

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060721\
 Data File : VX022541.D
 Acq On : 07 Jun 2021 18:04
 Operator : JC/MD
 Sample : M2583-21 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 39-41

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_X\Method\82X060721W.M
 Title : SW846 8260

Signal : TIC: VX022541.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.569	71	79	82	rVB7	4647	10148	2.41%	0.379%
2	2.386	205	213	218	rBV	15734	27060	6.42%	1.010%
3	2.550	234	240	247	rVB	6076	10651	2.53%	0.398%
4	4.580	564	573	583	rBV2	5120	16497	3.91%	0.616%
5	5.391	695	706	720	rBV2	42124	124895	29.63%	4.663%
6	5.556	724	733	748	rBV2	70304	201403	47.78%	7.520%
7	5.970	790	801	811	rBV	55613	147601	35.01%	5.511%
8	6.769	923	932	944	rBV	128734	301275	71.47%	11.249%
9	7.470	1042	1047	1055	rVB2	2923	5608	1.33%	0.209%
10	8.580	1221	1229	1234	rBV2	8212	13885	3.29%	0.518%
11	8.653	1234	1241	1249	rVV	274132	421537	100.00%	15.739%
12	8.720	1249	1252	1258	rVV	6592	10999	2.61%	0.411%
13	10.055	1462	1471	1485	rVB	257415	361696	85.80%	13.504%
14	10.220	1491	1498	1500	rBV2	3206	5291	1.26%	0.198%
15	10.549	1548	1552	1561	rVB	6204	8697	2.06%	0.325%
16	11.085	1634	1640	1646	rBV	202496	252077	59.80%	9.412%
17	11.305	1668	1676	1680	rVB6	2442	4745	1.13%	0.177%
18	11.360	1680	1685	1691	rBV	8573	12405	2.94%	0.463%
19	11.762	1744	1751	1759	rBV6	2091	5173	1.23%	0.193%
20	11.975	1778	1786	1789	rVV2	7634	9376	2.22%	0.350%
21	12.024	1789	1794	1803	rVB	260136	314695	74.65%	11.750%
22	12.110	1803	1808	1814	rBV6	2704	5529	1.31%	0.206%
23	12.219	1821	1826	1838	rBV	21832	37068	8.79%	1.384%
24	12.768	1909	1916	1917	rBV2	5598	6287	1.49%	0.235%
25	12.798	1917	1921	1926	rVB3	6770	11176	2.65%	0.417%
26	12.865	1926	1932	1937	rBV	37744	60386	14.33%	2.255%
27	12.975	1946	1950	1952	rBV2	11651	14897	3.53%	0.556%
28	13.067	1960	1965	1968	rBV3	14309	22681	5.38%	0.847%
29	13.109	1968	1972	1975	rBV2	32676	48734	11.56%	1.820%
30	13.213	1987	1989	1996	rVB7	3820	6843	1.62%	0.255%
31	13.268	1996	1998	2006	rVB8	3573	6273	1.49%	0.234%
32	13.408	2017	2021	2026	rVB5	5222	8669	2.06%	0.324%
33	13.591	2047	2051	2054	rVV4	9045	11809	2.80%	0.441%
34	13.701	2065	2069	2071	rBV3	9983	16463	3.91%	0.615%
35	13.731	2071	2074	2080	rVB	79422	108765	25.80%	4.061%
36	13.835	2087	2091	2094	rBV4	7256	12650	3.00%	0.472%

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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

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Title : SW846 8260

37	13.896	2098	2101	2110	rVB6	13125	29547	7.01%	1.103%
38	14.493	2196	2199	2209	rVB7	2120	4854	1.15%	0.181%

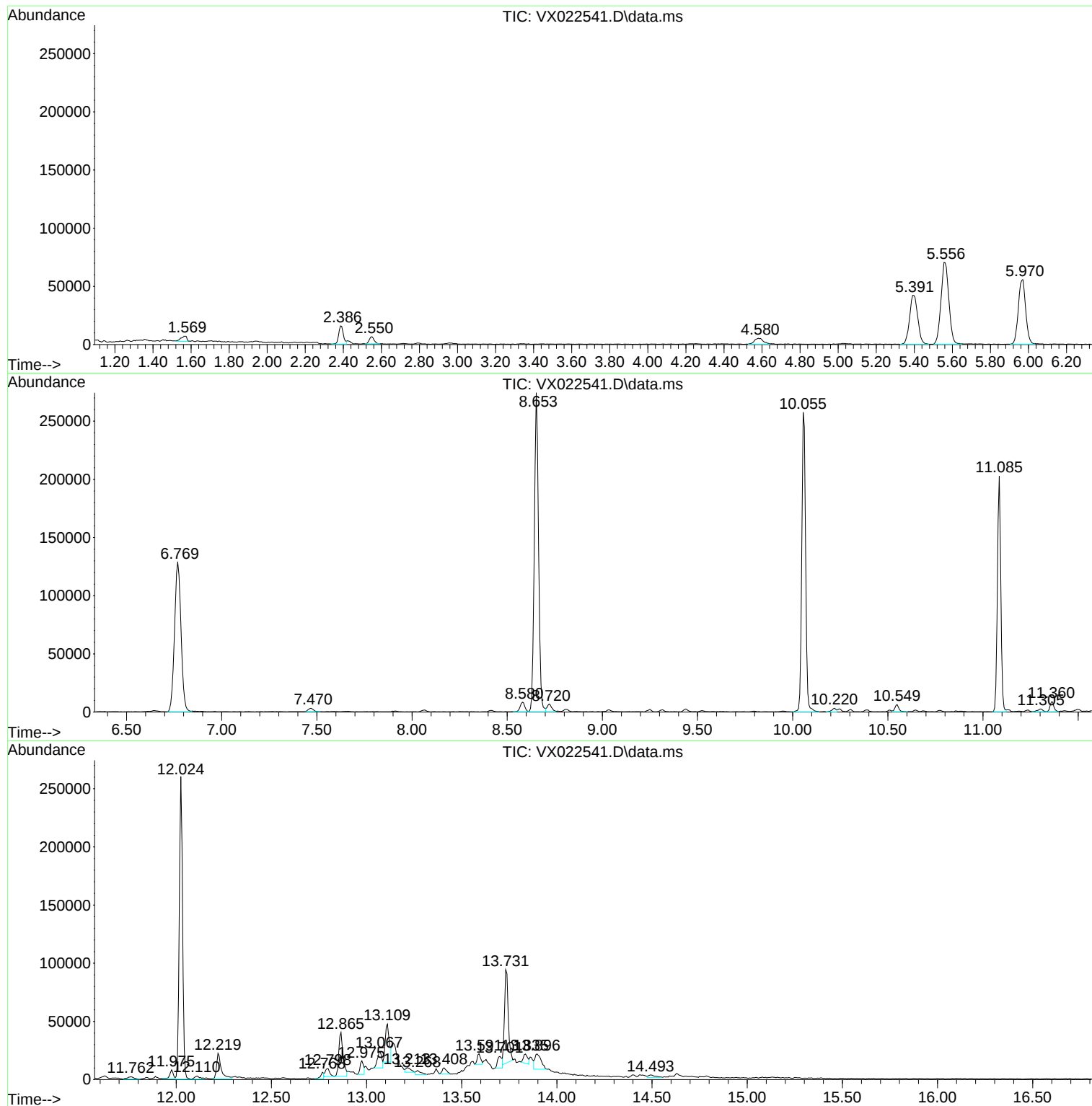
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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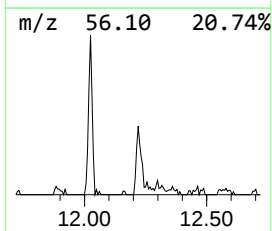
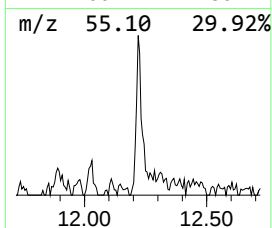
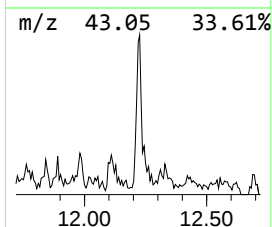
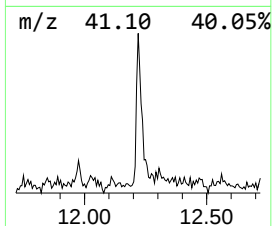
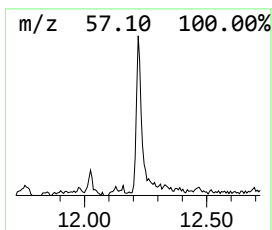
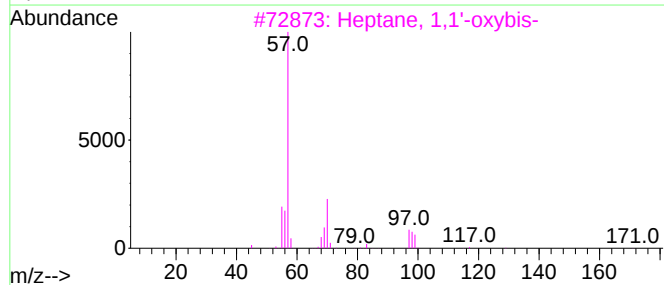
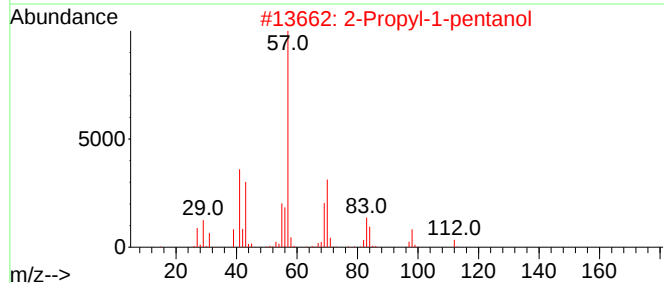
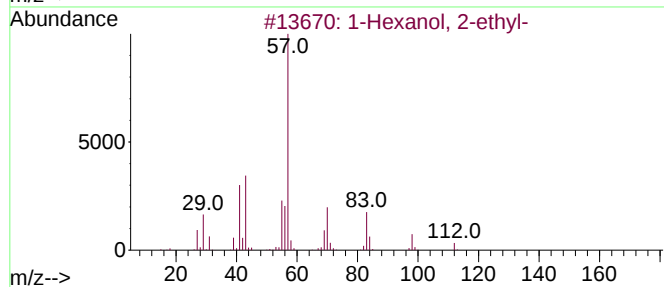
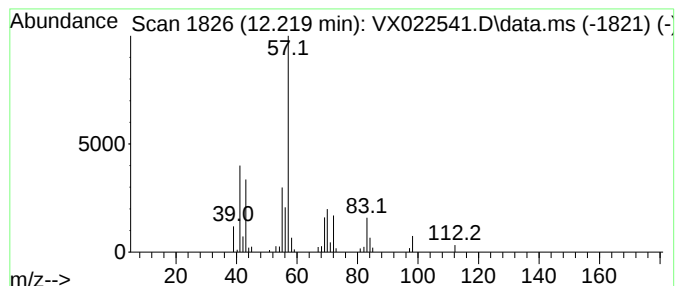
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	5.89 ug/l	37068	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4		1-Octyn-3-ol, 4-ethyl-	154	C10H18O	005877-42-9	50
5		Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	38



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Instrument :
MSVOA_X
ClientSampled :
39-41

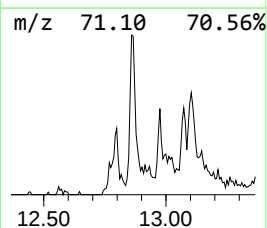
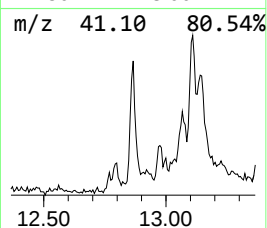
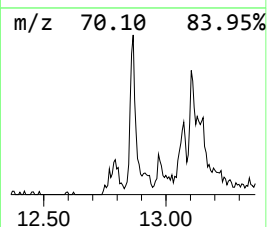
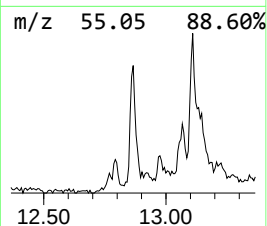
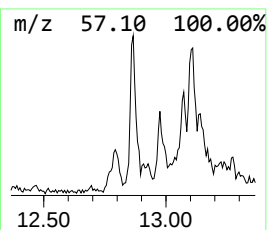
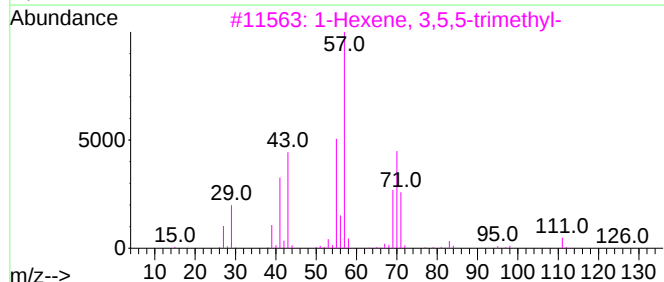
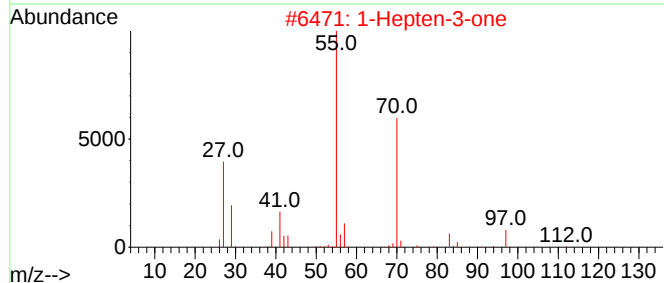
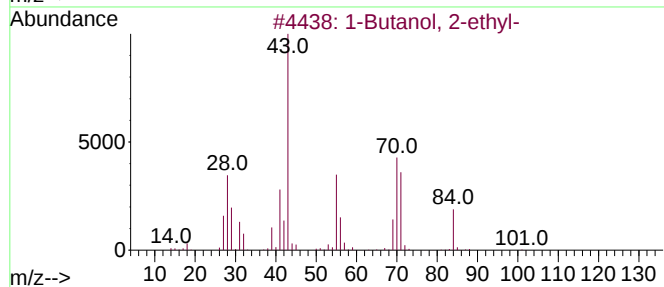
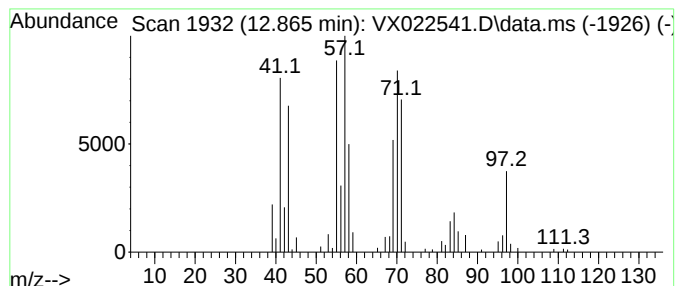
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Butanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.866	9.59 ug/l	60386	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	50
2			1-Hepten-3-one	112	C7H12O	002918-13-0	43
3			1-Hexene, 3,5,5-trimethyl-	126	C9H18	004316-65-8	38
4			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	38
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	37



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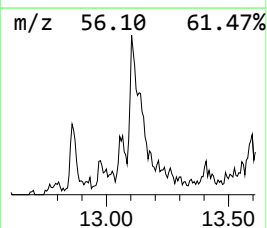
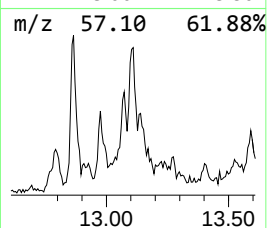
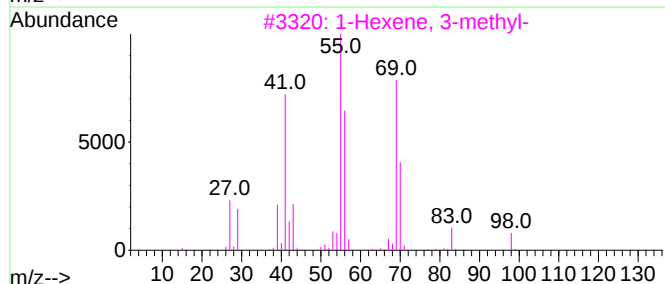
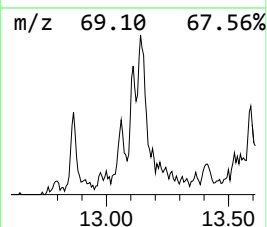
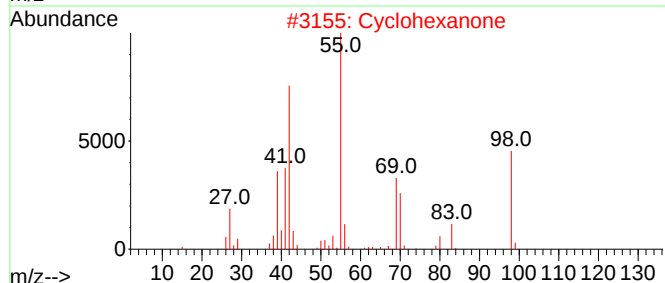
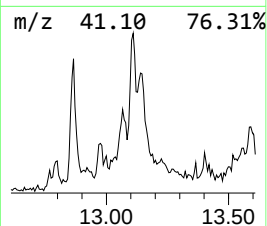
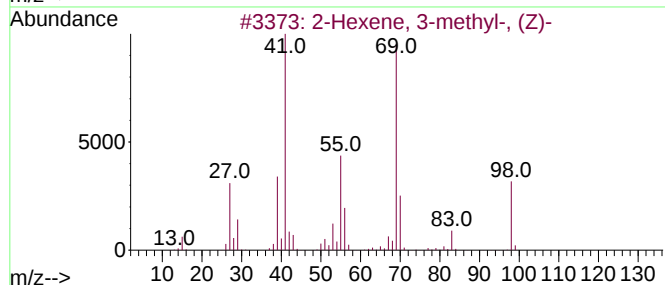
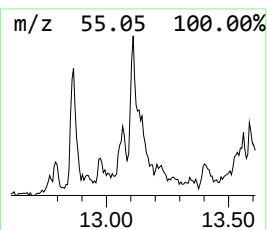
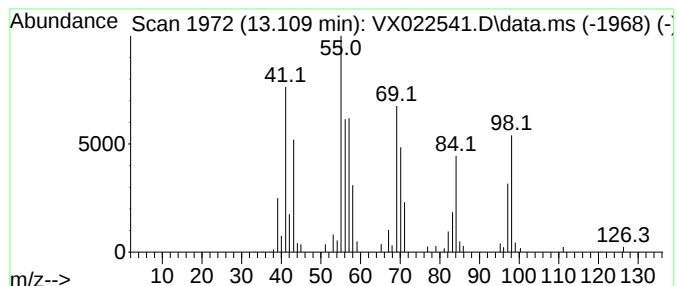
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown13.109 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.109	7.74 ug/l	48734	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 3-methyl-, (Z)-			98	C7H14	010574-36-4	43
2	Cyclohexanone			98	C6H10O	000108-94-1	38
3	1-Hexene, 3-methyl-			98	C7H14	003404-61-3	35
4	n-Heptyl hexanoate			214	C13H26O2	006976-72-3	35
5	2-Pentene, 3-methyl-, (Z)-			84	C6H12	000922-62-3	27



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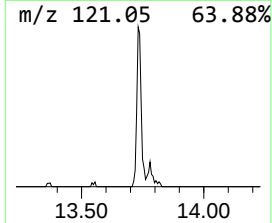
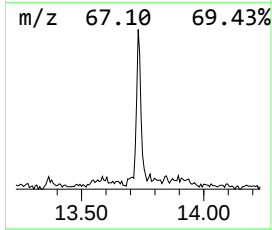
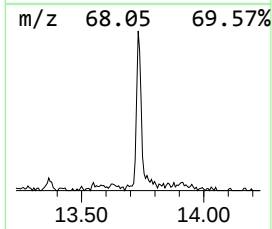
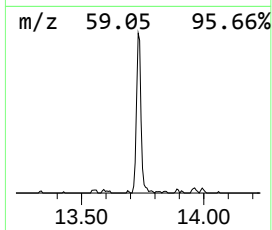
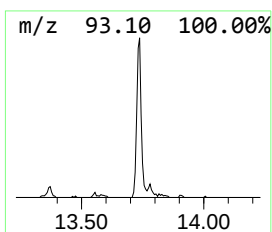
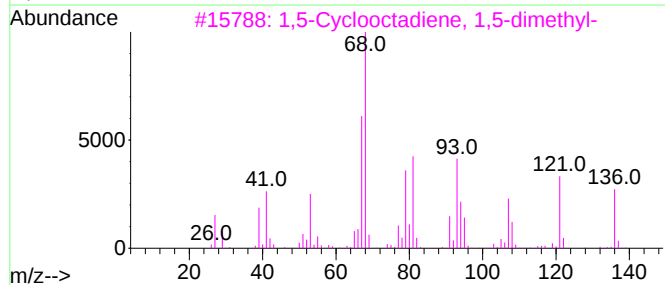
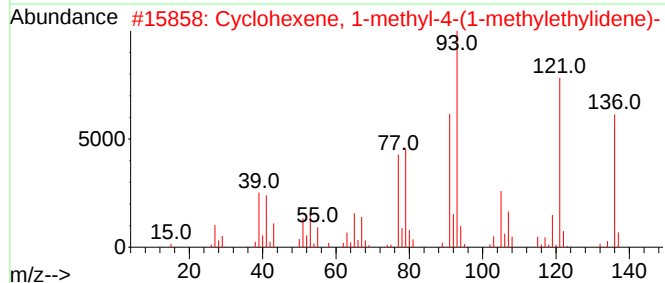
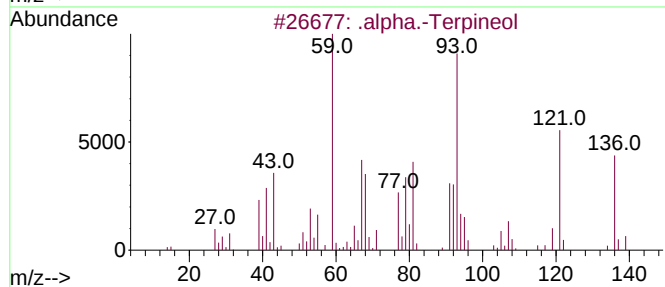
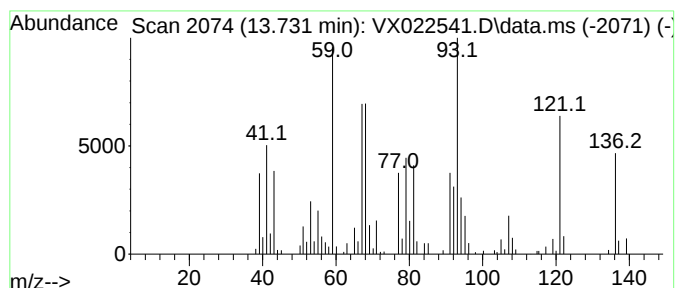
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 .alpha.-Terpineol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.731	17.28 ug/l	108765	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Terpineol	154	C10H18O	000098-55-5	87
2	Cyclohexene, 1-methyl-4-(1-methyl-2-propenyl)-	136	C10H16	000586-62-9	64
3	1,5-Cyclooctadiene, 1,5-dimethyl-	136	C10H16	003760-14-3	49
4	(1S)-2,6,6-Trimethylbicyclo[3.1.0]hex-2-ene	136	C10H16	007785-26-4	46
5	Bicyclo[2.2.1]hept-2-ene, 1,7,7-dimethyl-	136	C10H16	000464-17-5	46



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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	12.219	5.9	ug/l	37068	4	12.024	314695	50.0
1-Butanol, 2-et...	12.866	9.6	ug/l	60386	4	12.024	314695	50.0
unknown13.109	13.109	7.7	ug/l	48734	4	12.024	314695	50.0
.alpha.-Terpineol	13.731	17.3	ug/l	108765	4	12.024	314695	50.0