

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102621\
 Data File : VY006485.D
 Acq On : 26 Oct 2021 16:47
 Operator : SY/MD
 Sample : M4325-01
 Misc : 5.05G/5ML/MSVOA_Y/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 RED-BOX-1-225057

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\82Y102221S.M
 Title : SW846 8260

Signal : TIC: VY006485.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.010	29	31	33	rVB	496	449	1.49%	0.186%
2	2.034	33	35	42	rVB3	735	1260	4.17%	0.522%
3	2.113	45	48	49	rBV3	483	529	1.75%	0.219%
4	2.388	91	93	99	rBV5	467	594	1.96%	0.246%
5	2.644	132	135	137	rBV3	386	608	2.01%	0.252%
6	2.662	137	138	143	rVB4	1327	1587	5.25%	0.657%
7	2.741	147	151	152	rBV4	317	507	1.68%	0.210%
8	3.089	205	208	211	rVB2	351	416	1.38%	0.172%
9	4.101	367	374	377	rBV4	522	1092	3.61%	0.452%
10	4.716	470	475	476	rBV3	662	853	2.82%	0.353%
11	7.722	960	968	973	rVV4	1032	2584	8.55%	1.070%
12	7.795	973	980	990	rVV2	6645	13582	44.93%	5.625%
13	8.143	1029	1037	1046	rVB2	6037	12899	42.67%	5.343%
14	8.691	1119	1127	1133	rBV	10847	20510	67.84%	8.495%
15	9.307	1225	1228	1233	rBV2	316	465	1.54%	0.193%
16	9.466	1251	1254	1258	rVB2	408	535	1.77%	0.222%
17	9.917	1326	1328	1332	rBV2	311	398	1.32%	0.165%
18	10.185	1365	1372	1378	rVV2	17445	30232	100.00%	12.522%
19	10.295	1388	1390	1394	rBV3	260	402	1.33%	0.167%
20	10.484	1419	1421	1423	rBV2	530	534	1.77%	0.221%
21	10.526	1423	1428	1430	rVB4	485	800	2.65%	0.331%
22	11.093	1516	1521	1525	rBV6	988	1845	6.10%	0.764%
23	11.191	1531	1537	1539	rBV3	531	989	3.27%	0.410%
24	11.301	1552	1555	1559	rVV4	727	966	3.20%	0.400%
25	11.429	1572	1576	1579	rBV3	483	629	2.08%	0.261%
26	11.490	1579	1586	1593	rVB	16660	27233	90.08%	11.280%
27	11.624	1606	1608	1612	rBV4	572	722	2.39%	0.299%
28	11.672	1612	1616	1617	rBV2	475	608	2.01%	0.252%
29	11.740	1623	1627	1628	rVV4	704	822	2.72%	0.340%
30	11.849	1641	1645	1646	rBV2	469	420	1.39%	0.174%
31	11.996	1664	1669	1676	rVV4	881	2114	6.99%	0.876%
32	12.087	1680	1684	1686	rBV3	456	540	1.79%	0.224%
33	12.130	1686	1691	1693	rBV4	811	1263	4.18%	0.523%
34	12.203	1699	1703	1706	rBV3	1462	2295	7.59%	0.951%
35	12.319	1721	1722	1724	rBV2	700	444	1.47%	0.184%
36	12.367	1729	1730	1734	rBV4	505	564	1.87%	0.234%

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37	12.435	1738	1741	1743	rBV4	590	703	2.33%	0.291%
38	12.483	1743	1749	1756	rVB2	12862	19876	65.74%	8.232%
39	12.538	1756	1758	1759	rBV2	540	531	1.76%	0.220%
40	12.563	1760	1762	1766	rVB4	545	689	2.28%	0.285%
41	12.642	1768	1775	1780	rBV5	1332	2156	7.13%	0.893%
42	12.721	1786	1788	1789	rBV2	516	449	1.49%	0.186%
43	12.733	1789	1790	1793	rVB2	886	413	1.37%	0.171%
44	12.813	1796	1803	1806	rVV7	1767	3736	12.36%	1.547%
45	12.861	1808	1811	1815	rVB4	987	1180	3.90%	0.489%
46	12.953	1822	1826	1829	rBV5	1019	1429	4.73%	0.592%
47	12.989	1829	1832	1833	rBV2	483	493	1.63%	0.204%
48	13.038	1838	1840	1844	rVB4	1199	1530	5.06%	0.634%
49	13.075	1844	1846	1848	rVB3	684	577	1.91%	0.239%
50	13.123	1851	1854	1856	rBV4	470	541	1.79%	0.224%
51	13.172	1858	1862	1864	rVB5	758	1039	3.44%	0.430%
52	13.203	1864	1867	1870	rBV5	582	915	3.03%	0.379%
53	13.245	1871	1874	1876	rVV4	597	733	2.42%	0.304%
54	13.355	1889	1892	1894	rVB4	616	462	1.53%	0.191%
55	13.428	1897	1904	1910	rBV	12721	21267	70.35%	8.808%
56	13.599	1930	1932	1933	rBV2	813	563	1.86%	0.233%
57	13.660	1941	1942	1945	rBV3	586	520	1.72%	0.215%
58	13.697	1945	1948	1952	rBV4	775	1159	3.83%	0.480%
59	13.751	1952	1957	1962	rBV6	2372	5265	17.42%	2.181%
60	13.800	1962	1965	1968	rVB4	1128	1391	4.60%	0.576%
61	13.831	1968	1970	1971	rBV2	667	573	1.90%	0.237%
62	13.855	1971	1974	1977	rVB4	742	1146	3.79%	0.475%
63	13.922	1984	1985	1987	rBV	463	423	1.40%	0.175%
64	14.075	2007	2010	2017	rVB8	1125	2391	7.91%	0.990%
65	14.135	2017	2020	2021	rBV2	1085	1312	4.34%	0.543%
66	14.160	2021	2024	2026	rVV3	672	812	2.69%	0.336%
67	14.263	2037	2041	2046	rVB6	2103	3950	13.07%	1.636%
68	14.312	2046	2049	2052	rBV5	631	888	2.94%	0.368%
69	14.355	2054	2056	2058	rBV2	367	430	1.42%	0.178%
70	14.379	2058	2060	2062	rVB2	841	681	2.25%	0.282%
71	14.428	2062	2068	2069	rBV4	1377	2302	7.61%	0.953%
72	14.471	2073	2075	2078	rVV4	791	883	2.92%	0.366%
73	14.538	2082	2086	2087	rBV4	565	677	2.24%	0.280%
74	14.581	2091	2093	2094	rBV2	515	406	1.34%	0.168%
75	14.623	2097	2100	2101	rVB3	743	767	2.54%	0.318%
76	14.684	2104	2110	2112	rBV7	1460	2315	7.66%	0.959%

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77	14.733	2115	2118	2121	rVB5	1712	2154	7.12%	0.892%
78	14.904	2144	2146	2150	rVB4	866	1167	3.86%	0.483%
79	14.946	2150	2153	2155	rVB4	859	977	3.23%	0.405%
80	14.971	2155	2157	2160	rBV4	658	968	3.20%	0.401%
81	15.019	2163	2165	2166	rBV2	518	481	1.59%	0.199%
82	15.056	2168	2171	2173	rVB4	879	948	3.14%	0.393%
83	15.087	2173	2176	2179	rBV5	837	939	3.11%	0.389%
84	15.117	2179	2181	2183	rBV2	945	964	3.19%	0.399%
85	15.221	2194	2198	2201	rBV6	1272	1472	4.87%	0.610%
86	15.269	2204	2206	2207	rBV2	569	578	1.91%	0.239%
87	15.324	2213	2215	2216	rBV2	1057	767	2.54%	0.318%
88	15.556	2251	2253	2254	rBV2	697	509	1.68%	0.211%
89	15.653	2266	2269	2271	rBV3	777	873	2.89%	0.362%
90	15.678	2271	2273	2276	rVB4	867	737	2.44%	0.305%
91	15.757	2284	2286	2288	rVV3	714	560	1.85%	0.232%
92	15.794	2291	2292	2295	rVB3	705	555	1.84%	0.230%
93	15.910	2309	2311	2316	rBV6	806	1322	4.37%	0.548%
94	16.007	2323	2327	2330	rBV6	1067	1868	6.18%	0.774%
95	16.166	2349	2353	2357	rVB6	844	1353	4.48%	0.560%
96	16.391	2388	2390	2391	rBV2	571	465	1.54%	0.193%
97	16.434	2395	2397	2398	rBV2	706	460	1.52%	0.191%
98	16.507	2407	2409	2411	rVB3	869	543	1.80%	0.225%
99	16.745	2446	2448	2450	rBV2	604	501	1.66%	0.208%
100	16.769	2450	2452	2454	rVB3	580	414	1.37%	0.171%

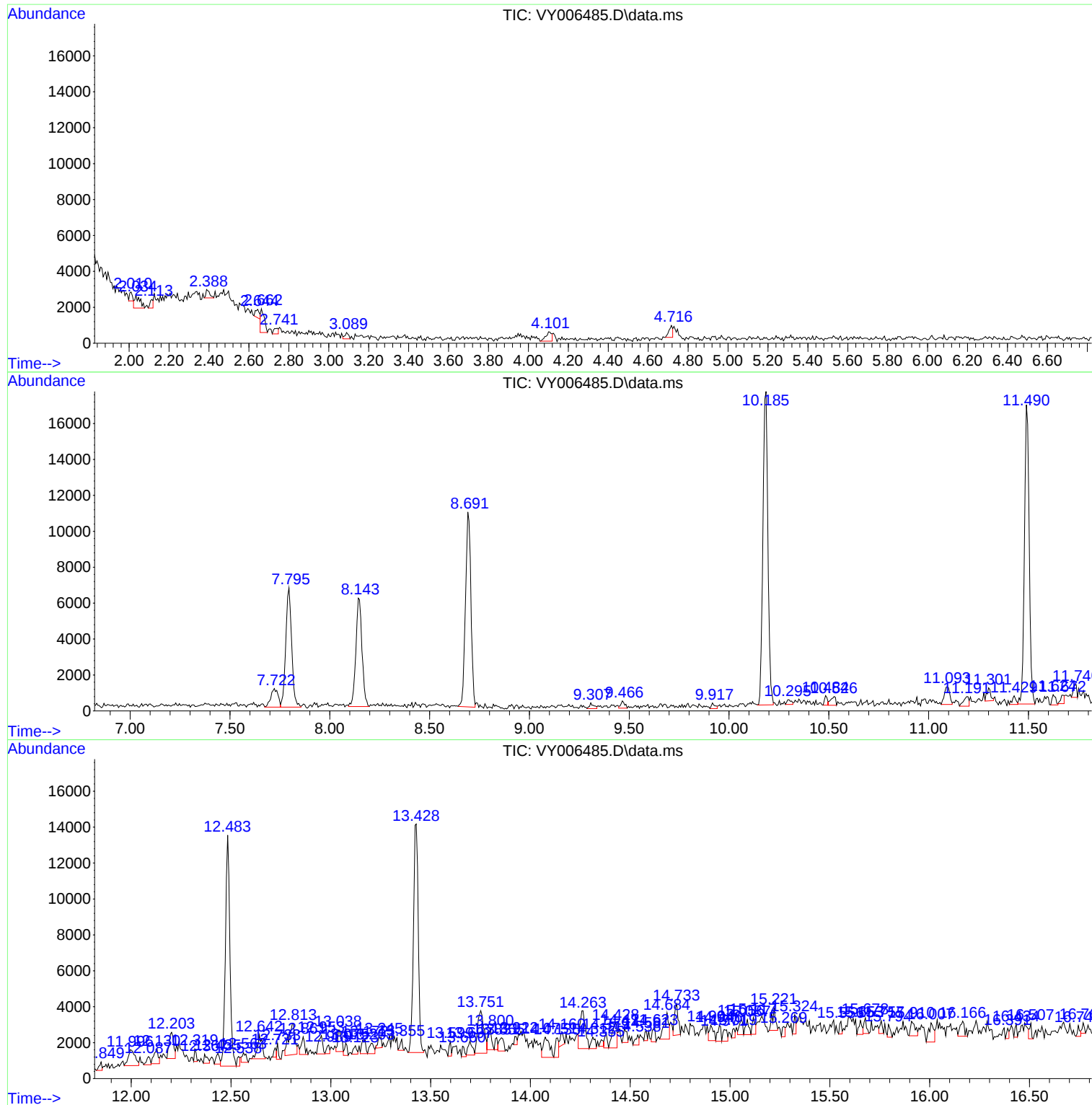
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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



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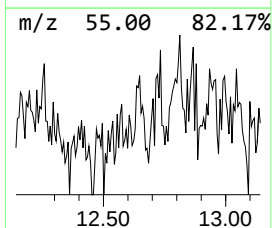
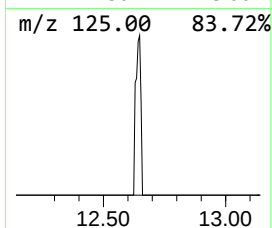
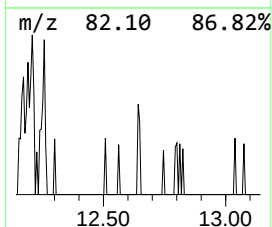
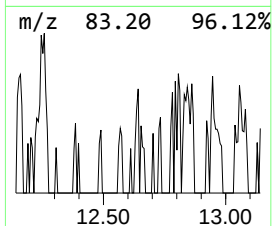
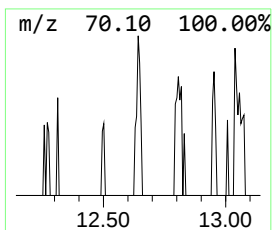
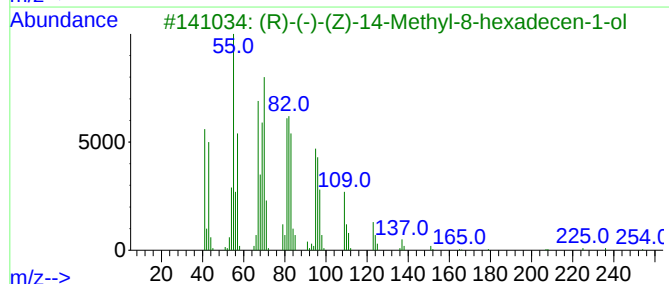
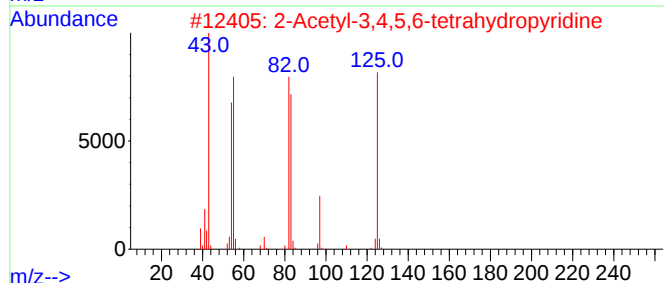
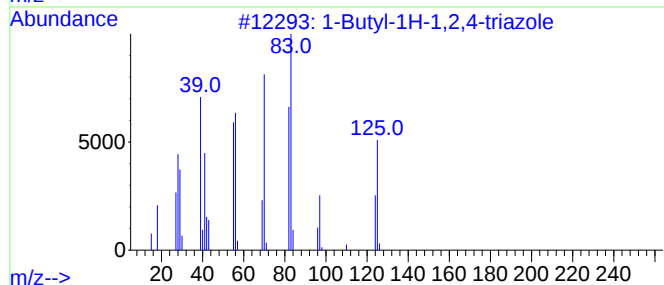
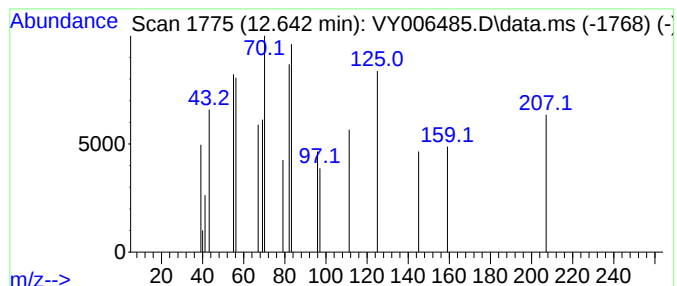
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.642 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.642	5.07 ug/l	2156	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butyl-1H-1,2,4-triazole	125	C6H11N3	006086-22-2	43
2			2-Acetyl-3,4,5,6-tetrahydropyridine	125	C7H11NO	027300-27-2	38
3			(R)-(-)-(Z)-14-Methyl-8-hexadecene-1-ol	254	C17H34O	030689-78-2	37
4			2,5-Dimethyl-1-aza-bicyclo[2.2.1]hept-2-ene	125	C8H15N	1000194-05-9	35
5			Undecanal	170	C11H22O	000112-44-7	27



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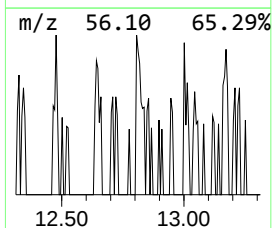
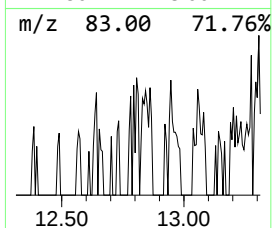
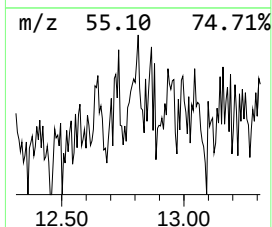
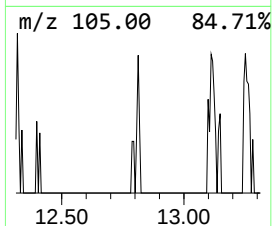
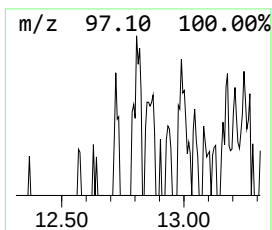
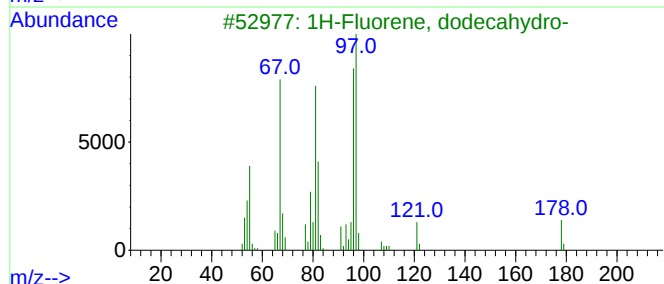
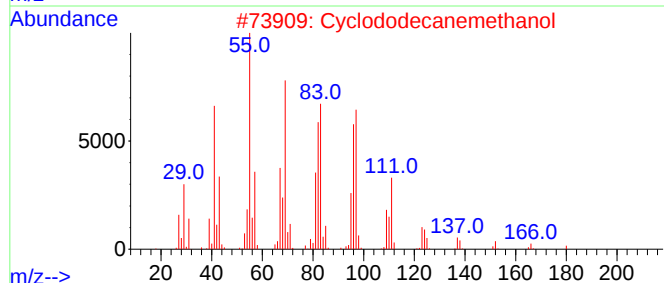
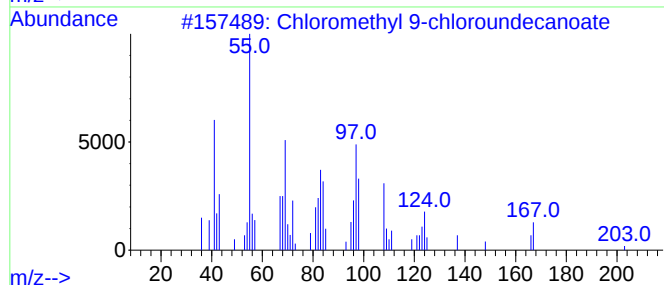
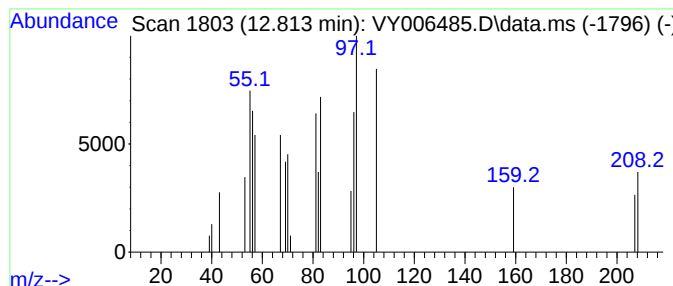
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.813 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.813	8.78 ug/l	3736	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Chloromethyl 9-chloroundecanoate	268	C12H22Cl2O2	080418-95-7	47
2			Cyclododecanemethanol	198	C13H26O	001892-12-2	38
3			1H-Fluorene, dodecahydro-	178	C13H22	005744-03-6	35
4			1-Cyclohexylheptene	180	C13H24	114614-83-4	35
5			Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-97-1	32



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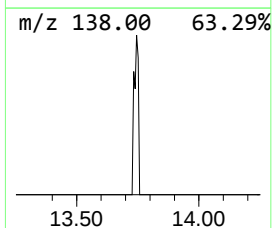
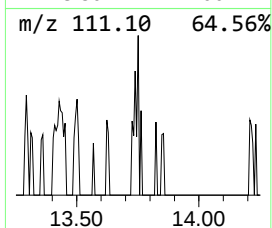
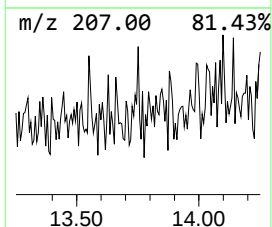
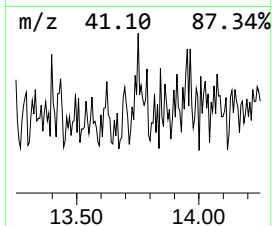
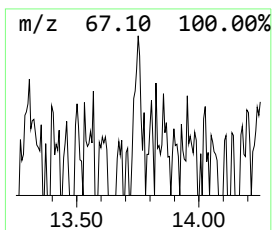
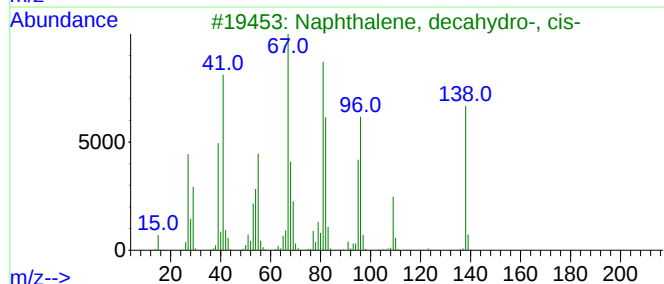
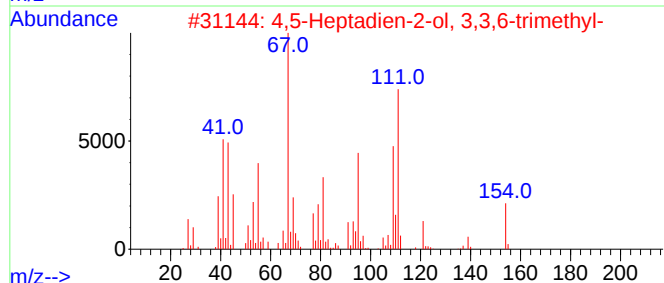
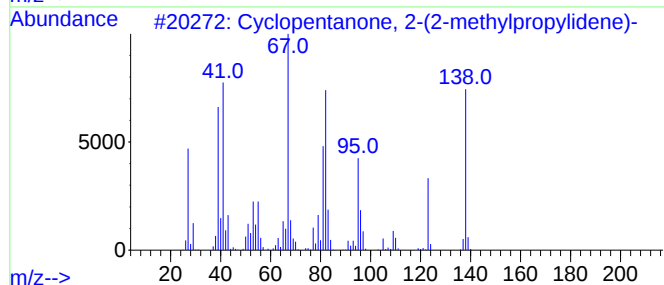
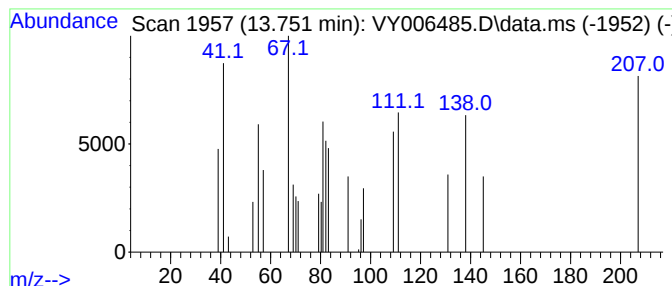
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown13.751 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	12.38 ug/l	5265	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone, 2-(2-methylpropy...	138	C9H14O	016856-72-7	30
2			4,5-Heptadien-2-ol, 3,3,6-trimet...	154	C10H18O	060432-69-1	27
3			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	27
4			4,6-Decadiene	138	C10H18	055682-65-0	27
5			1H-Inden-1-one, octahydro-, trans-	138	C9H14O	016783-22-5	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102621\
Data File : VY006485.D
Acq On : 26 Oct 2021 16:47
Operator : SY/MD
Sample : M4325-01
Misc : 5.05G/5ML/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RED-BOX-1-225057

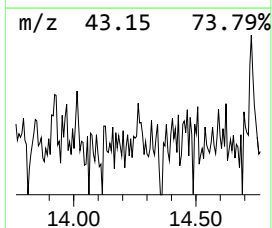
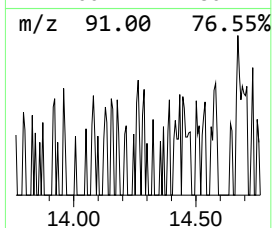
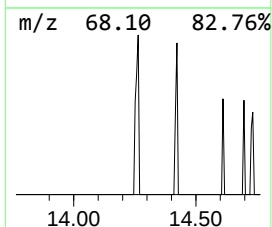
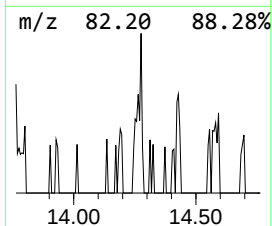
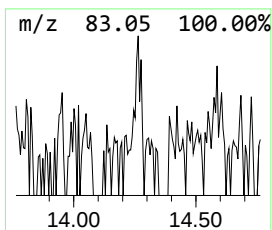
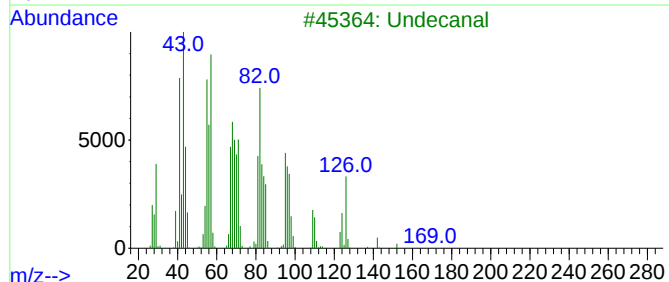
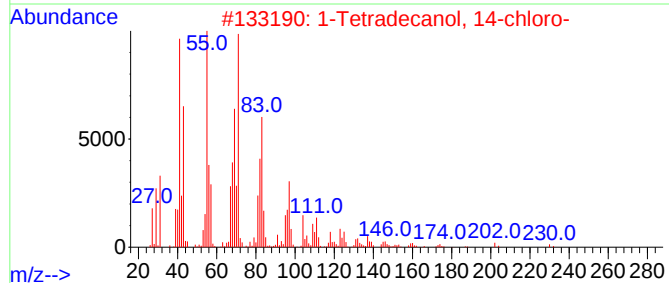
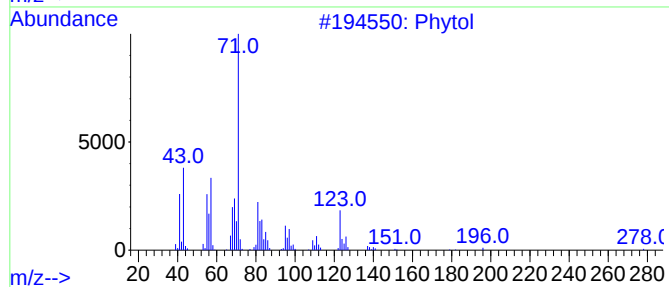
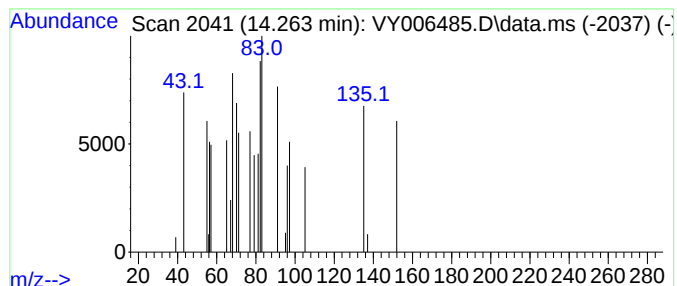
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Quant Title : SW846 8260

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

Peak Number 6 unknown14.264 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.264	9.29 ug/l	3950	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phytol	296	C20H40O	000150-86-7	32
2			1-Tetradecanol, 14-chloro-	248	C14H29ClO	073937-05-0	32
3			Undecanal	170	C11H22O	000112-44-7	16
4			Oxirane, decyl-	184	C12H24O	002855-19-8	12
5			Oxirane, dodecyl-	212	C14H28O	003234-28-4	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102621\
Data File : VY006485.D
Acq On : 26 Oct 2021 16:47
Operator : SY/MD
Sample : M4325-01
Misc : 5.05G/5ML/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RED-BOX-1-225057

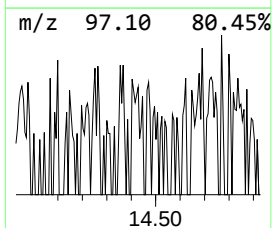
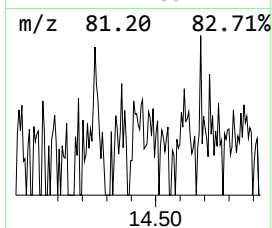
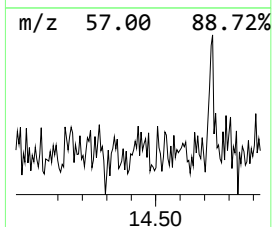
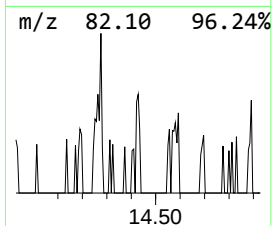
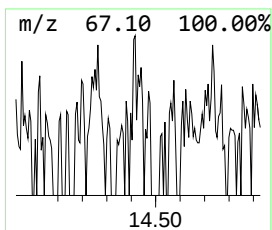
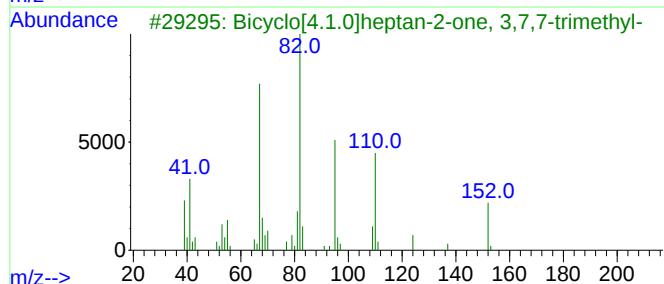
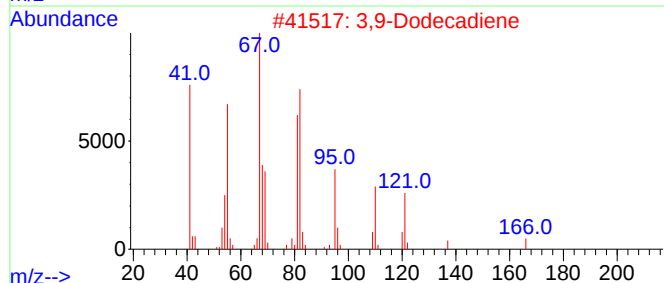
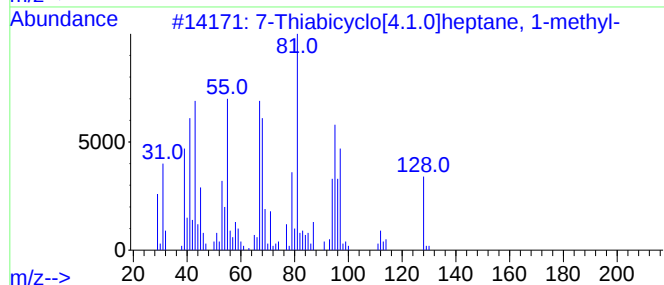
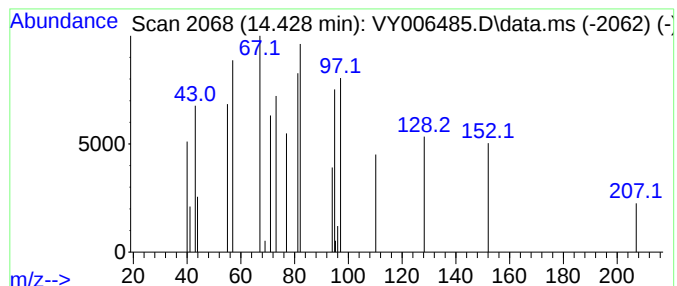
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.428 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.428	5.41 ug/l	2302	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Thiabicyclo[4.1.0]heptane, 1-m...	128	C7H12S	007272-23-3	43		
2	3,9-Dodecadiene	166	C12H22	054764-65-7	43		
3	Bicyclo[4.1.0]heptan-2-one, 3,7,...	152	C10H16O	000497-62-1	43		
4	Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	43		
5	Cyclohexene, 1,6-dimethyl-	110	C8H14	001759-64-4	43		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102621\
Data File : VY006485.D
Acq On : 26 Oct 2021 16:47
Operator : SY/MD
Sample : M4325-01
Misc : 5.05G/5ML/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RED-BOX-1-225057

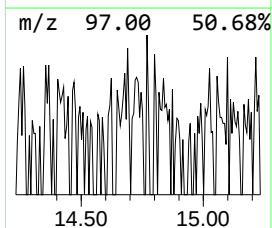
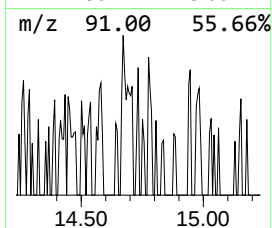
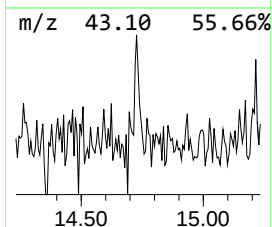
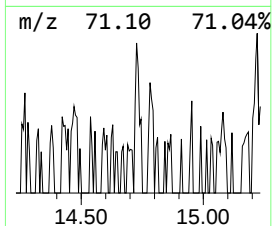
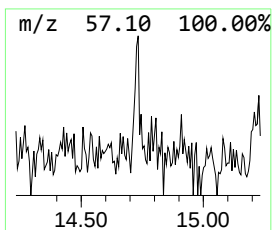
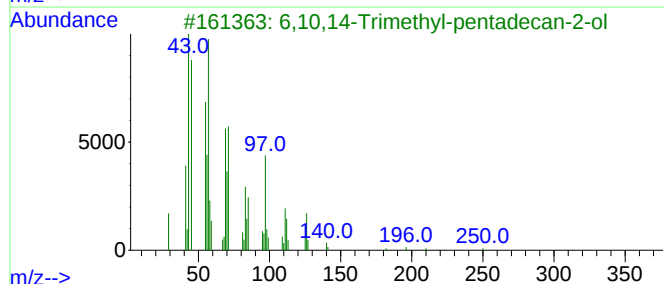
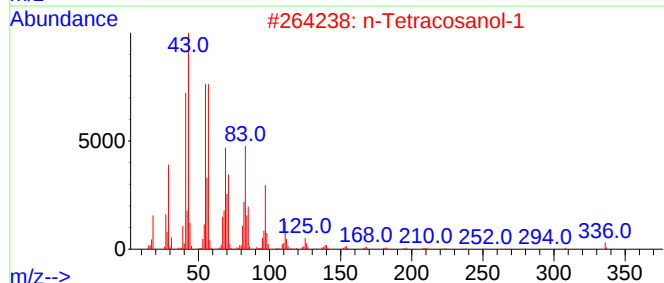
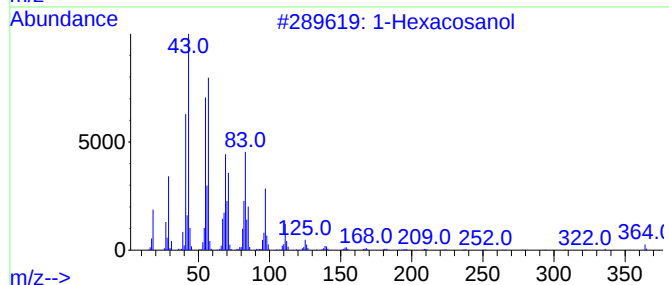
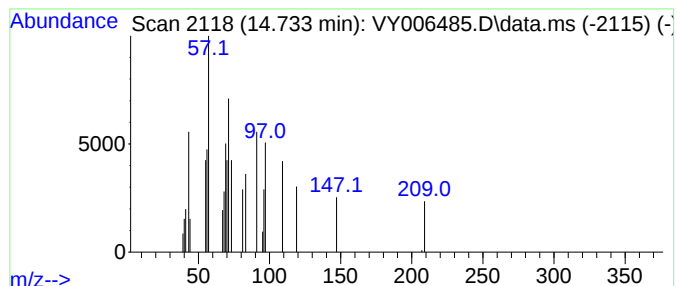
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 9 unknown14.733 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	5.06 ug/l	2154	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol			382	C26H54O	000506-52-5	38
2	n-Tetracosanol-1			354	C24H50O	000506-51-4	38
3	6,10,14-Trimethyl-pentadecan-2-ol			270	C18H38O	069729-17-5	37
4	Acetoxyacetic acid, nonyl ester			244	C13H24O4	1000308-31-4	35
5	2-Decanol, pentafluoropropionate			304	C13H21F5O2	1000352-32-7	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102621\
Data File : VY006485.D
Acq On : 26 Oct 2021 16:47
Operator : SY/MD
Sample : M4325-01
Misc : 5.05G/5ML/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RED-BOX-1-225057

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.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	8.8	ug/l	3736	4	13.428	21267	50.0
unknown13.751	13.751	12.4	ug/l	5265	4	13.428	21267	50.0
unknown14.264	14.264	9.3	ug/l	3950	4	13.428	21267	50.0
unknown14.428	14.428	5.4	ug/l	2302	4	13.428	21267	50.0
unknown14.733	14.733	5.1	ug/l	2154	4	13.428	21267	50.0