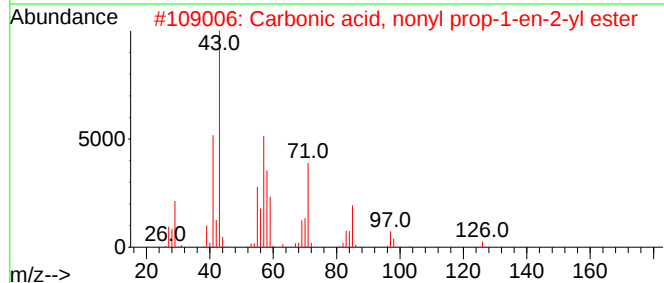
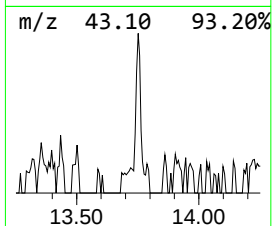
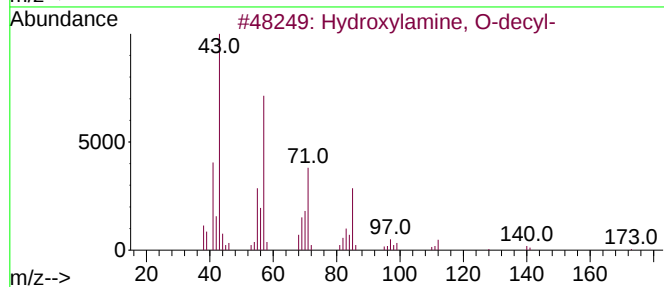
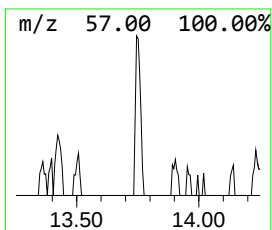
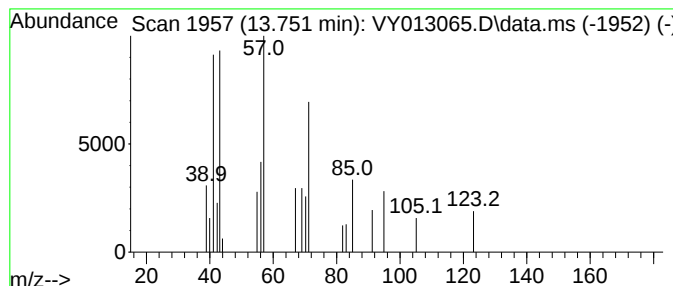
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown13.751 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	12.72 ug/l	4740	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	47
2			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	47
3			Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	47
4			Hexyl octyl ether	214	C14H30O	017071-54-4	43
5			Oxirane, octyl-	156	C10H20O	002404-44-6	42



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OK-02-032323

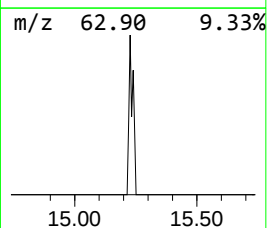
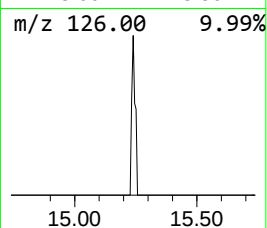
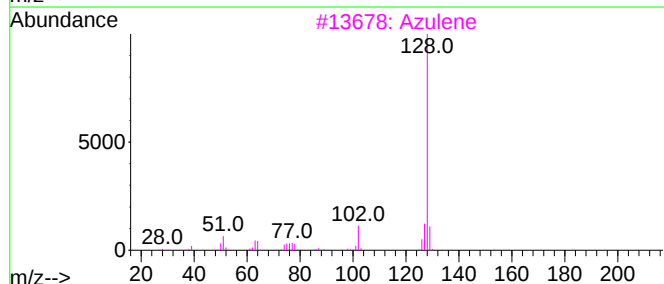
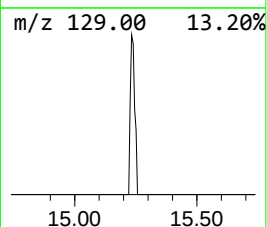
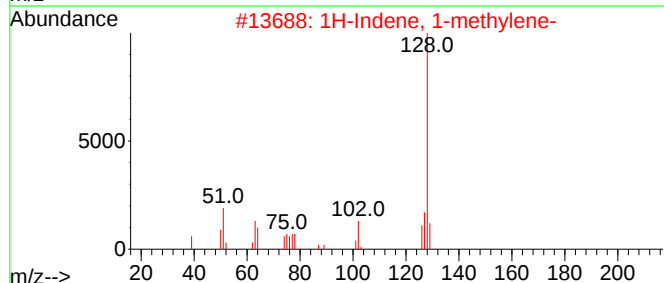
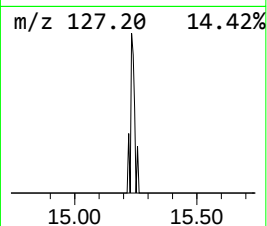
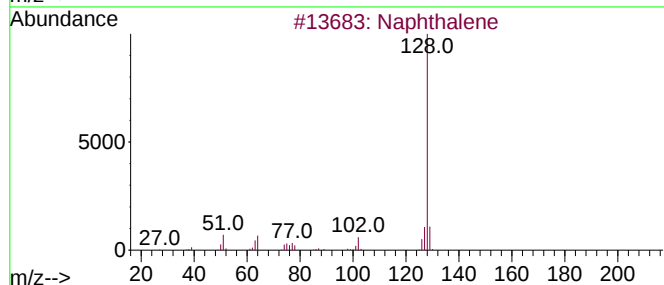
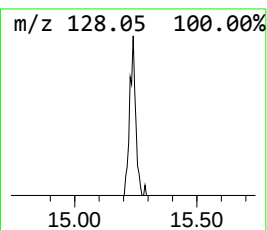
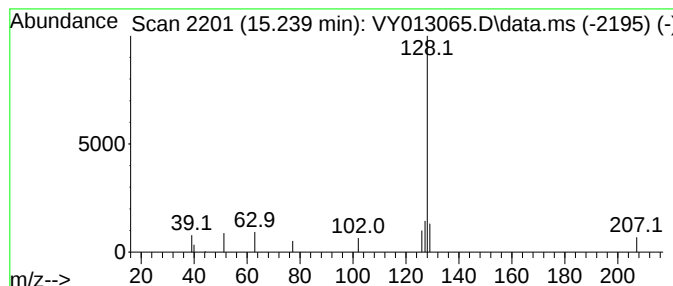
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Quant Title : SW846 8260

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

Peak Number 7 Azulene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.239	9.21 ug/l	3433	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	90
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	78
3			Azulene	128	C10H8	000275-51-4	78
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	56
5			4-Fluorothiophenol	128	C6H5FS	000371-42-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY032323\
Data File : VY013065.D
Acq On : 23 Mar 2023 17:12
Operator : KP/MD
Sample : 02049-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
OK-02-032323

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.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
unknown12.648	12.648	11.2	ug/l	4162	4	13.422	18628	50.0
unknown12.806	12.806	10.3	ug/l	3821	4	13.422	18628	50.0
unknown13.751	13.751	12.7	ug/l	4740	4	13.422	18628	50.0
Azulene	15.239	9.2	ug/l	3433	4	13.422	18628	50.0