

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100223\
 Data File : VV032192.D
 Acq On : 02 Oct 2023 11:16
 Operator : SY/MD
 Sample : PB155945TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 LEB945

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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_V\Method\SFAMVLM092523WMA.M
 Title : VOC Analysis

Signal : TIC: VV032192.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	67	74	88	rVB	84113	88005	12.23%	1.359%
2	1.426	112	120	126	rBV8	2824	4543	0.63%	0.070%
3	1.532	145	153	168	rVB	77470	92383	12.84%	1.427%
4	2.059	307	317	331	rBV	144442	209712	29.15%	3.239%
5	2.394	418	421	422	rBV2	229	139	0.02%	0.002%
6	2.449	429	438	449	rVB3	5437	8876	1.23%	0.137%
7	2.561	467	473	478	rBV4	767	967	0.13%	0.015%
8	2.661	501	504	507	rVV2	207	137	0.02%	0.002%
9	2.703	510	517	520	rBV2	248	304	0.04%	0.005%
10	2.783	539	542	544	rBV3	361	182	0.03%	0.003%
11	2.934	585	589	591	rVB2	345	155	0.02%	0.002%
12	2.957	593	596	600	rBV2	283	179	0.02%	0.003%
13	3.072	629	632	635	rBV2	211	179	0.02%	0.003%
14	3.397	731	733	738	rVB2	261	186	0.03%	0.003%
15	3.426	738	742	745	rBV	194	152	0.02%	0.002%
16	3.564	781	785	791	rVB2	251	228	0.03%	0.004%
17	3.622	797	803	808	rBV	235	202	0.03%	0.003%
18	3.670	814	818	819	rBV	249	125	0.02%	0.002%
19	3.789	845	855	884	rBV2	61521	175117	24.35%	2.705%
20	4.252	982	999	1029	rBV	113716	291895	40.58%	4.509%
21	4.506	1076	1078	1082	rBV2	423	263	0.04%	0.004%
22	4.580	1097	1101	1104	rVB4	310	235	0.03%	0.004%
23	4.715	1136	1143	1144	rBV3	207	248	0.03%	0.004%
24	4.789	1162	1166	1170	rBV2	164	133	0.02%	0.002%
25	4.873	1185	1192	1194	rBV	140	191	0.03%	0.003%
26	4.960	1201	1219	1246	rBV2	268019	719311	100.00%	11.111%
27	5.172	1283	1285	1286	rBV	278	153	0.02%	0.002%
28	5.211	1289	1297	1299	rBV5	5128	6250	0.87%	0.097%
29	5.339	1335	1337	1342	rVB3	373	224	0.03%	0.003%
30	5.374	1344	1348	1353	rVB4	417	310	0.04%	0.005%
31	5.477	1376	1380	1381	rBV2	190	139	0.02%	0.002%
32	5.535	1385	1398	1419	rBV	262133	536610	74.60%	8.289%
33	5.831	1479	1490	1508	rBV2	10957	23774	3.31%	0.367%
34	5.895	1508	1510	1513	rVB	282	162	0.02%	0.003%
35	5.992	1526	1540	1560	rBV	161940	338967	47.12%	5.236%
36	6.188	1598	1601	1606	rBV4	265	244	0.03%	0.004%

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 Title : VOC Analysis

37	6.223	1610	1612	1616	rVB2	239	141	0.02%	0.002%
38	6.249	1617	1620	1623	rBV3	327	183	0.03%	0.003%
39	6.272	1624	1627	1628	rBV2	288	141	0.02%	0.002%
40	6.294	1628	1634	1635	rBV3	1593	1590	0.22%	0.025%
41	6.397	1657	1666	1705	rBV	78120	162199	22.55%	2.505%
42	6.683	1751	1755	1757	rVB	324	222	0.03%	0.003%
43	6.706	1760	1762	1764	rBV2	314	136	0.02%	0.002%
44	6.821	1796	1798	1804	rBV3	192	179	0.02%	0.003%
45	6.915	1816	1827	1854	rBV	85183	165924	23.07%	2.563%
46	7.056	1869	1871	1873	rVB2	402	172	0.02%	0.003%
47	7.124	1882	1892	1902	rBV	18772	32864	4.57%	0.508%
48	7.246	1918	1930	1961	rBV	312340	556512	77.37%	8.596%
49	7.554	2016	2026	2057	rBV	80005	153807	21.38%	2.376%
50	7.754	2084	2088	2091	rBV3	288	304	0.04%	0.005%
51	7.796	2097	2101	2107	rVB4	301	202	0.03%	0.003%
52	7.866	2113	2123	2143	rBV2	25515	44230	6.15%	0.683%
53	7.979	2147	2158	2163	rBV3	5671	8591	1.19%	0.133%
54	8.027	2163	2173	2199	rVV2	173187	336407	46.77%	5.196%
55	8.133	2199	2206	2223	rVB	37467	65402	9.09%	1.010%
56	8.249	2234	2242	2268	rVB	21039	40659	5.65%	0.628%
57	8.362	2272	2277	2281	rBV6	1190	1473	0.20%	0.023%
58	8.468	2307	2310	2313	rBV2	233	183	0.03%	0.003%
59	8.542	2329	2333	2335	rVB	253	175	0.02%	0.003%
60	8.622	2346	2358	2383	rBV	73096	122240	16.99%	1.888%
61	8.786	2395	2409	2435	rBV	403384	676933	94.11%	10.456%
62	9.062	2490	2495	2497	rBV2	833	601	0.08%	0.009%
63	9.345	2577	2583	2584	rBV3	559	453	0.06%	0.007%
64	9.400	2597	2600	2603	rBV2	194	161	0.02%	0.002%
65	9.500	2621	2631	2642	rBV4	4054	8130	1.13%	0.126%
66	9.567	2650	2652	2657	rVB4	632	447	0.06%	0.007%
67	9.680	2680	2687	2692	rBV2	219	271	0.04%	0.004%
68	9.722	2697	2700	2704	rVB3	320	216	0.03%	0.003%
69	9.869	2743	2746	2748	rBV2	204	127	0.02%	0.002%
70	9.908	2756	2758	2766	rVB2	235	177	0.02%	0.003%
71	9.953	2767	2772	2775	rVB2	186	177	0.02%	0.003%
72	9.982	2775	2781	2784	rBV	201	197	0.03%	0.003%
73	10.111	2813	2821	2823	rBV	240	298	0.04%	0.005%
74	10.156	2823	2835	2857	rVV	221283	355512	49.42%	5.491%
75	10.294	2875	2878	2884	rBV2	216	213	0.03%	0.003%
76	10.918	3068	3072	3076	rBV2	151	135	0.02%	0.002%

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77	11.133	3137	3139	3145	rVB2	266	170	0.02%	0.003%
78	11.188	3145	3156	3176	rBV	450151	682903	94.94%	10.549%
79	11.342	3202	3204	3207	rBV2	284	128	0.02%	0.002%
80	11.429	3228	3231	3235	rBV2	145	161	0.02%	0.002%
81	11.564	3261	3273	3293	rBV	346132	544707	75.73%	8.414%
82	11.757	3330	3333	3335	rBV2	204	137	0.02%	0.002%
83	11.824	3351	3354	3359	rVB	388	200	0.03%	0.003%
84	12.287	3496	3498	3501	rBV2	232	128	0.02%	0.002%
85	12.390	3527	3530	3534	rBV2	212	144	0.02%	0.002%
86	12.818	3661	3663	3669	rVB2	310	285	0.04%	0.004%
87	12.847	3669	3672	3676	rBV	183	158	0.02%	0.002%
88	12.879	3676	3682	3683	rBV	242	229	0.03%	0.004%
89	13.217	3781	3787	3791	rBV4	530	560	0.08%	0.009%
90	13.310	3814	3816	3820	rBV2	329	250	0.03%	0.004%
91	13.377	3834	3837	3840	rVB2	240	159	0.02%	0.002%
92	13.458	3853	3862	3871	rVB5	1493	2410	0.34%	0.037%
93	13.660	3922	3925	3926	rBV2	415	227	0.03%	0.004%
94	13.689	3930	3934	3943	rVB4	573	849	0.12%	0.013%
95	13.728	3943	3946	3948	rBV2	284	174	0.02%	0.003%
96	13.776	3959	3961	3967	rBV3	507	360	0.05%	0.006%
97	13.863	3986	3988	3992	rVB	283	147	0.02%	0.002%
98	13.889	3993	3996	3999	rBV2	295	219	0.03%	0.003%
99	14.133	4070	4072	4074	rBV2	201	129	0.02%	0.002%
100	14.429	4161	4164	4166	rBV2	341	215	0.03%	0.003%

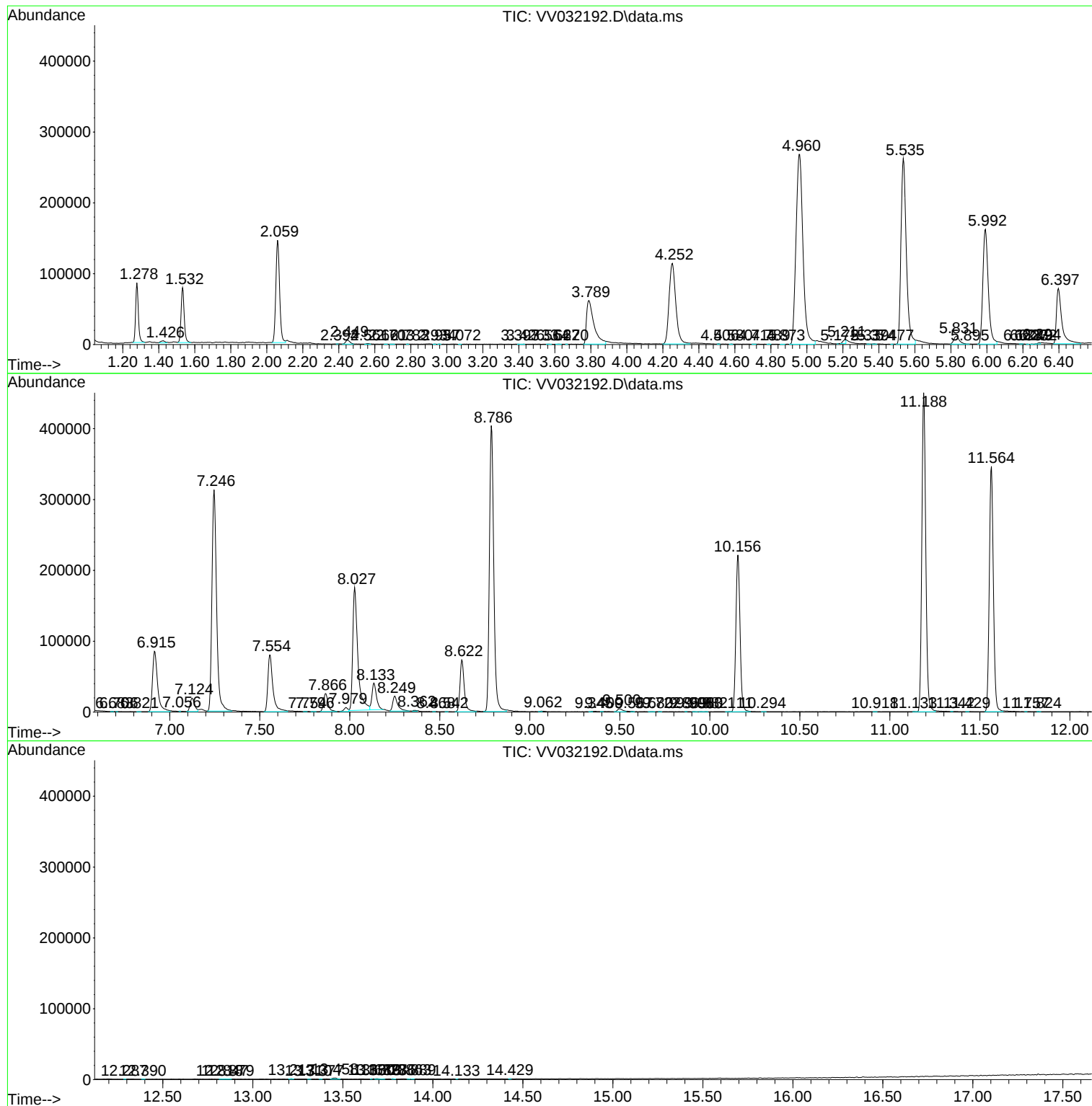
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092523WMA.M
Quant Title : VOC Analysis

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



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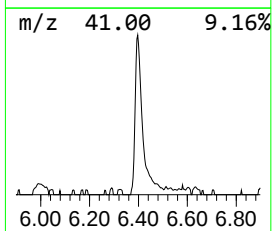
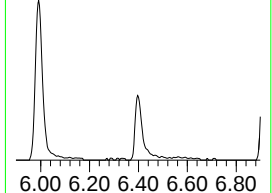
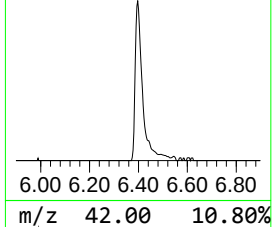
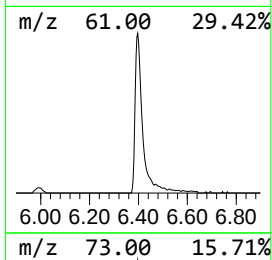
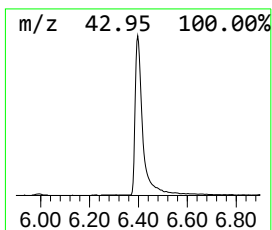
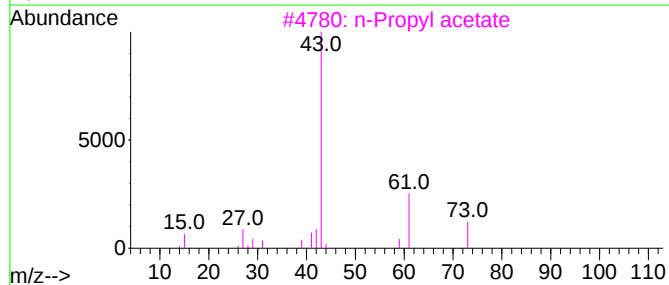
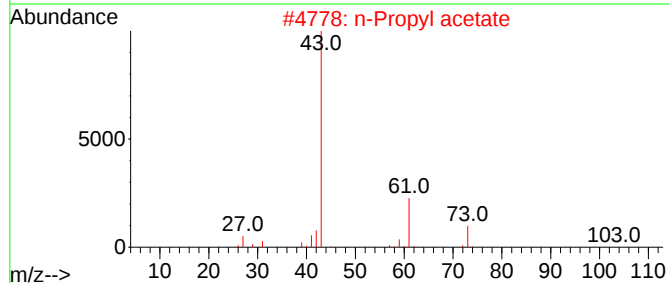
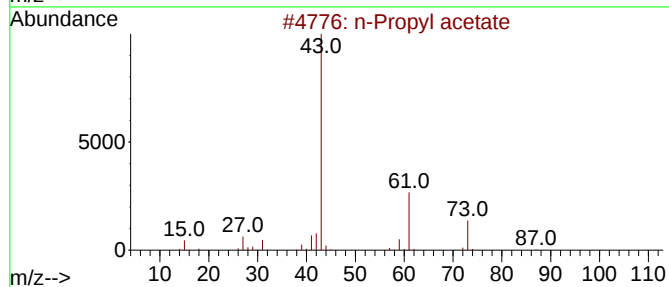
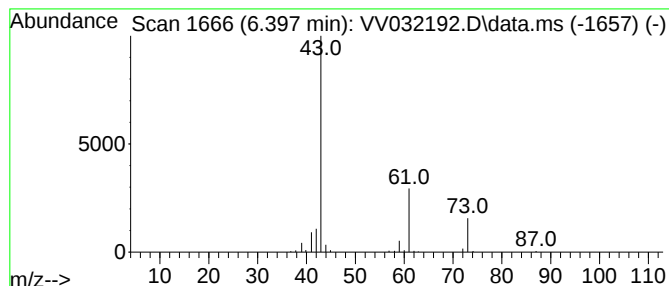
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.397	15.11 ug/L	162199	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	83
2	n-Propyl acetate			102	C5H10O2	000109-60-4	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	Isopropyl acetate			102	C5H10O2	000108-21-4	38



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Instrument :
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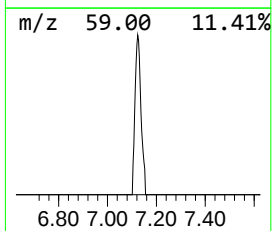
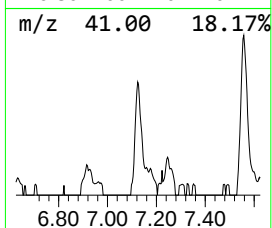
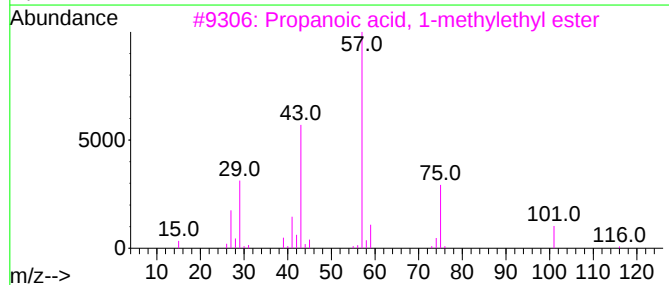
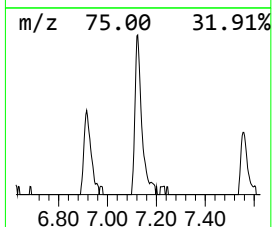
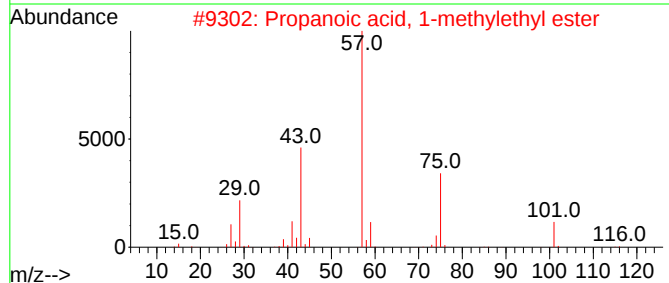
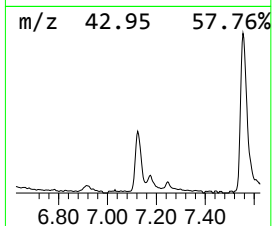
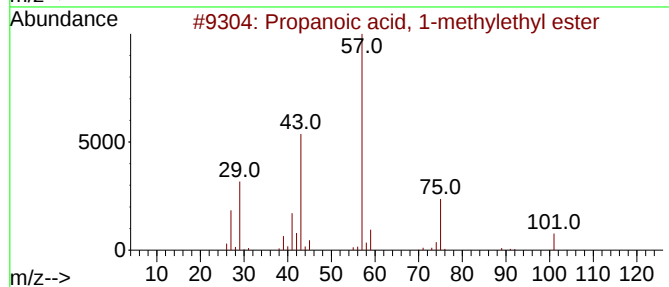
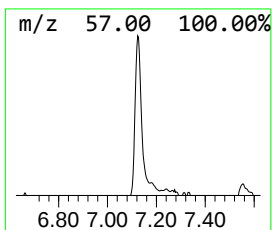
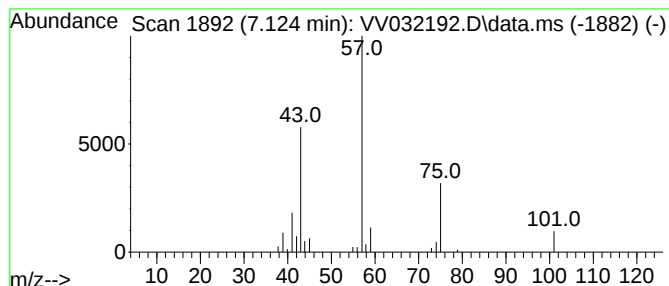
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.124	3.06 ug/L	32864	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	38



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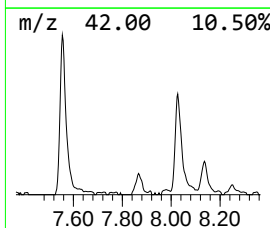
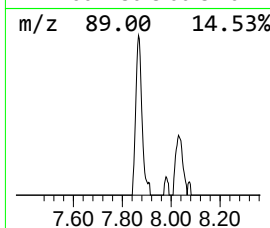
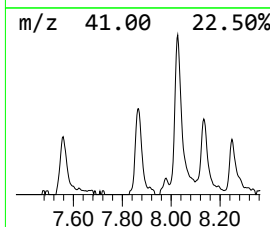
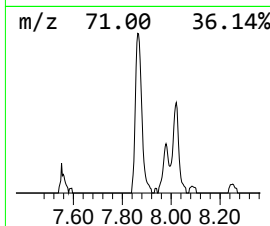
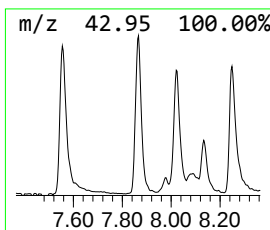
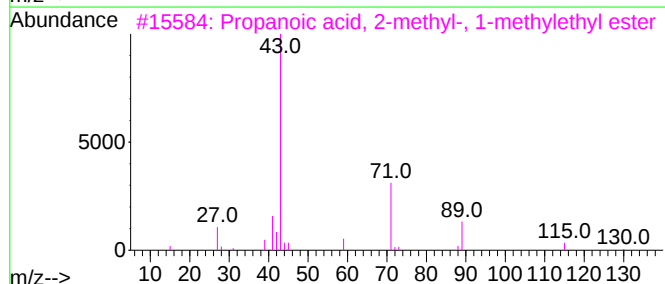
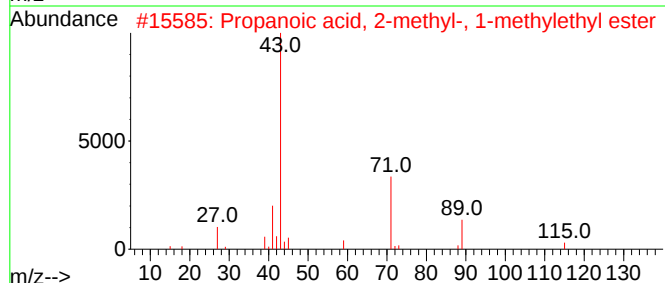
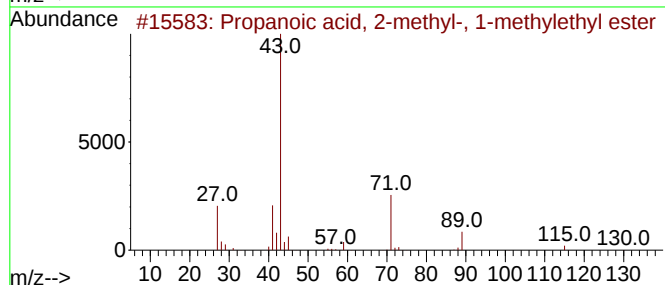
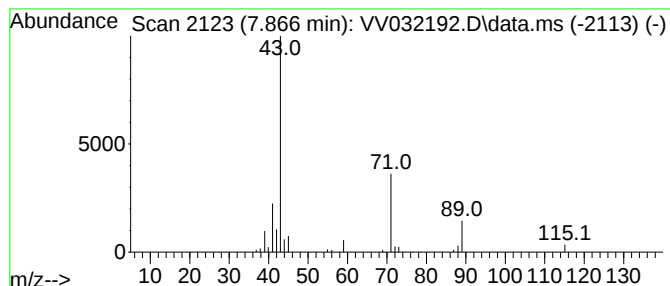
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Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.866	3.27 ug/L	44230	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100223\
Data File : VV032192.D
Acq On : 02 Oct 2023 11:16
Operator : SY/MD
Sample : PB155945TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB945

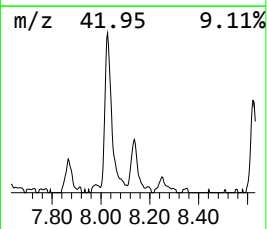
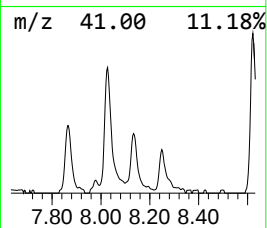
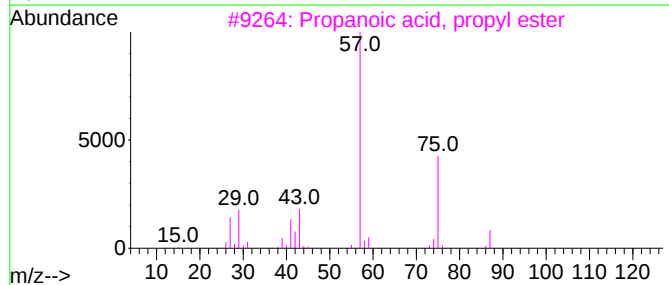
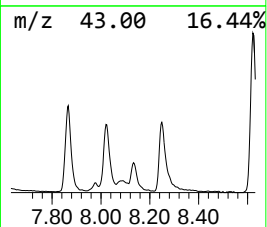
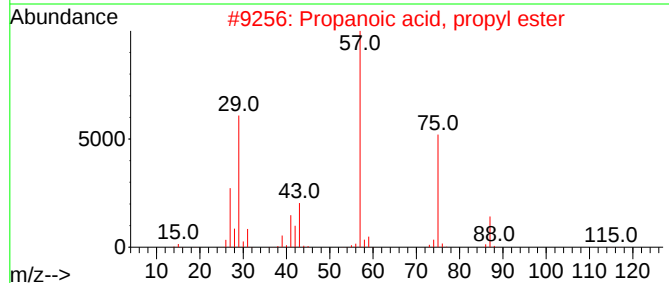
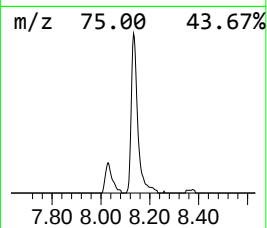
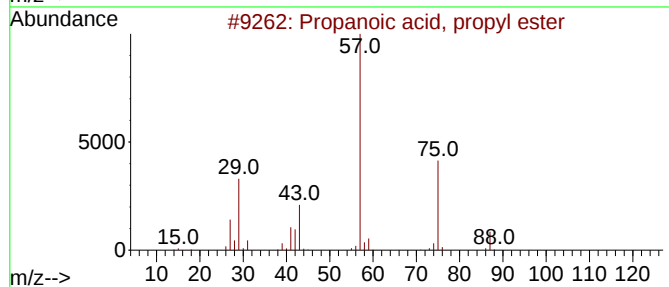
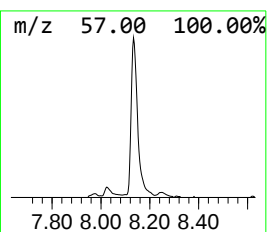
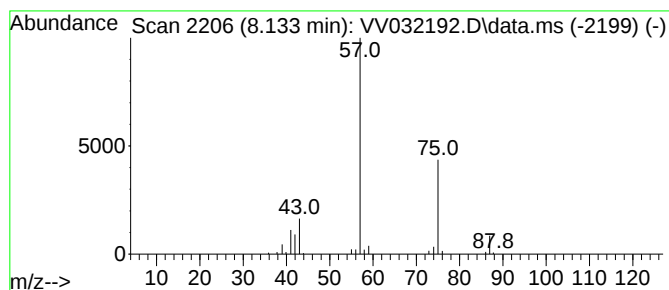
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.133	4.83 ug/L	65402	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	47
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100223\
Data File : VV032192.D
Acq On : 02 Oct 2023 11:16
Operator : SY/MD
Sample : PB155945TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB945

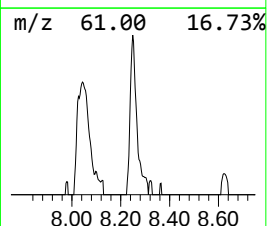
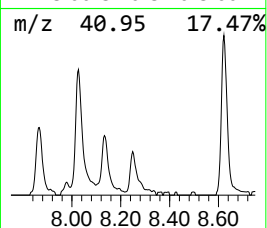
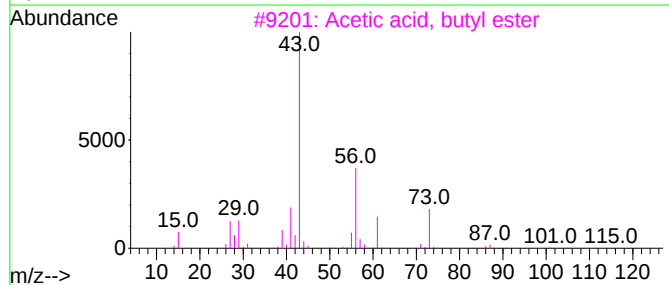
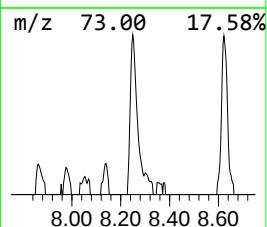
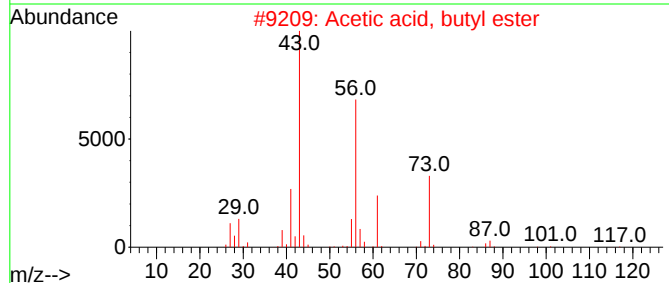
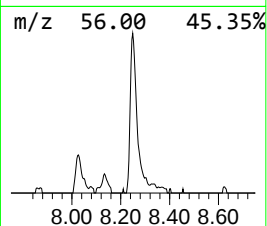
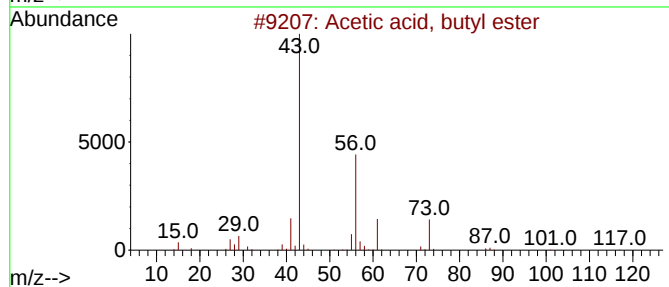
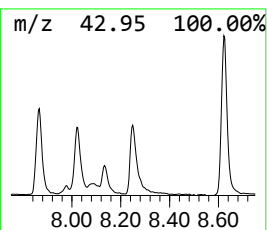
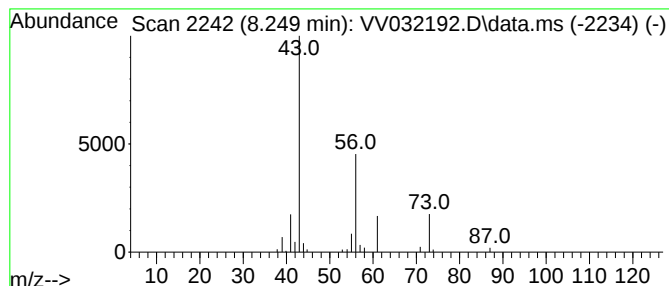
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.249	3.00 ug/L	40659	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83		
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64		
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	59		
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50		
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	42		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100223\
Data File : VV032192.D
Acq On : 02 Oct 2023 11:16
Operator : SY/MD
Sample : PB155945TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB945

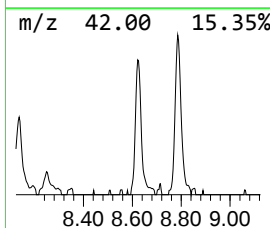
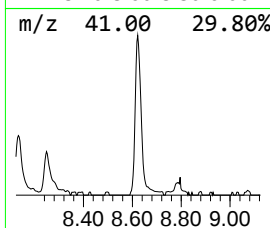
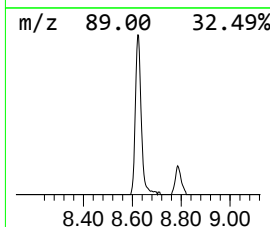
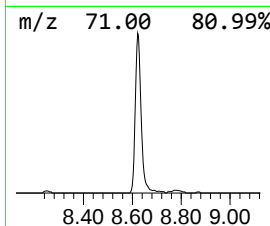
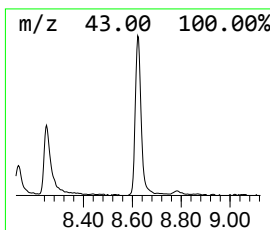
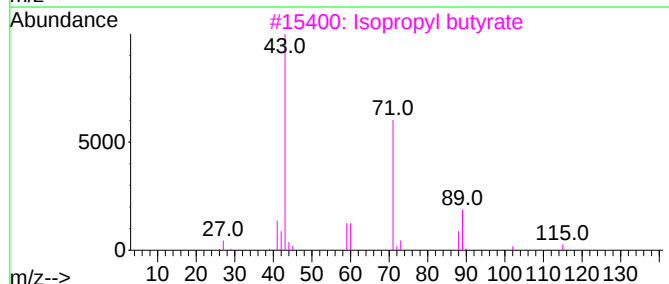
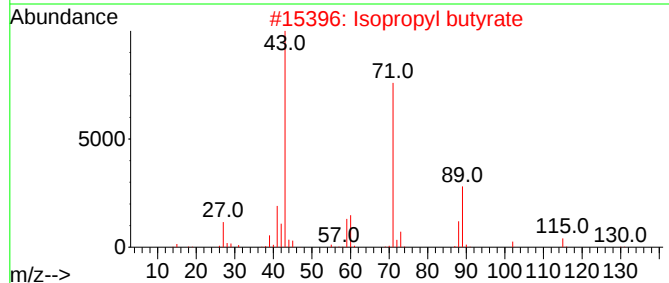
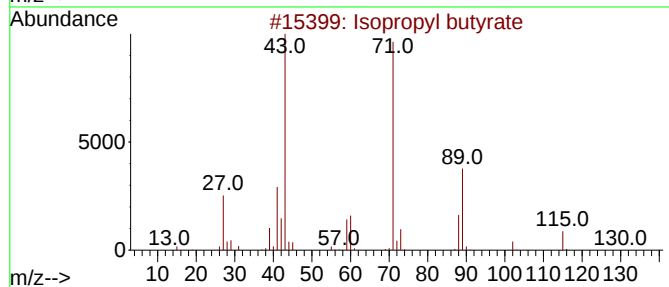
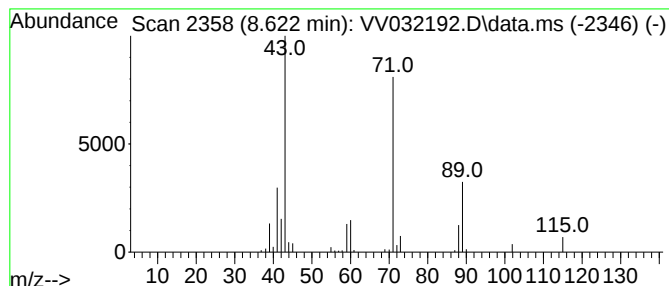
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092523WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.622	9.03 ug/L	122240	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100223\
Data File : VV032192.D
Acq On : 02 Oct 2023 11:16
Operator : SY/MD
Sample : PB155945TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB945

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092523WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.397	15.1	ug/L	162199	1	5.535	536610	50.0
Propanoic acid,...	7.124	3.1	ug/L	32864	1	5.535	536610	50.0
Propanoic acid,...	7.866	3.3	ug/L	44230	2	8.786	676933	50.0
Propanoic acid,...	8.133	4.8	ug/L	65402	2	8.786	676933	50.0
Acetic acid, bu...	8.249	3.0	ug/L	40659	2	8.786	676933	50.0
Isopropyl butyrate	8.622	9.0	ug/L	122240	2	8.786	676933	50.0