

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012924\
 Data File : VX040005.D
 Acq On : 29 Jan 2024 18:38
 Operator : JC/MD
 Sample : P1278-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 AUD-1316

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\82X011024W.M
 Title : SW846 8260

Signal : TIC: VX040005.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	22	rVB	55675	58406	19.42%	2.233%
2	1.270	24	30	34	rBV2	7521	8867	2.95%	0.339%
3	1.368	39	46	51	rBV	9723	11661	3.88%	0.446%
4	2.050	152	158	164	rBV4	2576	5096	1.69%	0.195%
5	2.380	206	212	218	rBV	12687	21190	7.04%	0.810%
6	2.532	229	237	243	rBV3	3661	7136	2.37%	0.273%
7	2.959	300	307	314	rBV3	2746	6159	2.05%	0.235%
8	3.331	360	368	375	rBV4	3016	6308	2.10%	0.241%
9	3.697	422	428	436	rVB4	2495	5592	1.86%	0.214%
10	4.227	503	515	533	rBV	77127	209074	69.51%	7.992%
11	5.385	694	705	717	rBV2	45285	134869	44.84%	5.155%
12	5.550	723	732	746	rVB3	72308	206478	68.65%	7.893%
13	5.952	789	798	807	rBV2	53977	147575	49.06%	5.641%
14	6.038	807	812	822	rVV3	13687	36766	12.22%	1.405%
15	6.763	921	931	947	rBV	123114	292702	97.31%	11.189%
16	7.232	1001	1008	1010	rBV3	2141	4051	1.35%	0.155%
17	7.531	1052	1057	1060	rBV3	2554	4478	1.49%	0.171%
18	7.580	1062	1065	1074	rVV3	2868	6389	2.12%	0.244%
19	7.684	1074	1082	1087	rVB5	1245	3059	1.02%	0.117%
20	8.647	1234	1240	1247	rBV	193839	300785	100.00%	11.498%
21	8.720	1247	1252	1261	rVB2	12515	22056	7.33%	0.843%
22	9.494	1374	1379	1381	rBV2	2277	3491	1.16%	0.133%
23	9.519	1381	1383	1391	rVB5	2999	4883	1.62%	0.187%
24	10.055	1465	1471	1482	rBV	196134	272904	90.73%	10.432%
25	10.305	1507	1512	1519	rVB	10405	15599	5.19%	0.596%
26	10.445	1530	1535	1541	rBV2	4322	6180	2.05%	0.236%
27	10.506	1541	1545	1557	rVB2	2128	3224	1.07%	0.123%
28	10.640	1562	1567	1572	rBV2	4940	7124	2.37%	0.272%
29	10.750	1580	1585	1594	rBV2	6659	10100	3.36%	0.386%
30	11.079	1634	1639	1645	rBV	153533	193586	64.36%	7.400%
31	11.134	1645	1648	1652	rVB2	3343	3867	1.29%	0.148%
32	11.573	1716	1720	1723	rBV4	3015	4641	1.54%	0.177%
33	11.610	1723	1726	1732	rVV5	3090	4715	1.57%	0.180%
34	11.683	1733	1738	1745	rVV	72122	86628	28.80%	3.311%
35	11.750	1746	1749	1754	rVB	4968	6423	2.14%	0.246%
36	12.018	1788	1793	1802	rVB	195178	256684	85.34%	9.812%

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37	12.219	1820	1826	1836	rBV	17142	31394	10.44%	1.200%
38	12.317	1839	1842	1850	rVB6	1536	3540	1.18%	0.135%
39	12.994	1950	1953	1958	rVB	5284	6644	2.21%	0.254%
40	13.170	1978	1982	1986	rVB4	2486	3153	1.05%	0.121%
41	13.292	1999	2002	2007	rVB3	5962	7854	2.61%	0.300%
42	13.420	2020	2023	2028	rBV2	3805	4482	1.49%	0.171%
43	13.585	2046	2050	2056	rVV5	2016	3993	1.33%	0.153%
44	13.676	2060	2065	2070	rVV3	16188	21269	7.07%	0.813%
45	13.774	2078	2081	2086	rVB2	3953	5187	1.72%	0.198%
46	13.853	2090	2094	2100	rVB5	4592	6404	2.13%	0.245%
47	13.920	2100	2105	2110	rBV6	4269	6334	2.11%	0.242%
48	14.036	2119	2124	2127	rBV3	5320	6888	2.29%	0.263%
49	14.073	2127	2130	2136	rVB4	4831	5928	1.97%	0.227%
50	14.140	2136	2141	2148	rVB3	4944	6854	2.28%	0.262%
51	14.225	2148	2155	2159	rBV3	15719	26031	8.65%	0.995%
52	14.274	2159	2163	2168	rVB3	3229	4667	1.55%	0.178%
53	14.371	2174	2179	2184	rBV3	6872	8953	2.98%	0.342%
54	14.475	2192	2196	2202	rBV3	12119	16212	5.39%	0.620%
55	14.615	2214	2219	2220	rBV2	8356	9708	3.23%	0.371%
56	14.634	2220	2222	2226	rVV	11063	14633	4.86%	0.559%
57	14.670	2226	2228	2233	rVB4	4416	4899	1.63%	0.187%
58	14.756	2239	2242	2244	rBV2	2941	3501	1.16%	0.134%
59	14.780	2244	2246	2250	rVB3	4725	4484	1.49%	0.171%
60	14.902	2261	2266	2272	rVB6	2724	4481	1.49%	0.171%
61	15.182	2304	2312	2314	rBV2	6542	9337	3.10%	0.357%
62	15.487	2356	2362	2365	rBV6	3757	6502	2.16%	0.249%
63	15.609	2379	2382	2386	rBV4	2647	3947	1.31%	0.151%

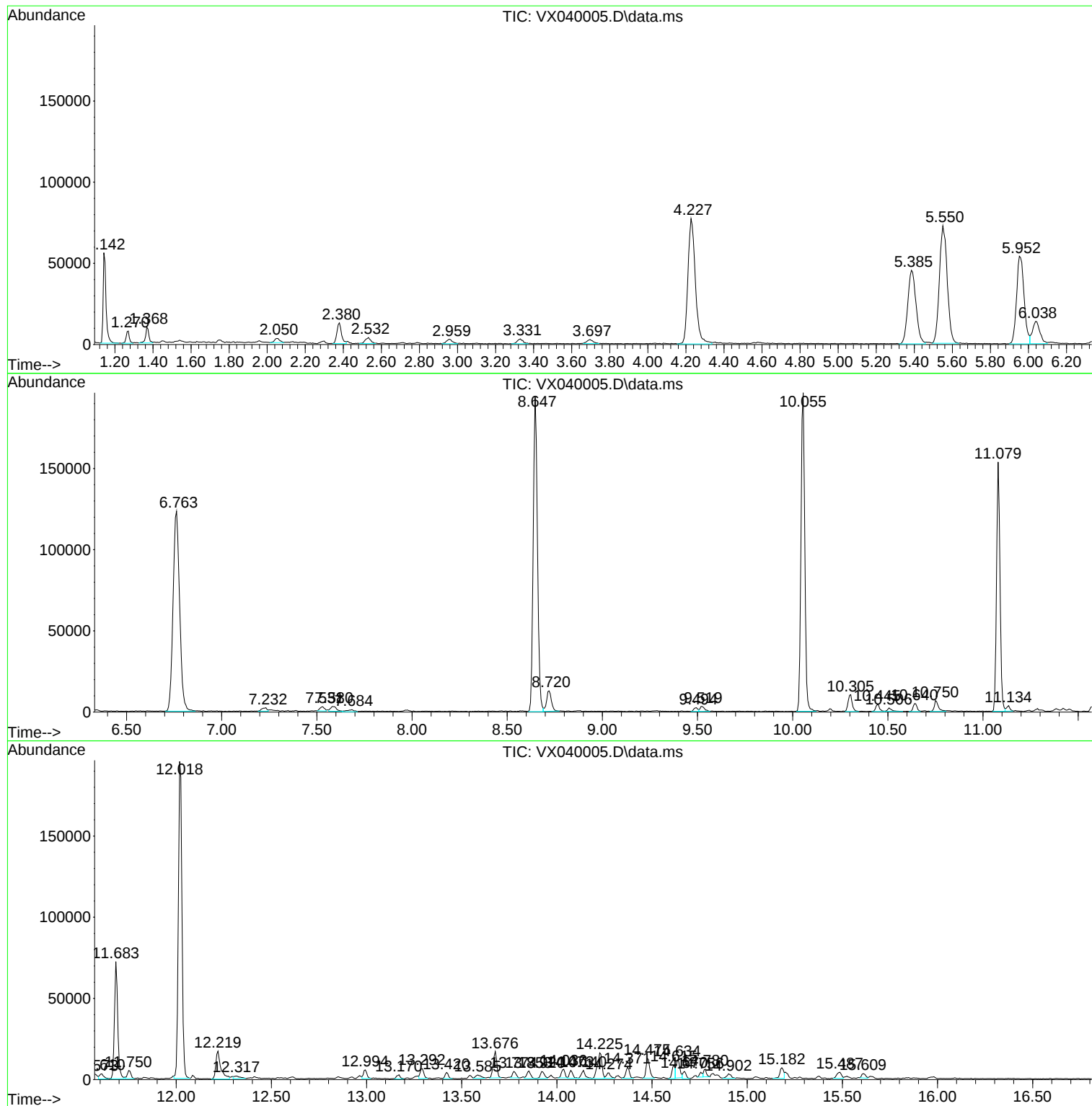
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
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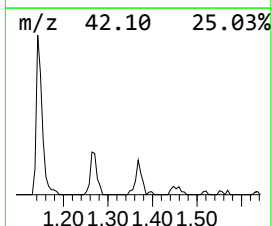
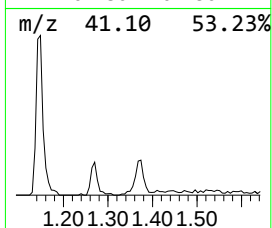
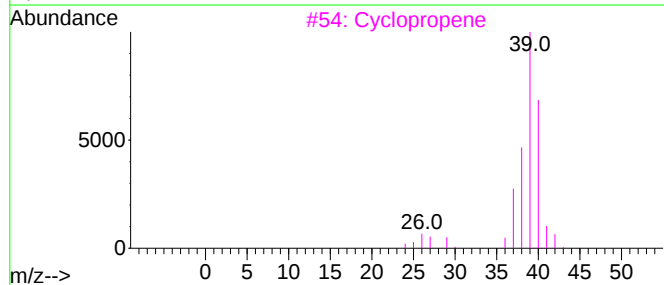
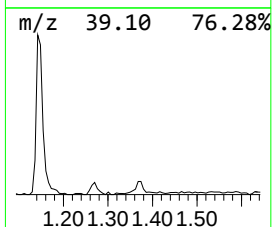
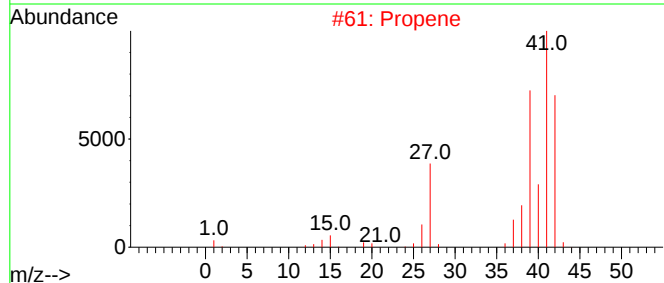
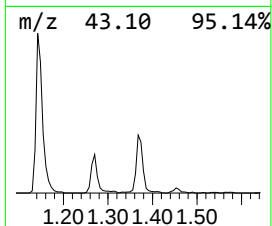
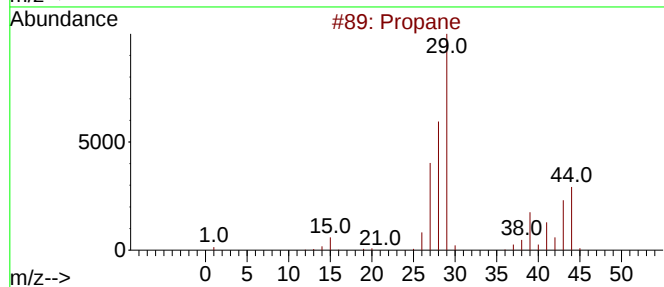
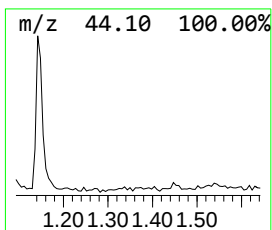
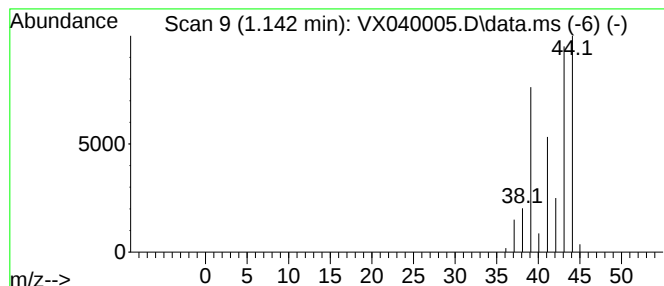
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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	14.14 ug/l	58406	Pentafluorobenzene	5.562

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	Propane, 2-nitro-			89	C3H7NO2	000079-46-9	2



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1316

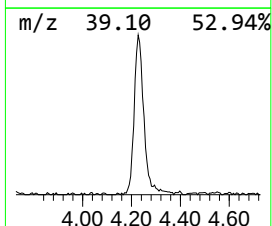
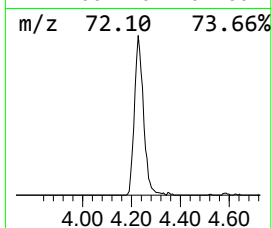
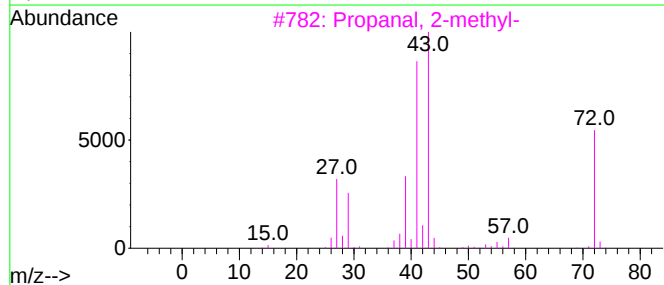
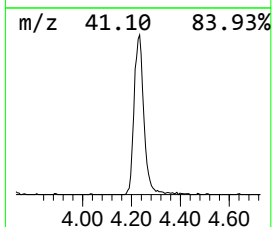
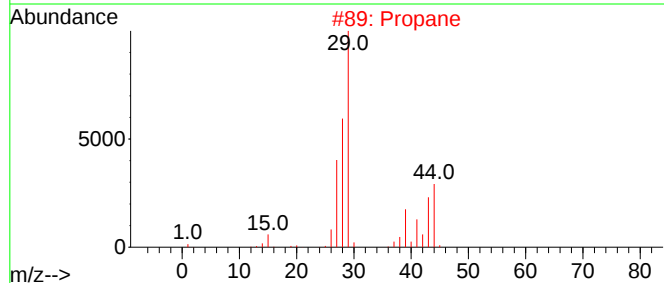
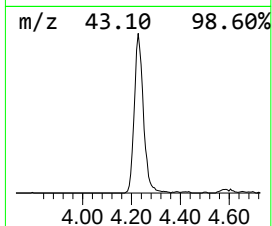
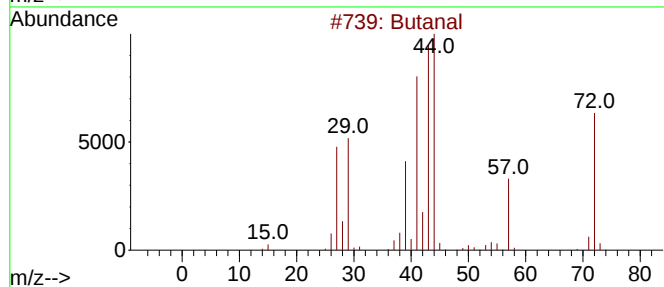
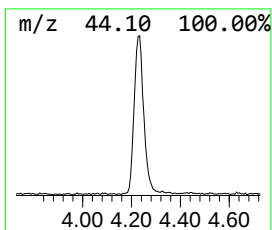
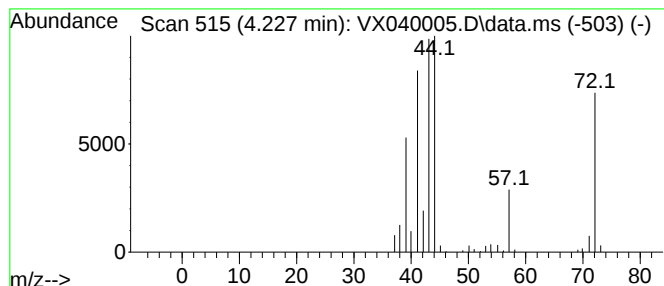
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	50.63 ug/l	209074	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propane	44	C3H8	000074-98-6	47
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4			Ethene, ethoxy-	72	C4H8O	000109-92-2	40
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012924\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
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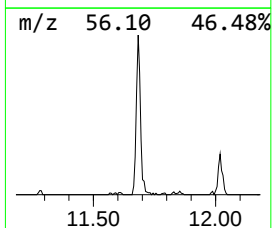
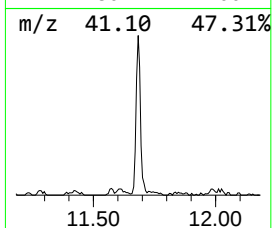
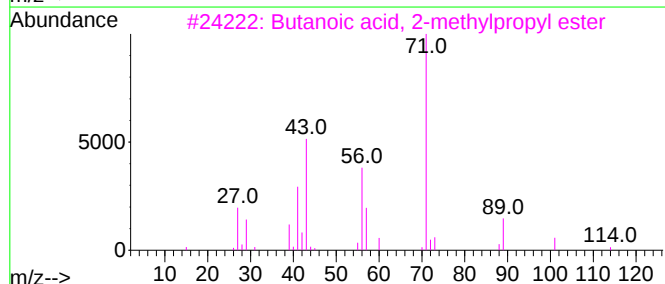
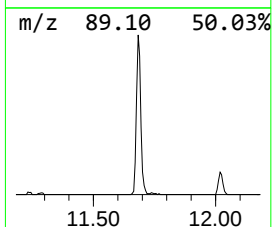
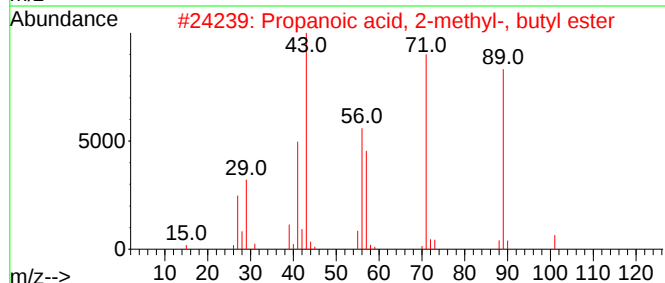
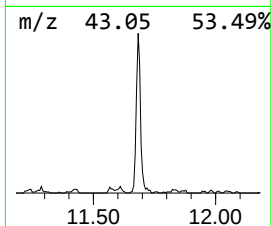
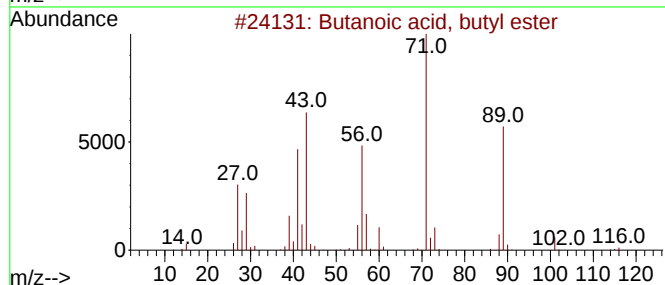
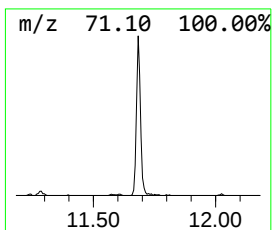
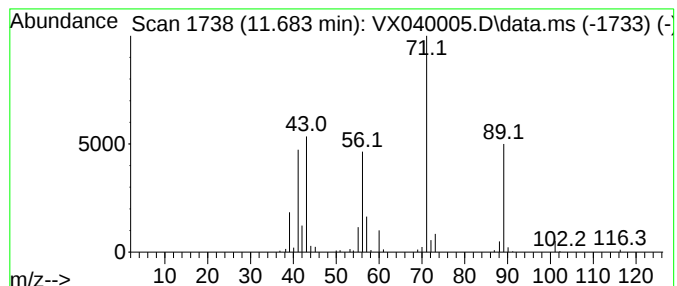
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	16.87 ug/l	86628	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
4			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59



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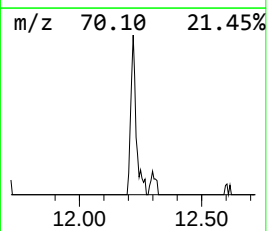
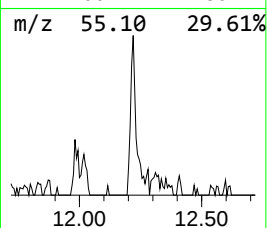
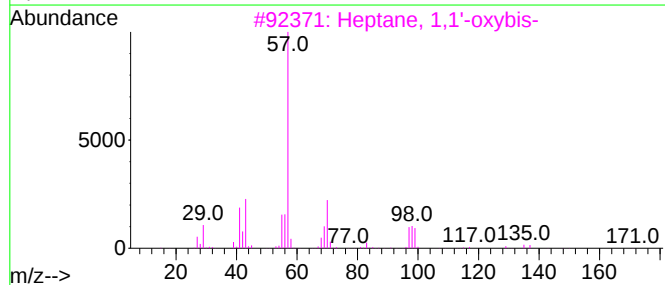
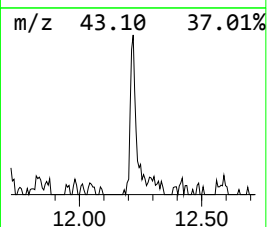
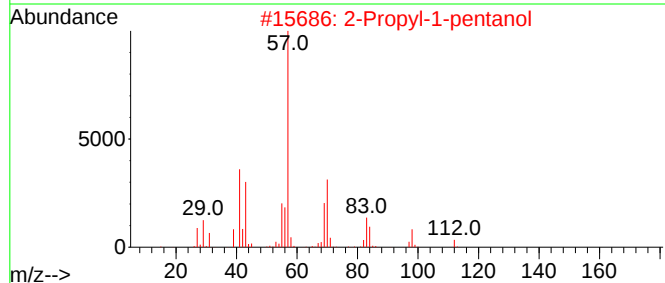
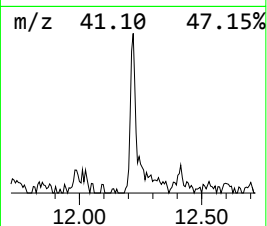
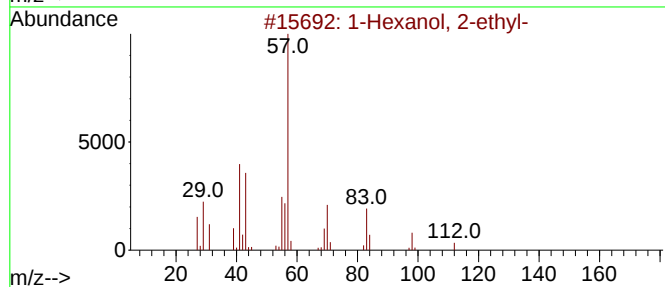
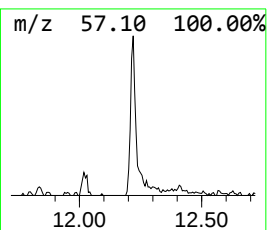
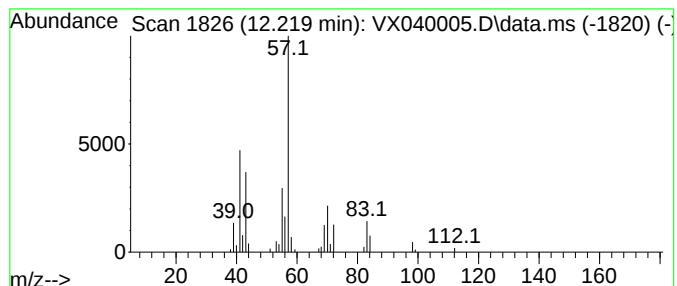
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	6.12 ug/l	31394	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	72
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4			Heptane, 3-ethyl-	128	C9H20	015869-80-4	50
5			1-Hexene, 4-methyl-	98	C7H14	003769-23-1	43



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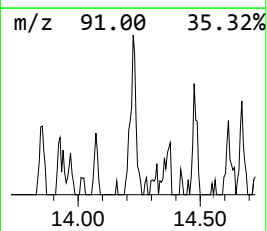
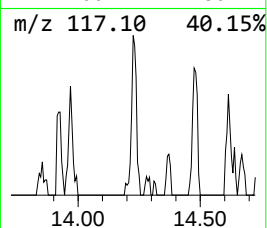
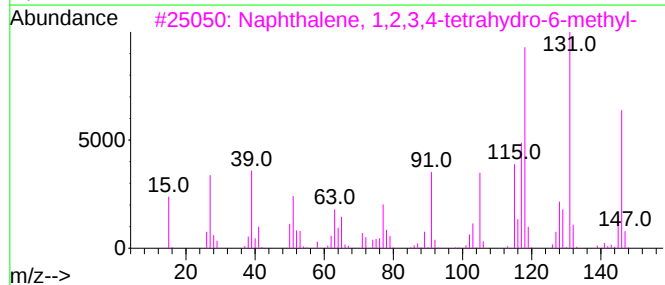
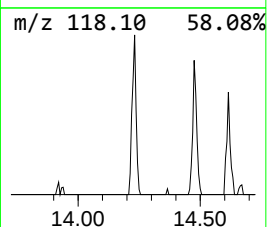
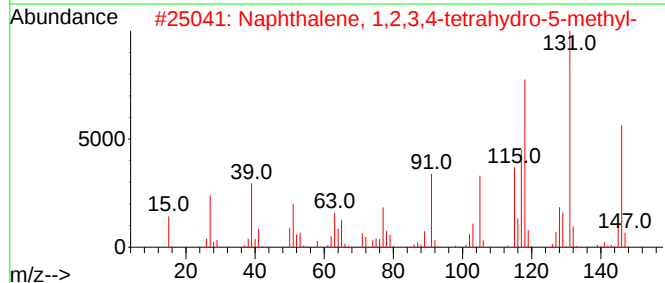
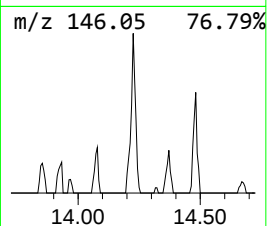
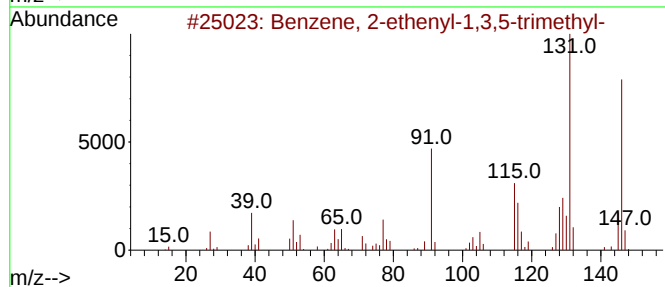
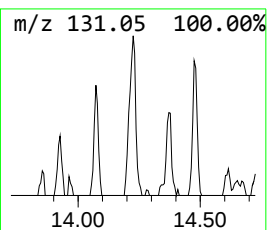
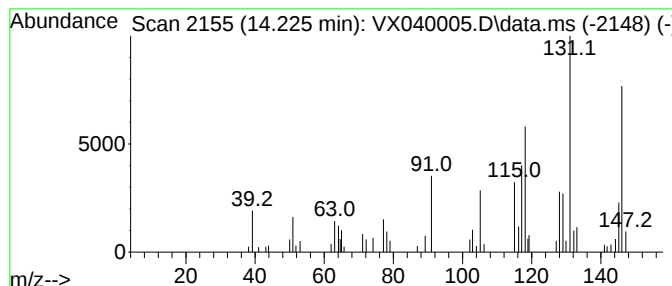
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-ethenyl-1,3,5-tr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.225	5.07 ug/l	26031	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	89
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	87
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	81
4			1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	70
5			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012924\
Data File : VX040005.D
Acq On : 29 Jan 2024 18:38
Operator : JC/MD
Sample : P1278-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1316

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
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	14.1	ug/l	58406	1	5.562	206478	50.0
Butanal	4.227	50.6	ug/l	209074	1	5.562	206478	50.0
Butanoic acid, ...	11.683	16.9	ug/l	86628	4	12.024	256684	50.0
1-Hexanol, 2-et...	12.219	6.1	ug/l	31394	4	12.024	256684	50.0
Benzene, 2-ethe...	14.225	5.1	ug/l	26031	4	12.024	256684	50.0