

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112322\
 Data File : VY011584.D
 Acq On : 23 Nov 2022 18:41
 Operator : KP/MD
 Sample : N5772-01
 Misc : 6.71g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 LOCATION-1

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: VY011584.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.710	464	474	495	rBV2	28820	94335	8.96%	1.391%
2	5.747	634	644	655	rBV4	4025	11654	1.11%	0.172%
3	7.716	957	967	973	rBV	150370	360495	34.23%	5.314%
4	7.789	973	979	991	rVB	231959	520329	49.40%	7.671%
5	8.142	1028	1037	1049	rBV	162375	347902	33.03%	5.129%
6	8.691	1118	1127	1139	rBV	397282	770953	73.20%	11.365%
7	10.179	1363	1371	1379	rBV	633932	1053248	100.00%	15.527%
8	11.489	1579	1586	1596	rBV	571479	886427	84.16%	13.068%
9	11.739	1623	1627	1638	rVB6	4699	12282	1.17%	0.181%
10	12.008	1662	1671	1677	rBV8	6067	17696	1.68%	0.261%
11	12.233	1704	1708	1713	rVB3	14313	25758	2.45%	0.380%
12	12.337	1714	1725	1732	rBV	215337	370267	35.15%	5.458%
13	12.483	1741	1749	1755	rBV	400154	652166	61.92%	9.614%
14	12.581	1755	1765	1770	rVV3	40265	91585	8.70%	1.350%
15	12.642	1770	1775	1782	rVB4	17710	40100	3.81%	0.591%
16	12.733	1782	1790	1793	rBV7	8874	22049	2.09%	0.325%
17	12.788	1794	1799	1813	rVV5	30708	97506	9.26%	1.437%
18	12.910	1815	1819	1823	rVV4	14646	27832	2.64%	0.410%
19	12.946	1823	1825	1829	rVB3	8918	11687	1.11%	0.172%
20	12.995	1829	1833	1837	rBV4	7222	12890	1.22%	0.190%
21	13.044	1837	1841	1842	rVV4	9730	14371	1.36%	0.212%
22	13.068	1842	1845	1851	rVB3	18301	27662	2.63%	0.408%
23	13.172	1858	1862	1868	rBV4	10635	19590	1.86%	0.289%
24	13.282	1868	1880	1884	rVV2	32257	70705	6.71%	1.042%
25	13.367	1884	1894	1898	rVV2	85220	194340	18.45%	2.865%
26	13.428	1898	1904	1909	rVV	385510	621637	59.02%	9.164%
27	13.477	1909	1912	1919	rVV2	29052	60028	5.70%	0.885%
28	13.562	1923	1926	1931	rVB5	8033	11108	1.05%	0.164%
29	13.641	1932	1939	1943	rBV4	11244	20156	1.91%	0.297%
30	13.745	1951	1956	1960	rBV6	21149	38327	3.64%	0.565%
31	13.873	1974	1977	1982	rVB5	14366	20458	1.94%	0.302%
32	13.965	1987	1992	2000	rVB5	15598	31832	3.02%	0.469%
33	14.141	2015	2021	2027	rBV10	10179	24890	2.36%	0.367%
34	14.257	2035	2040	2045	rBV7	16345	36299	3.45%	0.535%
35	14.306	2046	2048	2056	rVB7	9778	15139	1.44%	0.223%
36	14.385	2056	2061	2064	rBV4	18499	36601	3.48%	0.540%

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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

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

37	14.684	2104	2110	2114	rBV7	9723	20940	1.99%	0.309%
38	14.733	2115	2118	2125	rVB9	7910	15172	1.44%	0.224%
39	15.220	2193	2198	2204	rBV4	9050	17673	1.68%	0.261%
40	15.611	2258	2262	2266	rVB5	10552	17060	1.62%	0.251%
41	16.159	2347	2352	2356	rVB6	6282	11534	1.10%	0.170%
42	16.482	2399	2405	2417	rVB6	9114	30729	2.92%	0.453%

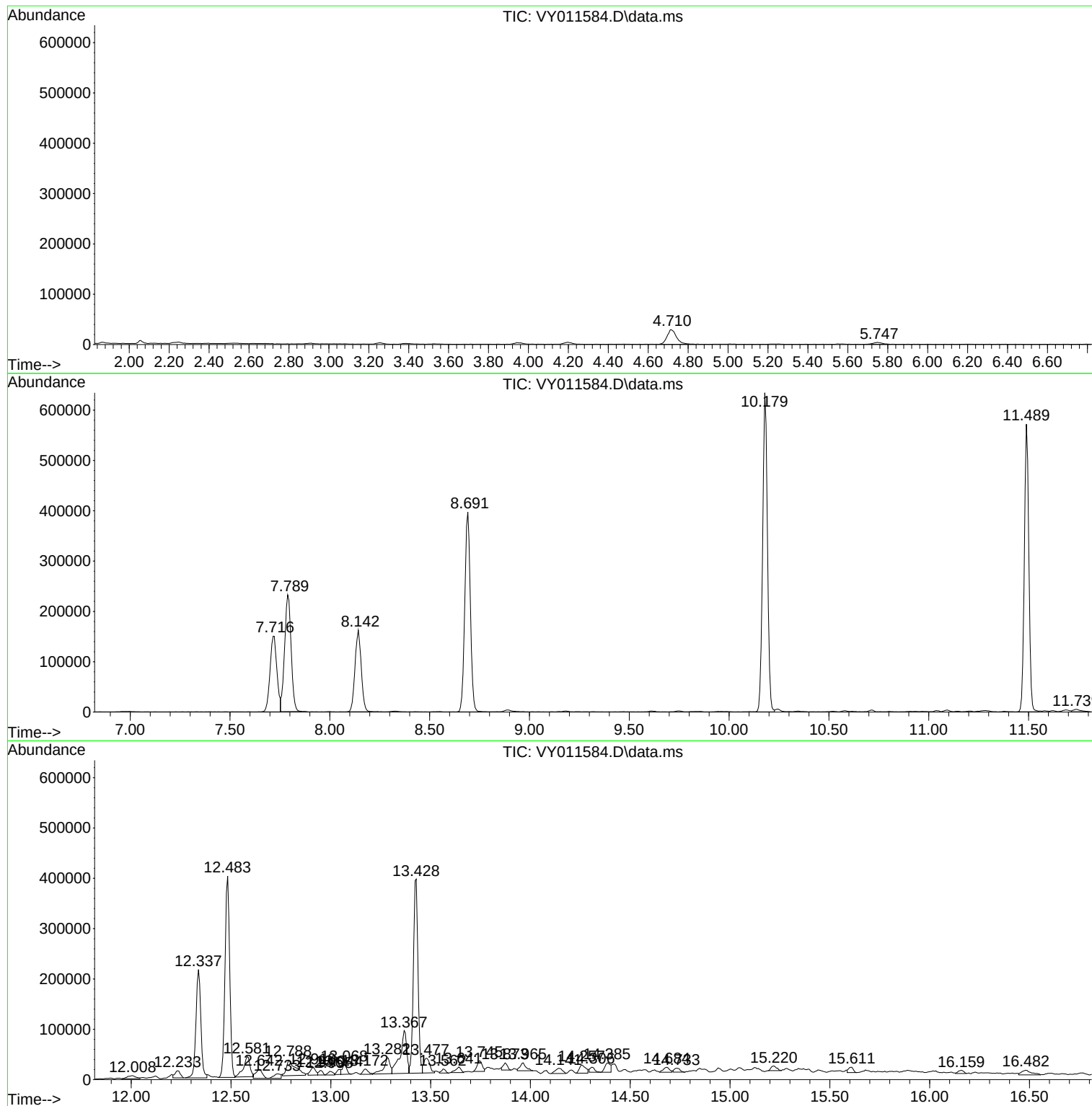
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111822S.M
Quant Title : SW846 8260

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



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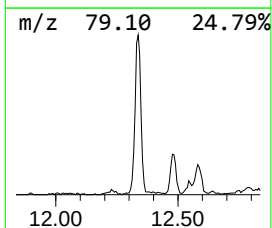
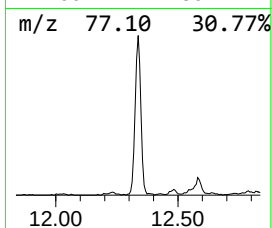
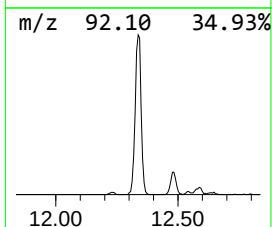
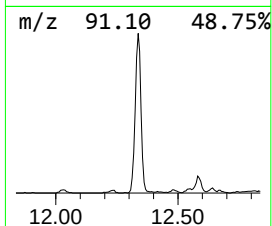
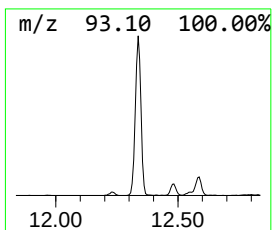
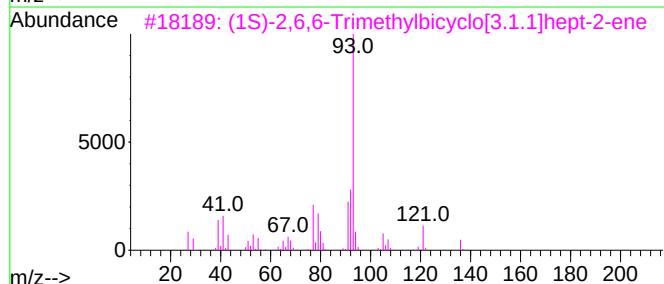
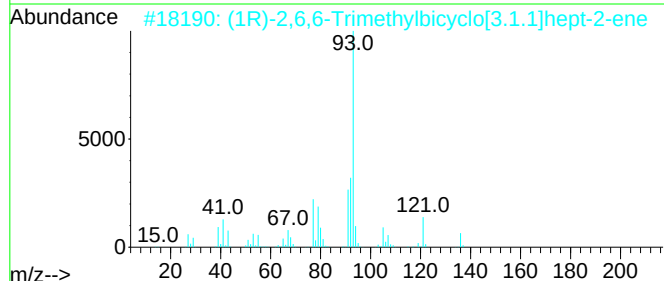
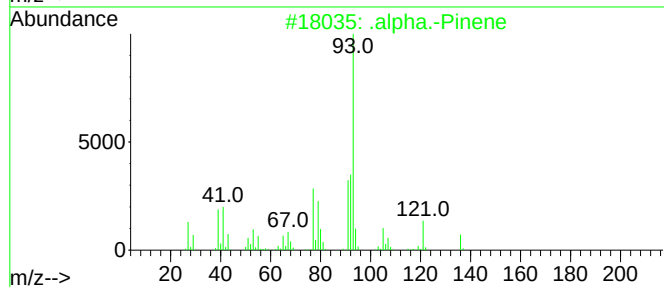
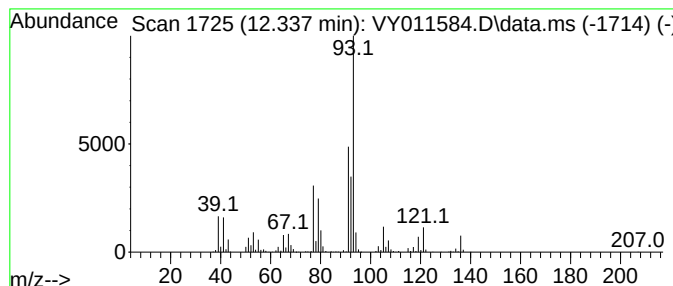
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111822S.M
Quant Title : SW846 8260

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

Peak Number 2 .alpha.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.337	20.89 ug/l	370267	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Pinene	136	C10H16	000080-56-8	97
2			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
3			(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	91
4			(+)-3-Carene	136	C10H16	000498-15-7	90
5			(+)-4-Carene	136	C10H16	029050-33-7	90



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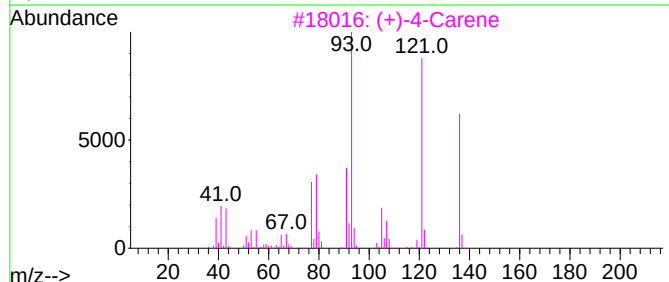
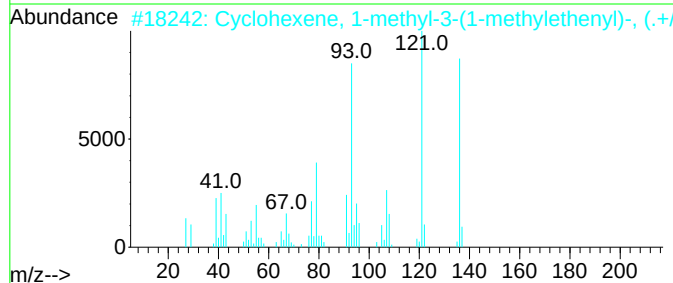
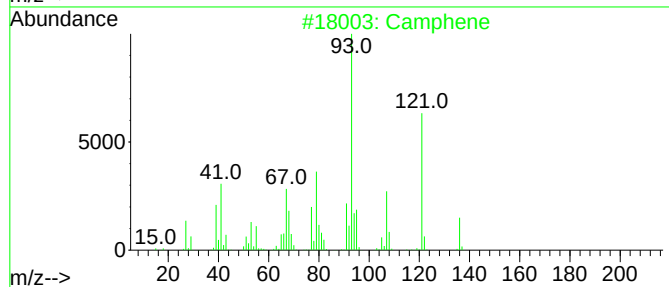
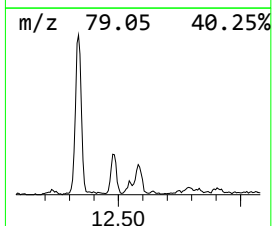
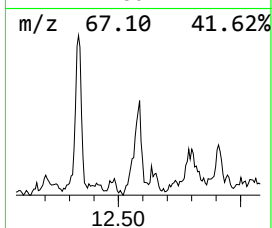
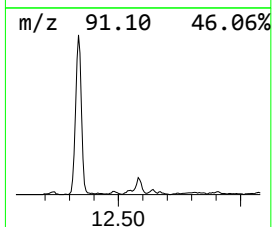
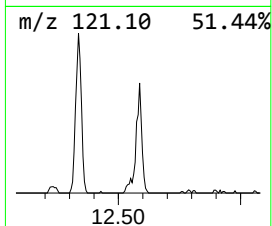
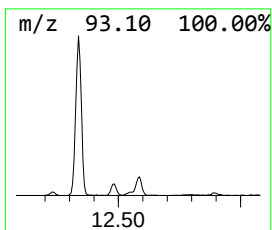
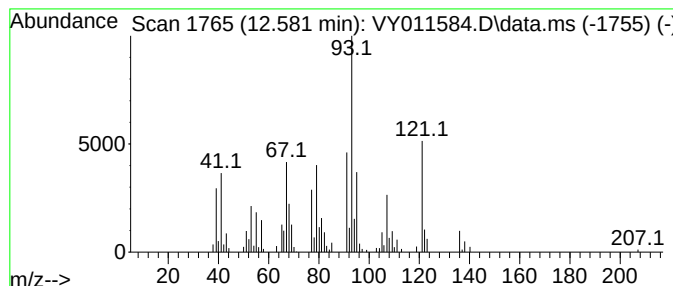
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Peak Number 3 Camphene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.581	7.37 ug/l	91585	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphene	136	C10H16	000079-92-5	95
2			Cyclohexene, 1-methyl-3-(1-methy...	136	C10H16	000499-03-6	58
3			(+)-4-Carene	136	C10H16	029050-33-7	58
4			1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	029548-02-5	55
5			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	52



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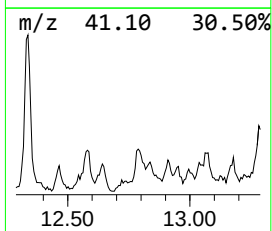
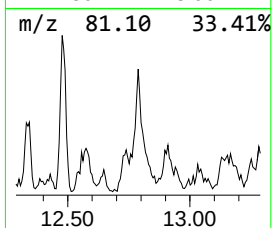
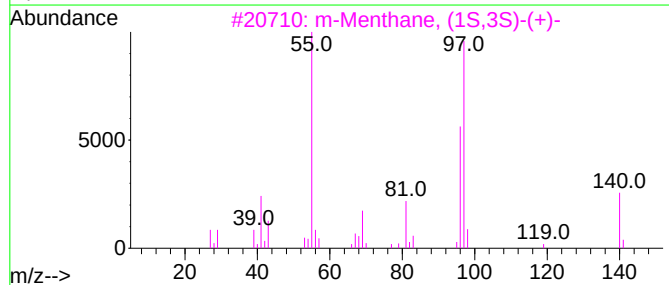
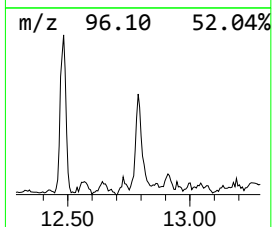
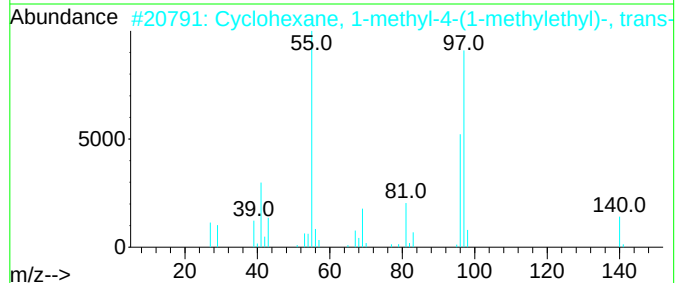
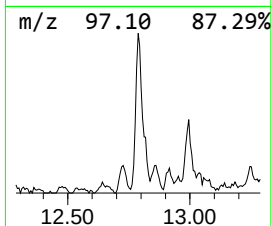
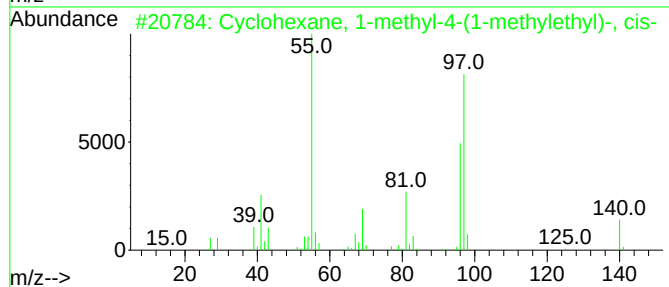
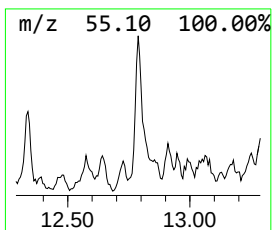
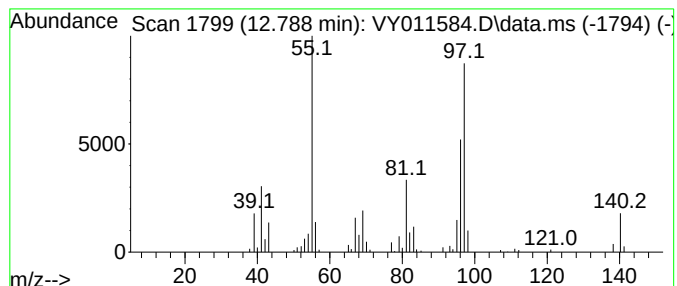
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111822S.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, 1-methyl-4-(1-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.788	7.84 ug/l	97506	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	95
2			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	90
3			m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	80
4			Oxalic acid, di(cyclohexylmethyl...	282	C16H26O4	1000309-68-5	80
5			1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	72



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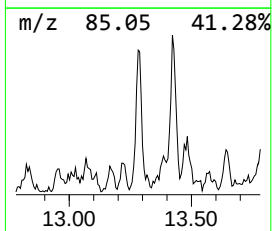
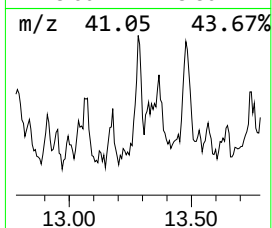
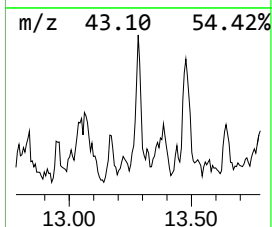
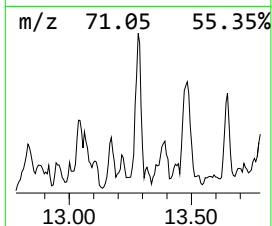
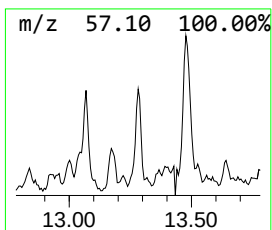
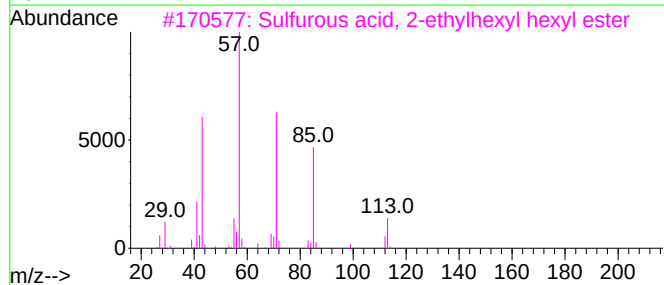
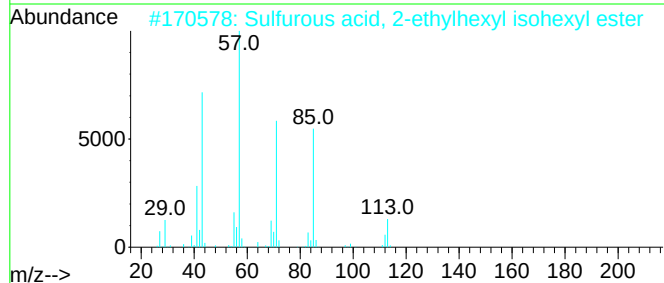
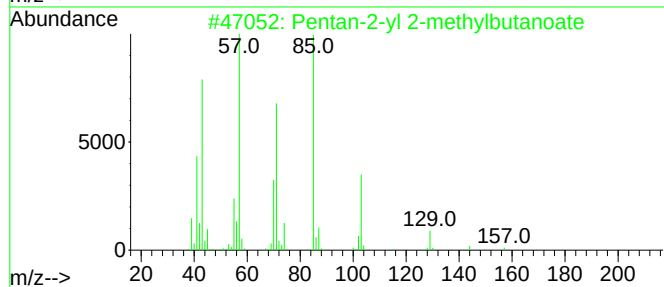
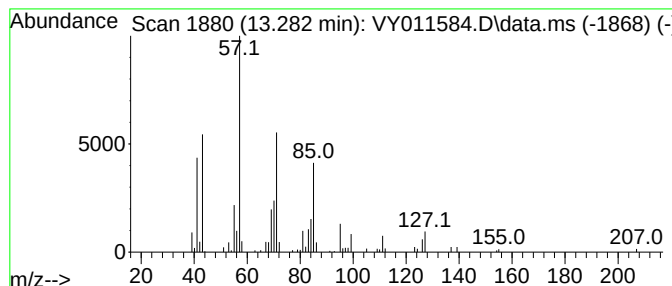
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Pentan-2-yl 2-methylbutanoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	5.69 ug/l	70705	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	53
2			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	50
3			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	50
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	47
5			Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	47



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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
.alpha.-Pinene	12.337	20.9	ug/l	370267	3	11.489	886427	50.0
Camphene	12.581	7.4	ug/l	91585	4	13.428	621637	50.0
Cyclohexane, 1-...	12.788	7.8	ug/l	97506	4	13.428	621637	50.0
Pentan-2-yl 2-m...	13.282	5.7	ug/l	70705	4	13.428	621637	50.0