

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112222\
 Data File : VY011560.D
 Acq On : 22 Nov 2022 19:54
 Operator : KP/MD
 Sample : N5754-01
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 PSC-124019

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\82Y111822S.M
 Title : SW846 8260

Signal : TIC: VY011560.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.138	50	52	55	rVB	667	644	1.03%	0.181%
2	2.253	65	71	75	rBV4	1625	3368	5.38%	0.946%
3	2.656	135	137	141	rVB2	630	831	1.33%	0.233%
4	3.021	192	197	198	rVV4	747	1202	1.92%	0.338%
5	3.064	202	204	211	rVV2	840	1183	1.89%	0.332%
6	3.942	342	348	358	rVB4	1184	3299	5.27%	0.927%
7	4.186	382	388	389	rBV2	480	703	1.12%	0.198%
8	4.716	465	475	493	rVB2	20010	62658	100.00%	17.604%
9	5.753	635	645	657	rVB5	5483	16906	26.98%	4.750%
10	6.978	835	846	861	rVV	17690	54788	87.44%	15.393%
11	7.728	962	969	973	rBV3	345	703	1.12%	0.198%
12	8.100	1027	1030	1033	rBV2	666	979	1.56%	0.275%
13	8.691	1119	1127	1132	rVB3	1084	1734	2.77%	0.487%
14	10.185	1367	1372	1378	rBV2	1851	3434	5.48%	0.965%
15	10.581	1431	1437	1445	rBV2	9361	15752	25.14%	4.426%
16	10.947	1489	1497	1506	rBV	16166	27406	43.74%	7.700%
17	11.044	1509	1513	1517	rVB2	440	627	1.00%	0.176%
18	11.313	1553	1557	1564	rBV	2587	4633	7.39%	1.302%
19	11.489	1579	1586	1591	rBV3	3121	5437	8.68%	1.528%
20	12.337	1719	1725	1731	rVV	12692	20202	32.24%	5.676%
21	12.489	1743	1750	1758	rVB	21050	34752	55.46%	9.764%
22	12.825	1798	1805	1812	rBV3	2849	4298	6.86%	1.208%
23	12.898	1812	1817	1820	rVV3	869	1381	2.20%	0.388%
24	13.184	1858	1864	1868	rBV2	1457	2217	3.54%	0.623%
25	13.428	1899	1904	1909	rVB3	5491	8417	13.43%	2.365%
26	13.788	1960	1963	1967	rVB4	621	843	1.35%	0.237%
27	13.904	1980	1982	1986	rVV4	574	885	1.41%	0.249%
28	13.965	1986	1992	1997	rVV3	4788	7709	12.30%	2.166%
29	14.257	2038	2040	2044	rVB3	729	915	1.46%	0.257%
30	14.330	2050	2052	2056	rVB3	673	780	1.24%	0.219%
31	14.379	2056	2060	2064	rBV5	931	1250	1.99%	0.351%
32	14.586	2089	2094	2096	rBV3	583	827	1.32%	0.232%
33	14.611	2096	2098	2105	rVB5	958	1420	2.27%	0.399%
34	14.666	2105	2107	2108	rBV	965	699	1.12%	0.196%
35	14.733	2113	2118	2125	rVB7	1357	2831	4.52%	0.795%
36	14.824	2129	2133	2135	rBV3	569	976	1.56%	0.274%

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37	14.934	2149	2151	2154	rBV2	590	680	1.09%	0.191%
38	15.019	2160	2165	2167	rBV4	1927	3132	5.00%	0.880%
39	15.050	2167	2170	2176	rVB5	3560	5335	8.51%	1.499%
40	15.153	2186	2187	2191	rVB3	966	678	1.08%	0.190%
41	15.214	2193	2197	2201	rBV6	1316	2845	4.54%	0.799%
42	15.324	2204	2215	2217	rBV6	2498	6570	10.49%	1.846%
43	15.361	2217	2221	2223	rBV4	1797	2024	3.23%	0.569%
44	15.385	2223	2225	2229	rVB5	1091	1215	1.94%	0.341%
45	15.434	2229	2233	2238	rVB8	1448	2186	3.49%	0.614%
46	15.538	2242	2250	2255	rBV8	4121	8159	13.02%	2.292%
47	15.696	2270	2276	2279	rBV7	3093	5955	9.50%	1.673%
48	15.824	2293	2297	2299	rVV3	913	1117	1.78%	0.314%
49	15.891	2304	2308	2310	rVB4	636	742	1.18%	0.208%
50	16.031	2325	2331	2337	rBV6	2484	4886	7.80%	1.373%
51	16.153	2348	2351	2353	rBV3	778	941	1.50%	0.264%
52	16.233	2359	2364	2369	rVB4	2145	3868	6.17%	1.087%
53	16.348	2380	2383	2385	rVB4	554	647	1.03%	0.182%
54	16.391	2385	2390	2393	rBV4	1161	2038	3.25%	0.573%
55	16.476	2402	2404	2407	rBV3	763	911	1.45%	0.256%
56	16.537	2412	2414	2420	rVB4	1334	1922	3.07%	0.540%
57	16.623	2425	2428	2435	rVB6	1048	2311	3.69%	0.649%
58	16.732	2442	2446	2450	rBV5	674	1080	1.72%	0.303%

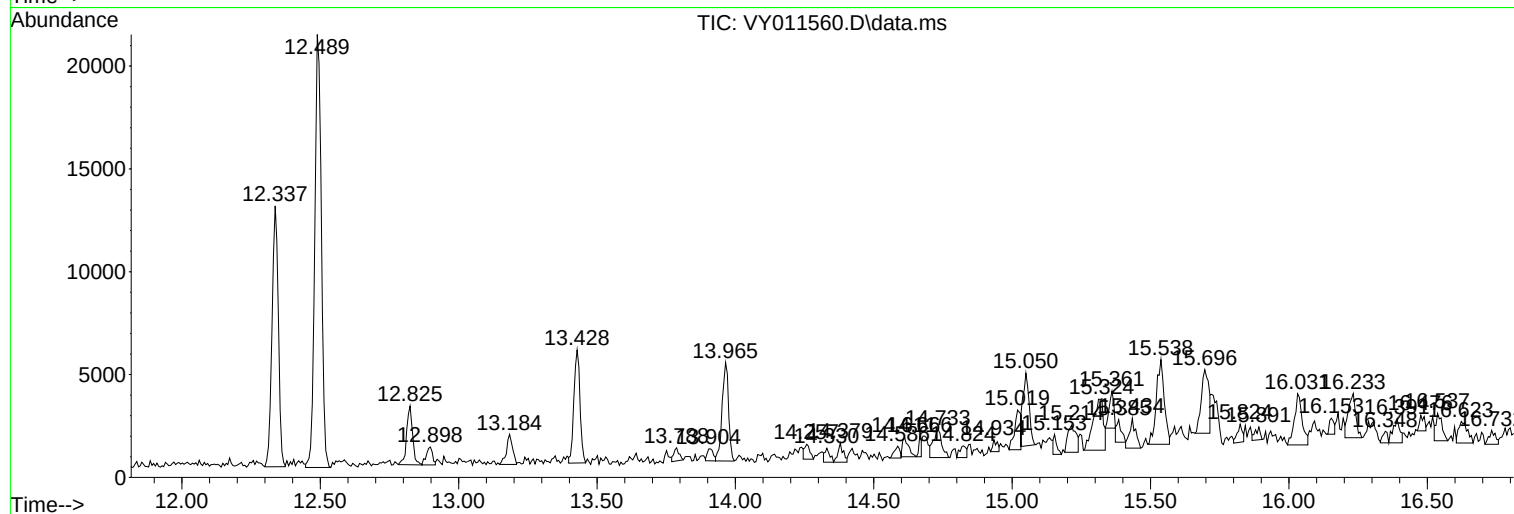
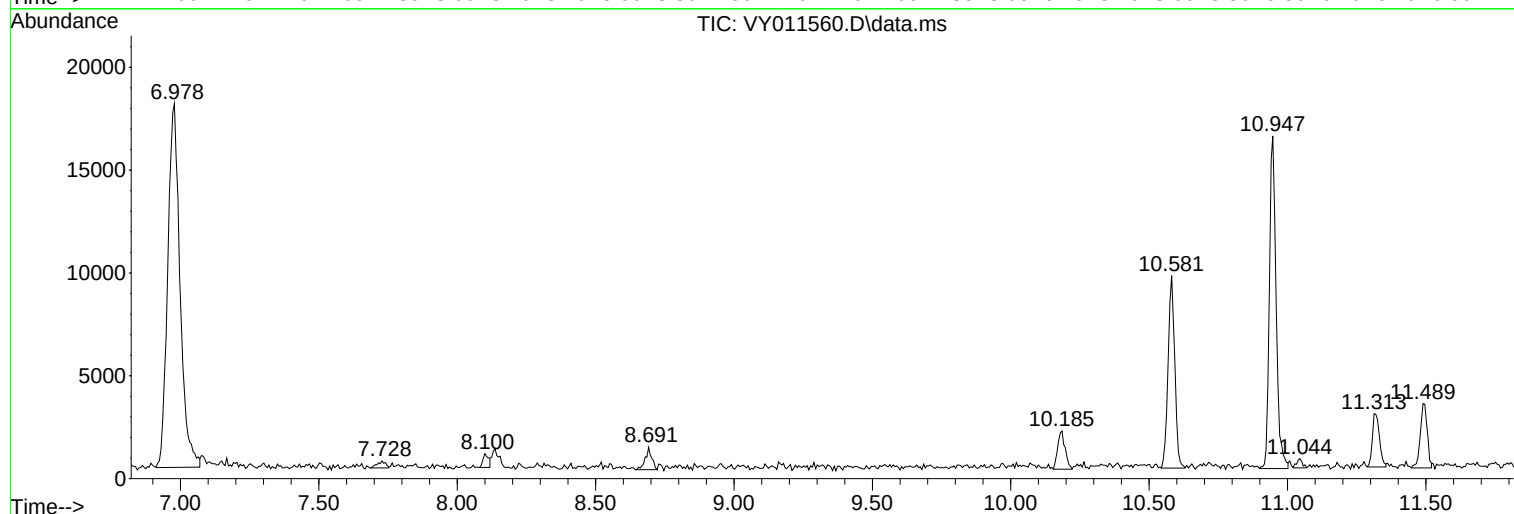
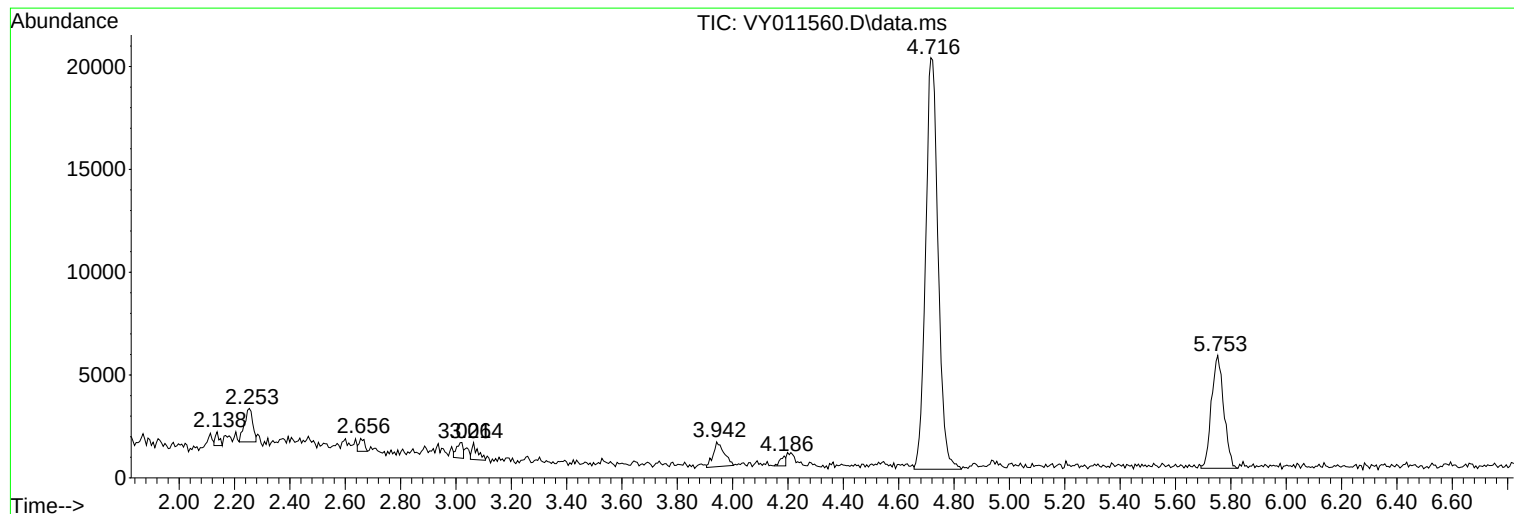
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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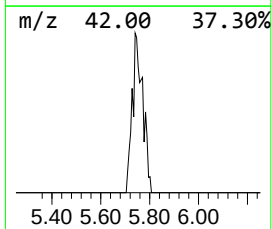
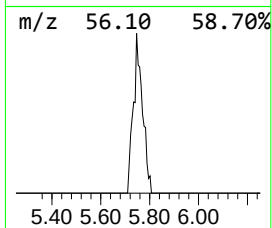
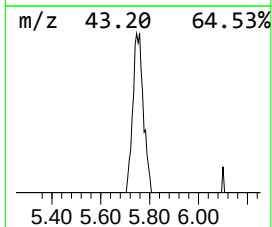
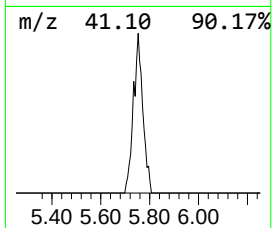
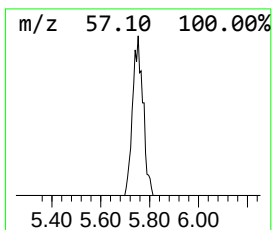
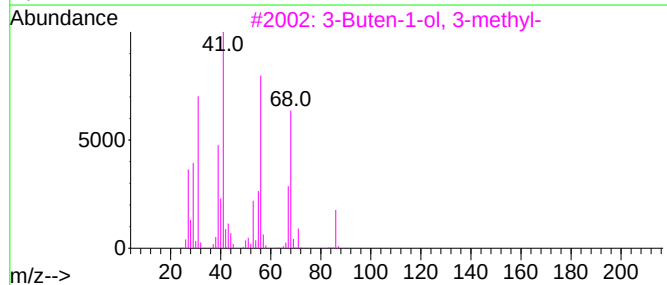
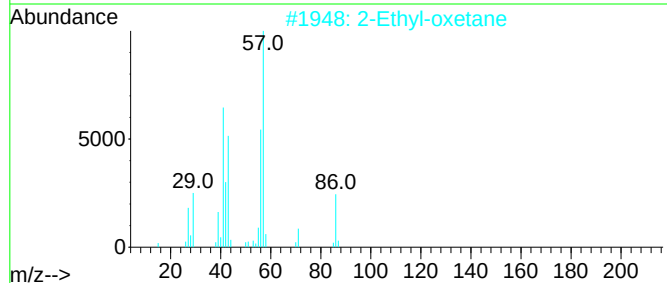
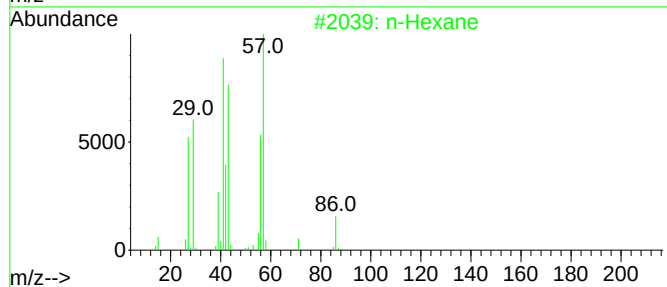
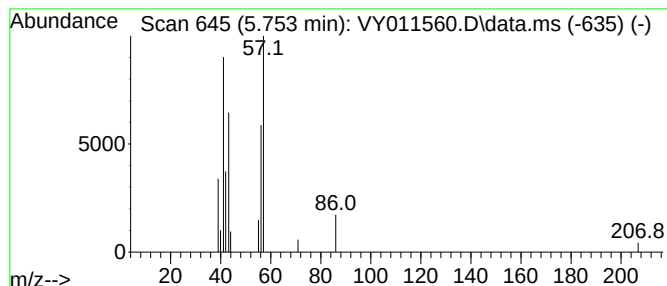
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111822S.M
Quant Title : SW846 8260

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

Peak Number 6 n-Hexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.753	1202.42 ug/l	16906	Pentafluorobenzene	7.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	80
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	72
3			3-Buten-1-ol, 3-methyl-	86	C5H10O	000763-32-6	25
4			Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	9
5			1-Heptene	98	C7H14	000592-76-7	9



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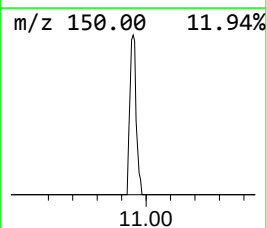
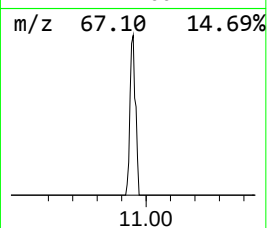
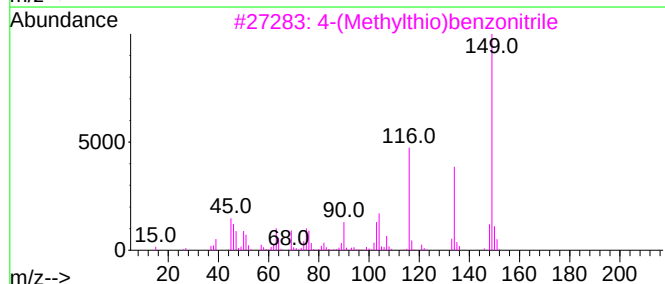
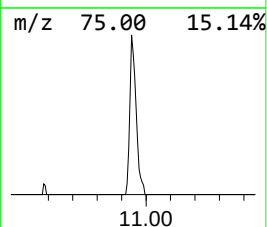
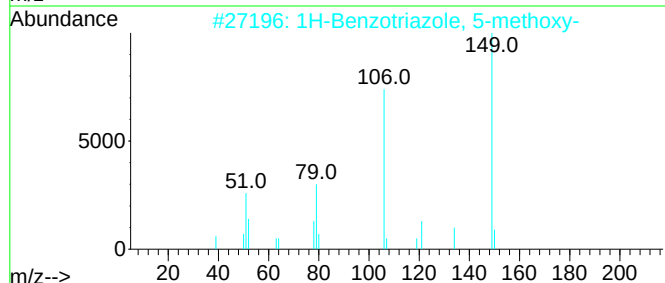
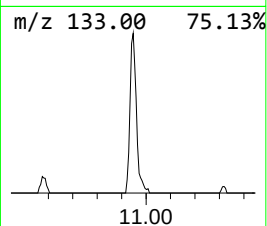
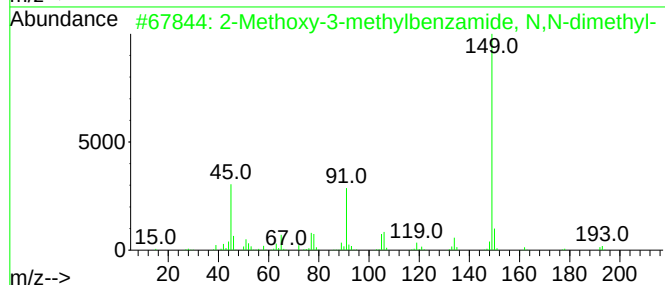
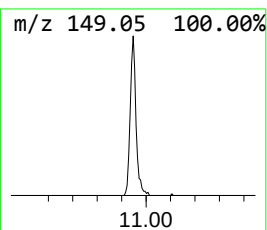
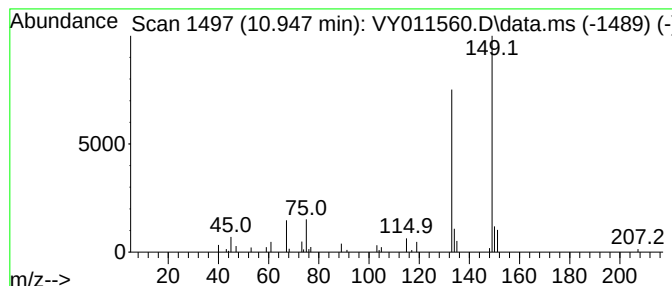
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111822S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown10.947 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	252.03 ug/l	27406	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methoxy-3-methylbenzamide, N,N...	193	C11H15NO2	1369798-01-5	32
2			1H-Benzotriazole, 5-methoxy-	149	C7H7N3O	027799-91-3	25
3			4-(Methylthio)benzonitrile	149	C8H7NS	021382-98-9	25
4			2-tert-Butyl-6-methyl-phenol, ac...	206	C13H18O2	125829-28-9	25
5			(1-t-Butylthiovinyl)oxy)trimethyl...	204	C9H20OSSI	063584-47-4	23



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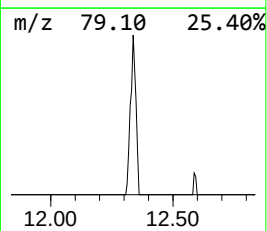
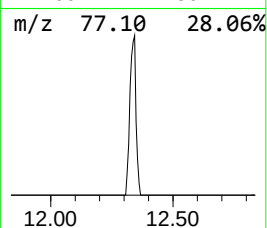
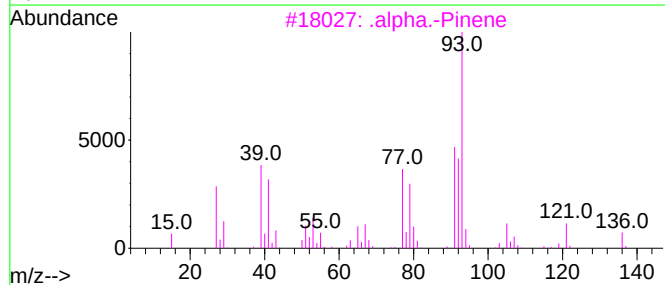
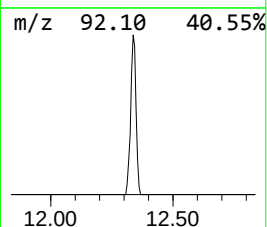
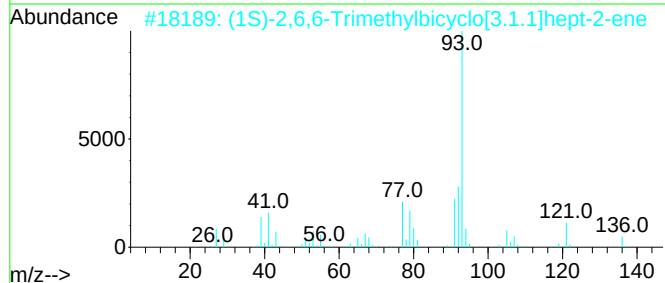
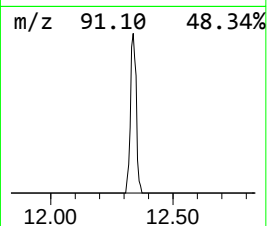
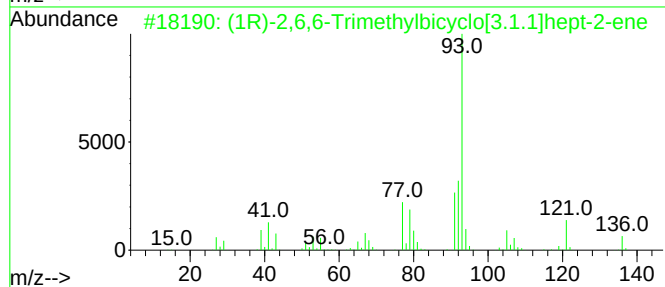
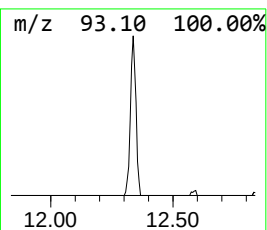
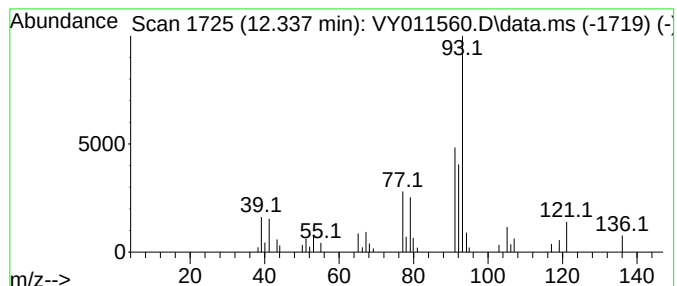
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Peak Number 9 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.337	185.78 ug/l	20202	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	91		
2	(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	91		
3	.alpha.-Pinene	136	C10H16	000080-56-8	91		
4	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	87		
5	1,3,6-Octatriene, 3,7-dimethyl-, (1R)-	136	C10H16	003338-55-4	87		



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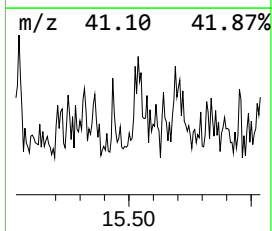
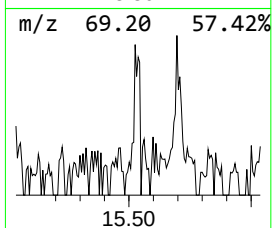
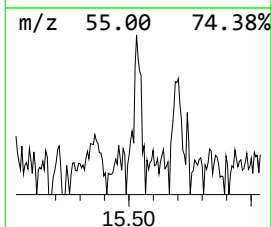
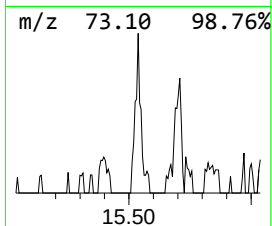
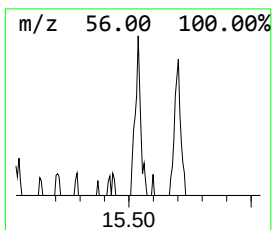
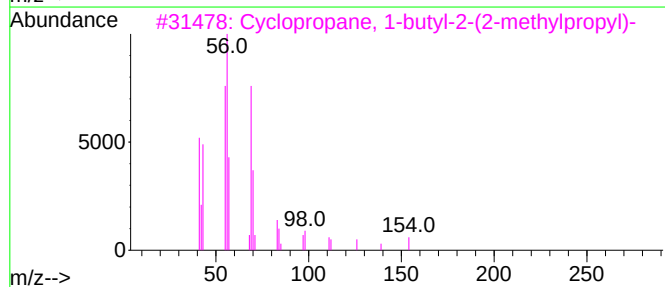
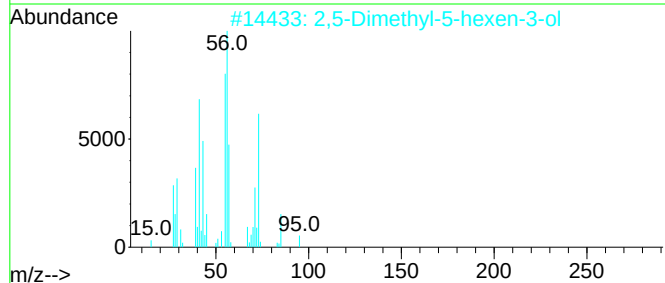
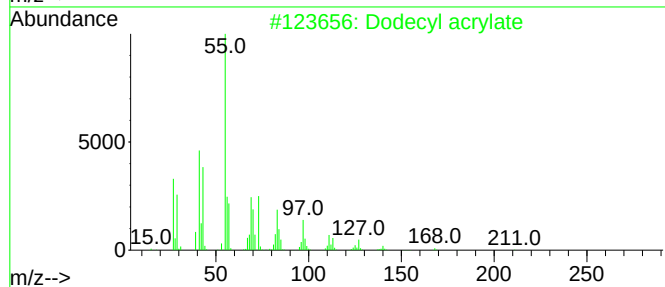
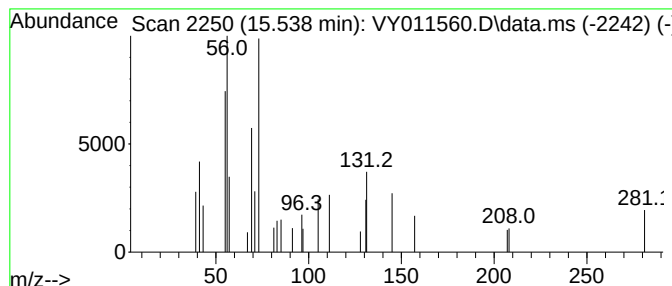
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TIC Library : C:\Database\NIST20.L
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Peak Number 10 unknown15.538 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.538	48.47 ug/l	8159	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecyl acrylate	240	C15H28O2	002156-97-0	23
2			2,5-Dimethyl-5-hexen-3-ol	128	C8H16O	067760-91-2	22
3			Cyclopropane, 1-butyl-2-(2-methy...	154	C11H22	041977-35-9	22
4			Tridecane, 7-methylene-	196	C14H28	019780-80-4	16
5			(S)-3,4-Dimethylpentanol	116	C7H16O	1000143-83-9	14



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexane	5.753	1202.4	ug/l	16906	1	7.801	703	50.0
unknown10.947	10.947	252.0	ug/l	27406	3	11.490	5437	50.0
(1R)-2,6,6-Trim...	12.337	185.8	ug/l	20202	3	11.490	5437	50.0
unknown15.538	15.538	48.5	ug/l	8159	4	13.428	8417	50.0