

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111422\
 Data File : VX032798.D
 Acq On : 14 Nov 2022 16:36
 Operator : JC/MD
 Sample : N5572-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31912

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\82X102622W.M
 Title : SW846 8260

Signal : TIC: VX032798.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	20	rVB	55860	56518	5.29%	1.175%
2	1.367	40	46	50	rBV2	7953	12148	1.14%	0.252%
3	1.501	64	68	72	rVB	9143	10874	1.02%	0.226%
4	2.385	207	213	224	rBV	25485	50824	4.76%	1.056%
5	4.227	506	515	529	rBV	74703	199368	18.66%	4.143%
6	4.568	560	571	585	rBV	4779	14978	1.40%	0.311%
7	5.385	693	705	722	rBV2	63849	187596	17.56%	3.899%
8	5.549	722	732	750	rVB	102736	290089	27.15%	6.028%
9	5.952	787	798	806	rBV	67527	179137	16.77%	3.723%
10	6.043	806	813	822	rVB2	18011	50484	4.72%	1.049%
11	6.763	919	931	945	rBV	158994	376896	35.27%	7.832%
12	7.256	1002	1012	1025	rBV5	4205	16525	1.55%	0.343%
13	7.580	1060	1065	1074	rVB2	7218	13420	1.26%	0.279%
14	8.646	1234	1240	1247	rBV	339070	524556	49.09%	10.901%
15	8.720	1247	1252	1257	rVV	39753	60056	5.62%	1.248%
16	8.781	1257	1262	1272	rVB2	7677	15560	1.46%	0.323%
17	9.250	1333	1339	1346	rBV2	5674	10817	1.01%	0.225%
18	10.055	1465	1471	1484	rVB	329707	443579	41.52%	9.218%
19	10.158	1484	1488	1491	rBV2	9321	13053	1.22%	0.271%
20	10.299	1506	1511	1520	rVB	23010	33318	3.12%	0.692%
21	10.445	1527	1535	1541	rVB	15510	21263	1.99%	0.442%
22	10.646	1563	1568	1572	rBV2	15602	28499	2.67%	0.592%
23	10.756	1581	1586	1591	rBV2	18839	27365	2.56%	0.569%
24	11.079	1634	1639	1645	rBV	311130	401525	37.58%	8.344%
25	11.573	1715	1720	1723	rBV2	9306	13260	1.24%	0.276%
26	11.756	1746	1750	1754	rBV2	11557	15626	1.46%	0.325%
27	11.890	1770	1772	1779	rVB4	9143	13520	1.27%	0.281%
28	12.024	1789	1794	1801	rVB	355614	449781	42.10%	9.347%
29	12.219	1821	1826	1837	rBV	858557	1068469	100.00%	22.204%
30	12.304	1837	1840	1848	rVB5	26173	46071	4.31%	0.957%
31	12.414	1854	1858	1864	rVB	26517	32964	3.09%	0.685%
32	12.566	1879	1883	1889	rVB8	6895	11201	1.05%	0.233%
33	13.749	2073	2077	2079	rBV3	9045	11635	1.09%	0.242%
34	13.774	2079	2081	2085	rVB	22636	27155	2.54%	0.564%
35	13.847	2090	2093	2100	rVB2	11159	16597	1.55%	0.345%
36	13.914	2100	2104	2111	rBV2	12356	16394	1.53%	0.341%

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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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37	14.639	2215	2223	2229	rVB2	11170	18328	1.72%	0.381%
38	15.968	2435	2441	2452	rBV3	15628	32554	3.05%	0.677%

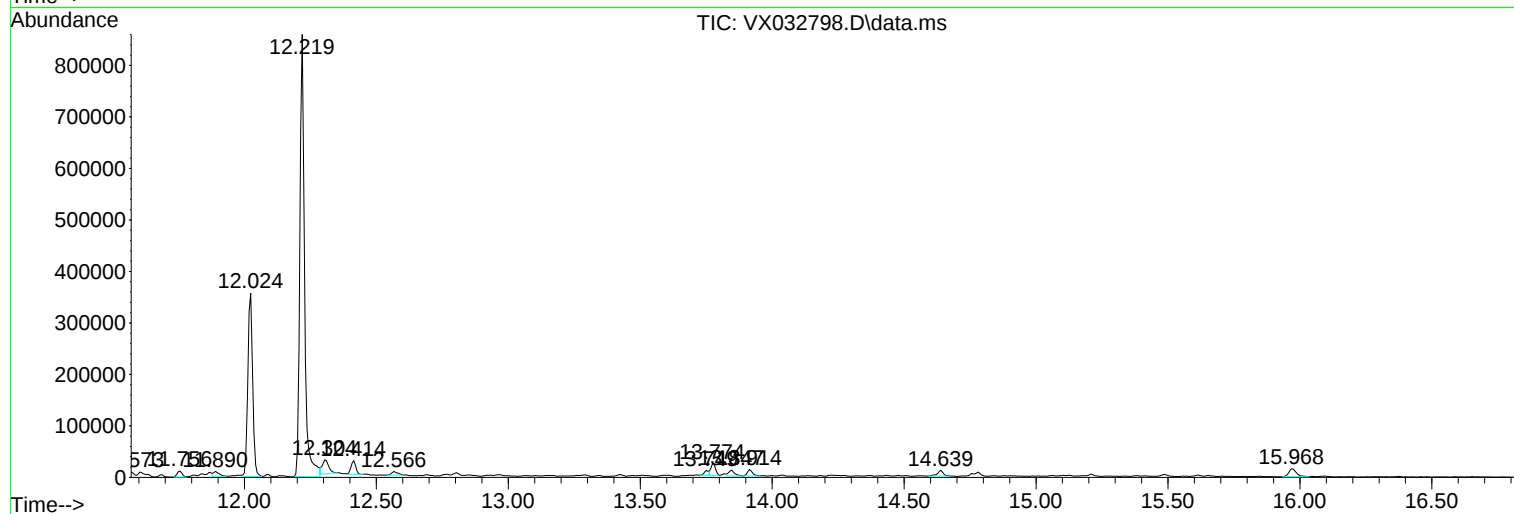
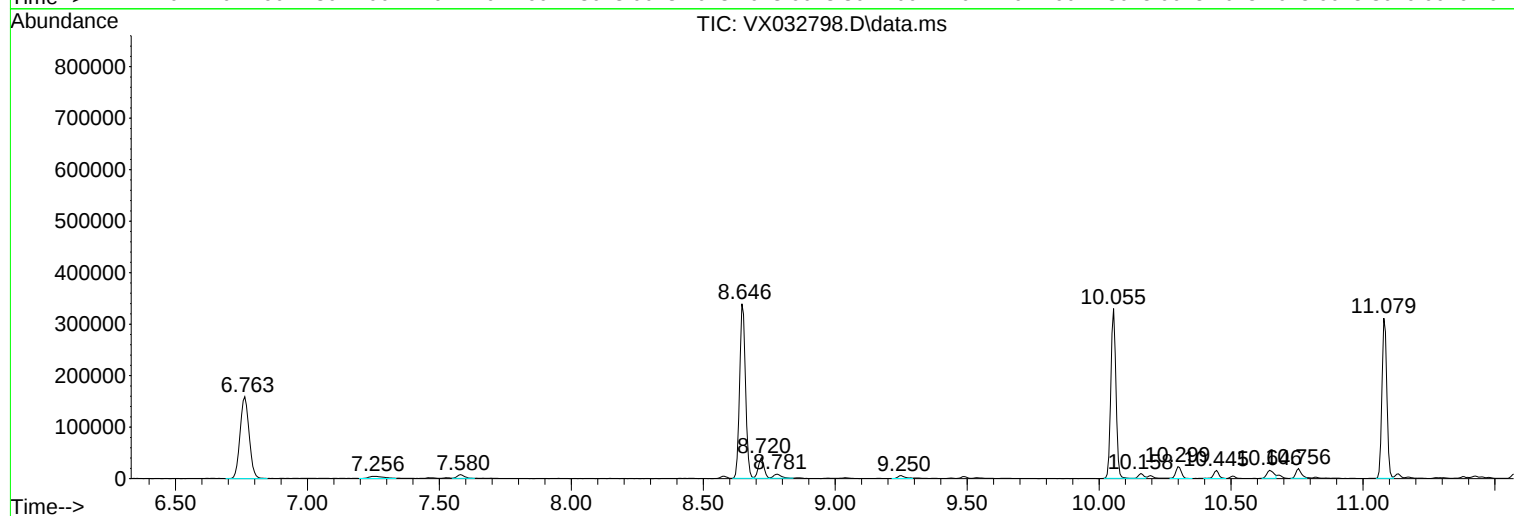
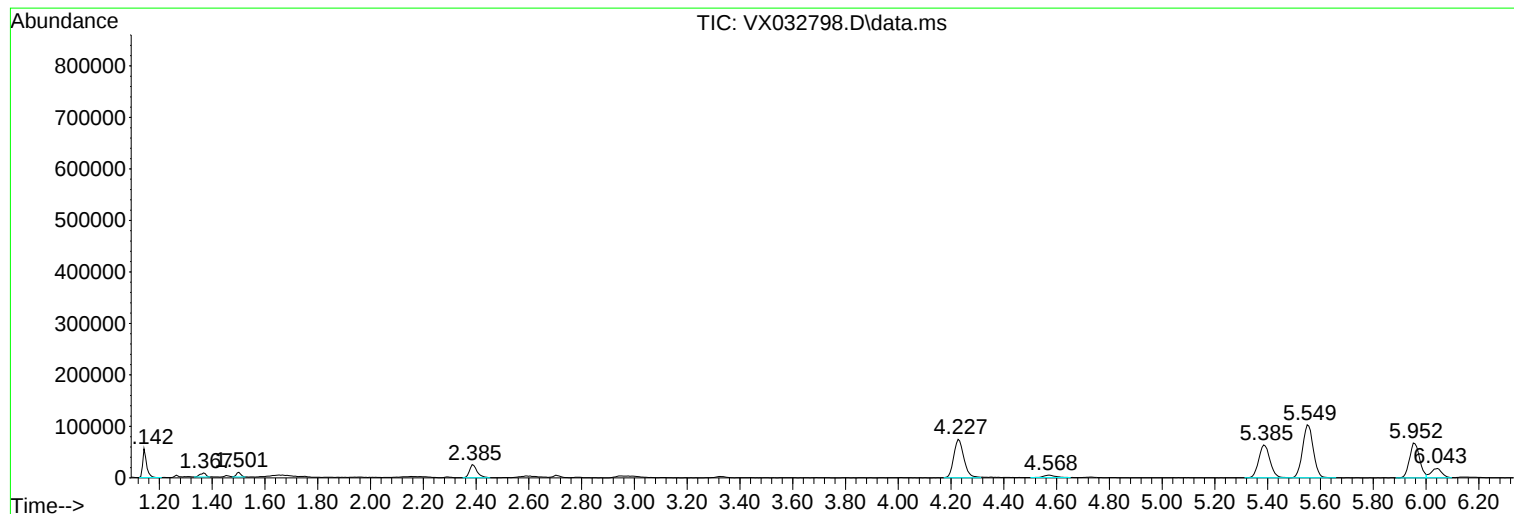
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



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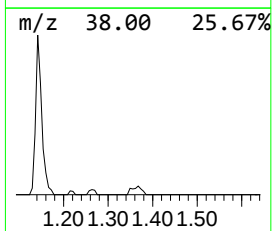
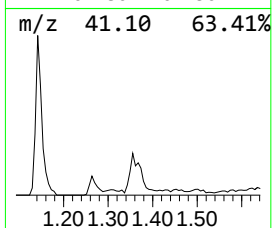
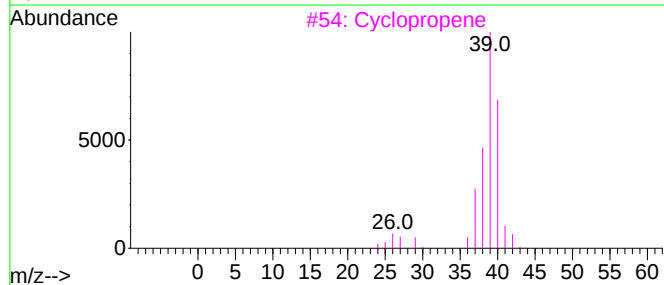
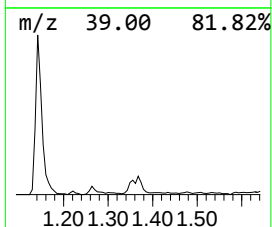
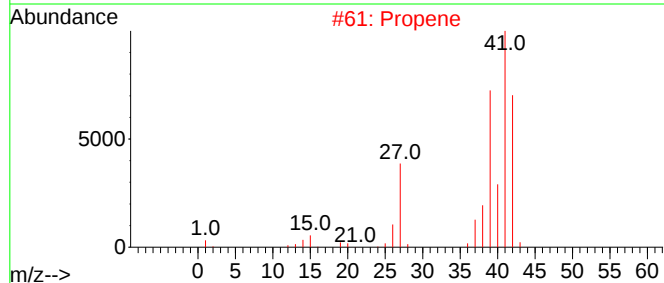
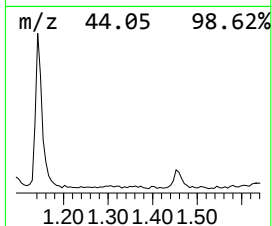
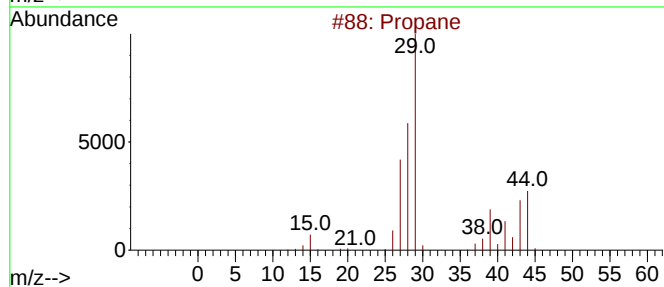
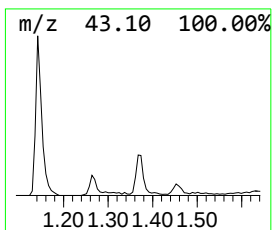
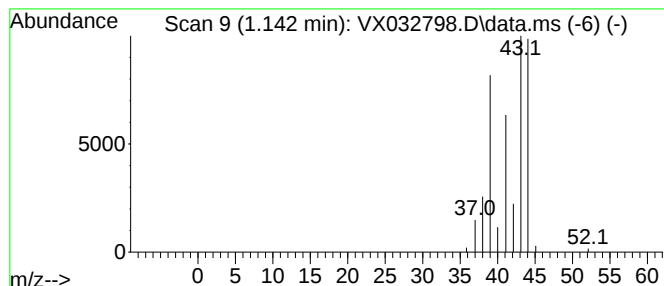
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	9.74 ug/l	56518	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane			44	C3H8	000074-98-6	83
2	Propene			42	C3H6	000115-07-1	9
3	Cyclopropene			40	C3H4	002781-85-3	2
4	Alanine			89	C3H7NO2	000056-41-7	2
5	1-(Methylamino)propan-2-ol			89	C4H11NO	1000486-79-1	1



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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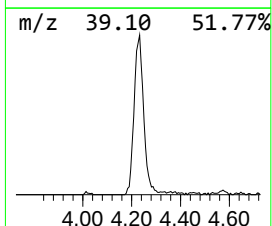
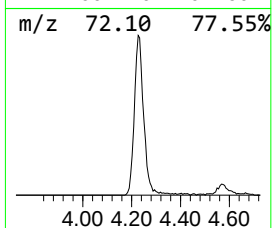
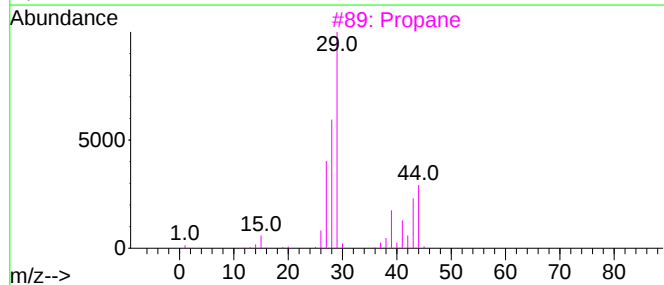
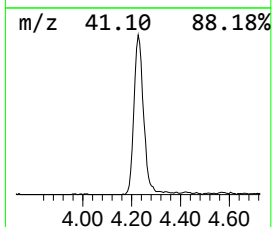
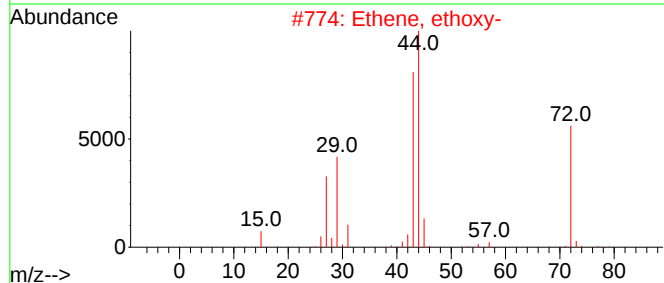
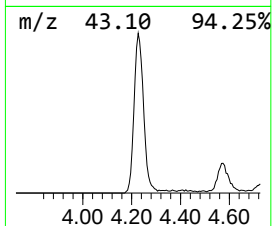
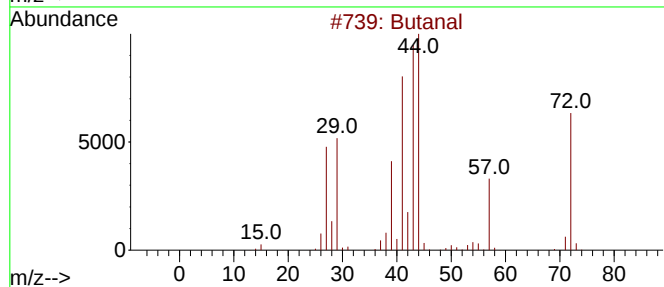
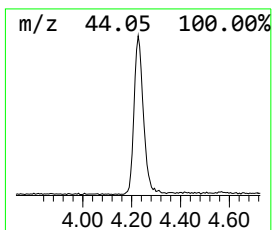
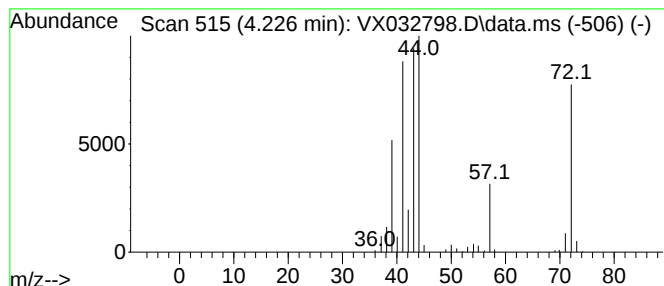
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.226	34.36 ug/l	199368	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3			Propane	44	C3H8	000074-98-6	47
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38



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ALS Vial : 18 Sample Multiplier: 1

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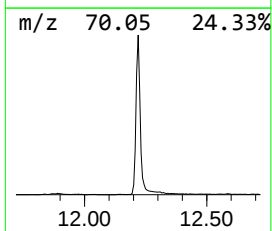
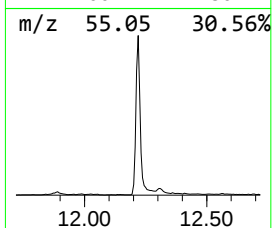
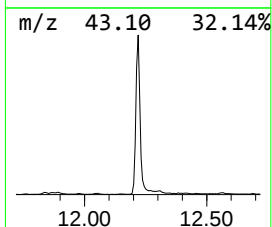
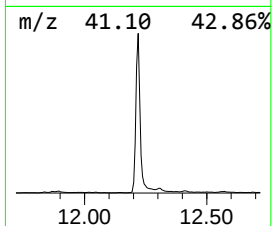
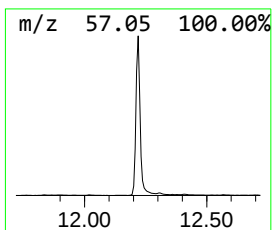
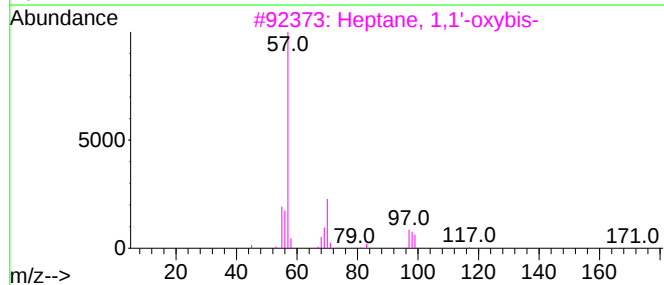
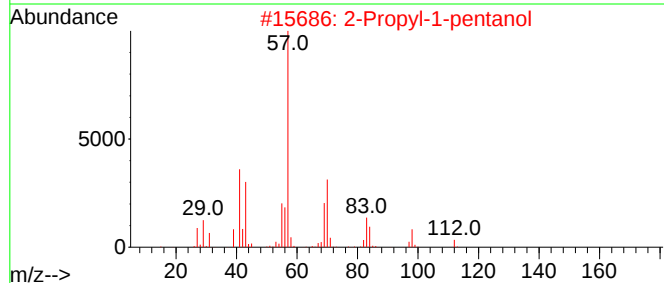
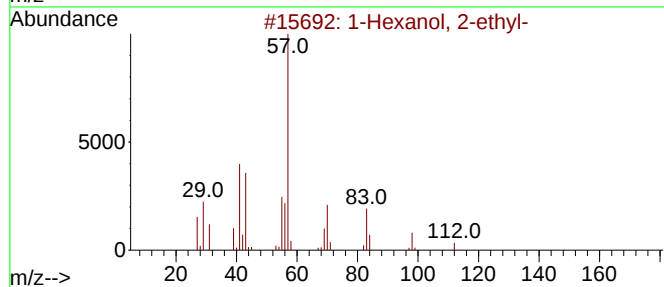
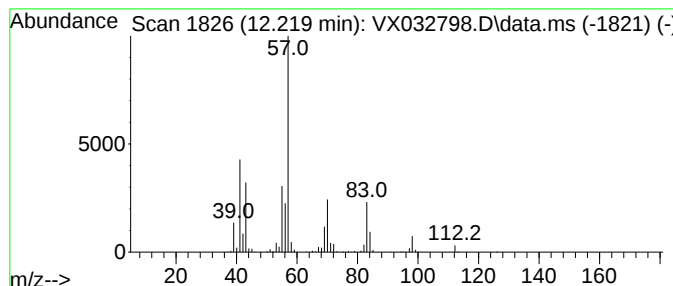
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	118.78 ug/l	1068470	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	90
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	43



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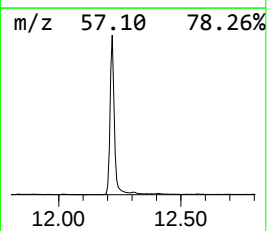
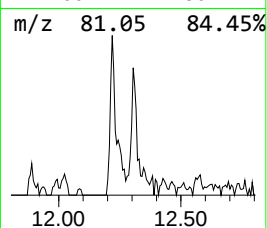
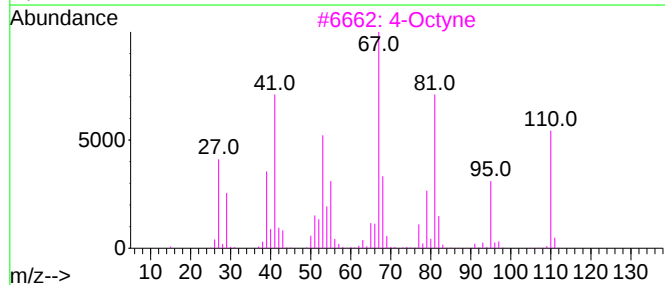
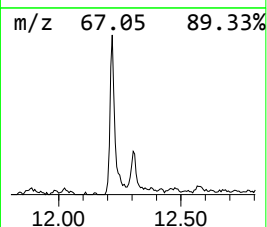
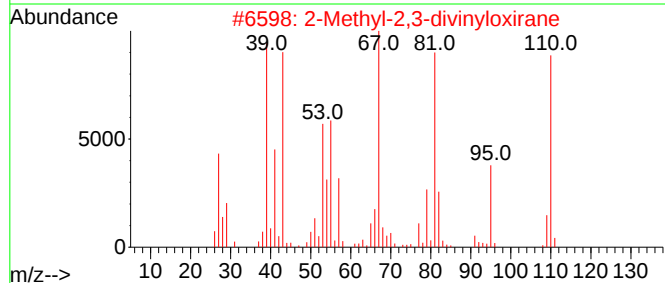
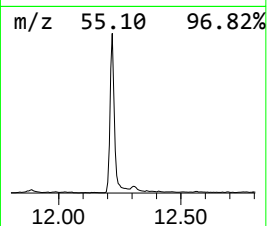
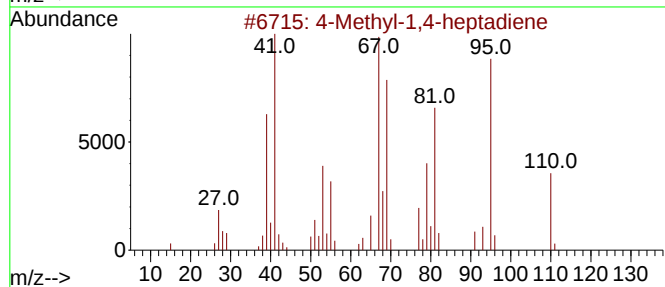
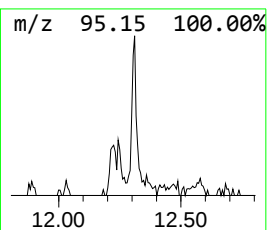
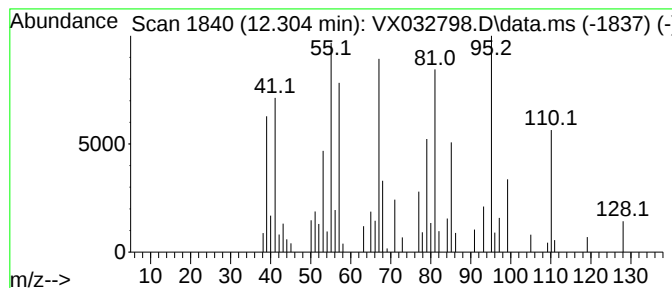
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4-Methyl-1,4-heptadiene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	5.12 ug/l	46071	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methyl-1,4-heptadiene	110	C8H14	013857-55-1	86
2			2-Methyl-2,3-divinyloxirane	110	C7H10O	070597-50-1	58
3			4-Octyne	110	C8H14	001942-45-6	58
4			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	52
5			4-Ethylcyclohexene	110	C8H14	003742-42-5	49



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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
Propane	1.142	9.7	ug/l	56518	1	5.556	290089	50.0
Butanal	4.226	34.4	ug/l	199368	1	5.556	290089	50.0
1-Hexanol, 2-et...	12.219	118.8	ug/l	1068470	4	12.024	449781	50.0
4-Methyl-1,4-he...	12.304	5.1	ug/l	46071	4	12.024	449781	50.0