

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032724\
 Data File : VV034859.D
 Acq On : 27 Mar 2024 12:53
 Operator : SY/MD
 Sample : PB159796TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

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\SFAMVLM032624WMA.M

Title : VOC Analysis

Signal : TIC: VV034859.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	68	74	90	rVB	165256	182123	13.62%	1.829%
2	1.526	146	151	168	rVB	143039	163411	12.22%	1.641%
3	2.056	306	316	330	rBV	306712	447161	33.43%	4.491%
4	2.449	431	438	449	rVB2	5375	8937	0.67%	0.090%
5	2.558	460	472	484	rBV3	5335	12113	0.91%	0.122%
6	2.751	528	532	534	rBV3	420	252	0.02%	0.003%
7	2.799	545	547	550	rBV3	318	179	0.01%	0.002%
8	2.854	558	564	566	rBV2	409	319	0.02%	0.003%
9	2.892	571	576	581	rBV3	574	606	0.05%	0.006%
10	2.944	589	592	594	rBV3	338	210	0.02%	0.002%
11	2.992	603	607	610	rBV2	408	254	0.02%	0.003%
12	3.044	620	623	627	rVB3	387	246	0.02%	0.002%
13	3.114	634	645	658	rBV6	3121	8631	0.65%	0.087%
14	3.400	731	734	739	rVB4	372	359	0.03%	0.004%
15	3.429	739	743	746	rBV3	311	233	0.02%	0.002%
16	3.613	796	800	804	rVB3	400	306	0.02%	0.003%
17	3.638	804	808	810	rBV	382	267	0.02%	0.003%
18	3.793	847	856	902	rBV	91171	295624	22.10%	2.969%
19	4.246	981	997	1030	rBV	214543	556764	41.63%	5.592%
20	4.478	1066	1069	1071	rBV	477	325	0.02%	0.003%
21	4.506	1076	1078	1081	rBV2	527	304	0.02%	0.003%
22	4.728	1142	1147	1151	rBV4	488	348	0.03%	0.003%
23	4.773	1157	1161	1164	rBV4	360	336	0.03%	0.003%
24	4.953	1201	1217	1252	rBV2	501781	1337527	100.00%	13.434%
25	5.432	1362	1366	1370	rBV6	386	310	0.02%	0.003%
26	5.532	1386	1397	1422	rBV	262413	551157	41.21%	5.536%
27	5.786	1474	1476	1479	rVB	773	317	0.02%	0.003%
28	5.831	1479	1490	1504	rBV4	9515	22104	1.65%	0.222%
29	5.941	1519	1524	1526	rBV4	782	627	0.05%	0.006%
30	5.986	1526	1538	1565	rBV	297759	622837	46.57%	6.256%
31	6.320	1633	1642	1644	rBV6	1947	3228	0.24%	0.032%
32	6.397	1658	1666	1698	rBV	80108	173193	12.95%	1.740%
33	6.748	1773	1775	1778	rBV2	645	408	0.03%	0.004%
34	6.799	1789	1791	1794	rVB3	393	201	0.02%	0.002%
35	6.912	1815	1826	1859	rBV	159427	311523	23.29%	3.129%
36	7.124	1884	1892	1905	rBV	20565	36187	2.71%	0.363%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
 Title : VOC Analysis

37	7.243	1918	1929	1960	rBV	548766	982880	73.48%	9.872%
38	7.555	2016	2026	2051	rBV2	131573	257228	19.23%	2.584%
39	7.760	2088	2090	2092	rVB3	705	290	0.02%	0.003%
40	7.863	2110	2122	2140	rBV	30202	54439	4.07%	0.547%
41	7.979	2148	2158	2163	rBV6	6789	10496	0.78%	0.105%
42	8.027	2164	2173	2198	rBV	301394	640361	47.88%	6.432%
43	8.252	2237	2243	2264	rVB2	21177	41979	3.14%	0.422%
44	8.551	2334	2336	2339	rVB4	513	208	0.02%	0.002%
45	8.622	2348	2358	2374	rBV	86913	145755	10.90%	1.464%
46	8.783	2398	2408	2429	rBV	428746	704429	52.67%	7.075%
47	9.169	2524	2528	2533	rVB5	403	449	0.03%	0.005%
48	9.214	2538	2542	2544	rBV	398	262	0.02%	0.003%
49	9.227	2544	2546	2548	rVB2	464	185	0.01%	0.002%
50	9.268	2554	2559	2563	rVB4	613	650	0.05%	0.007%
51	9.288	2563	2565	2568	rBV3	382	270	0.02%	0.003%
52	9.365	2580	2589	2593	rBV5	796	1470	0.11%	0.015%
53	9.432	2608	2610	2615	rVB3	578	319	0.02%	0.003%
54	9.503	2623	2632	2642	rBV6	4502	9233	0.69%	0.093%
55	9.841	2732	2737	2739	rBV2	219	203	0.02%	0.002%
56	9.863	2742	2744	2748	rBV3	607	485	0.04%	0.005%
57	9.950	2769	2771	2774	rVB	588	226	0.02%	0.002%
58	9.979	2774	2780	2781	rBV2	298	176	0.01%	0.002%
59	10.021	2791	2793	2796	rBV3	264	214	0.02%	0.002%
60	10.153	2821	2834	2858	rBV	447927	721955	53.98%	7.251%
61	10.349	2893	2895	2896	rBV2	499	206	0.02%	0.002%
62	10.387	2902	2907	2909	rVB4	453	325	0.02%	0.003%
63	10.413	2909	2915	2919	rVB6	484	515	0.04%	0.005%
64	10.461	2926	2930	2934	rBV3	436	470	0.04%	0.005%
65	10.603	2972	2974	2980	rBV3	396	351	0.03%	0.004%
66	10.673	2990	2996	2998	rBV2	294	226	0.02%	0.002%
67	10.754	3018	3021	3023	rBV	328	207	0.02%	0.002%
68	10.776	3023	3028	3030	rVV3	378	343	0.03%	0.003%
69	10.808	3034	3038	3040	rBV2	347	308	0.02%	0.003%
70	10.853	3050	3052	3058	rBV3	496	553	0.04%	0.006%
71	10.992	3093	3095	3100	rVV2	257	178	0.01%	0.002%
72	11.050	3110	3113	3116	rVB	337	218	0.02%	0.002%
73	11.185	3144	3155	3177	rBV	429627	665392	49.75%	6.683%
74	11.374	3211	3214	3221	rBV5	669	529	0.04%	0.005%
75	11.468	3240	3243	3247	rBV2	666	530	0.04%	0.005%
76	11.490	3247	3250	3251	rBV2	365	203	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M

Title : VOC Analysis

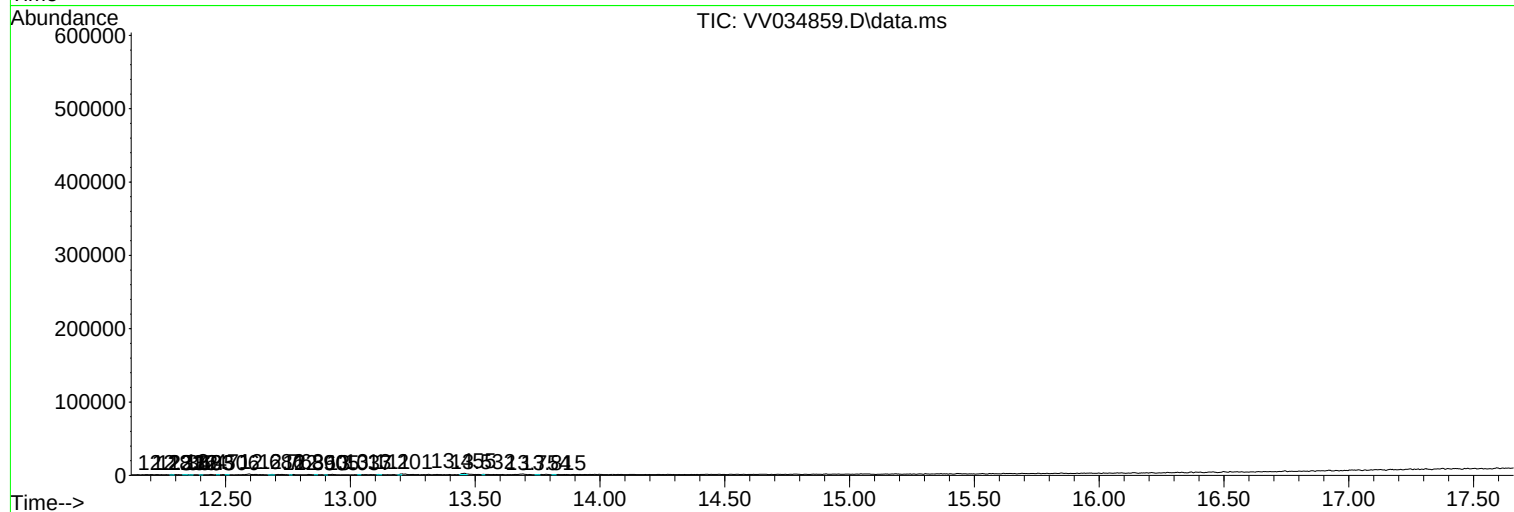
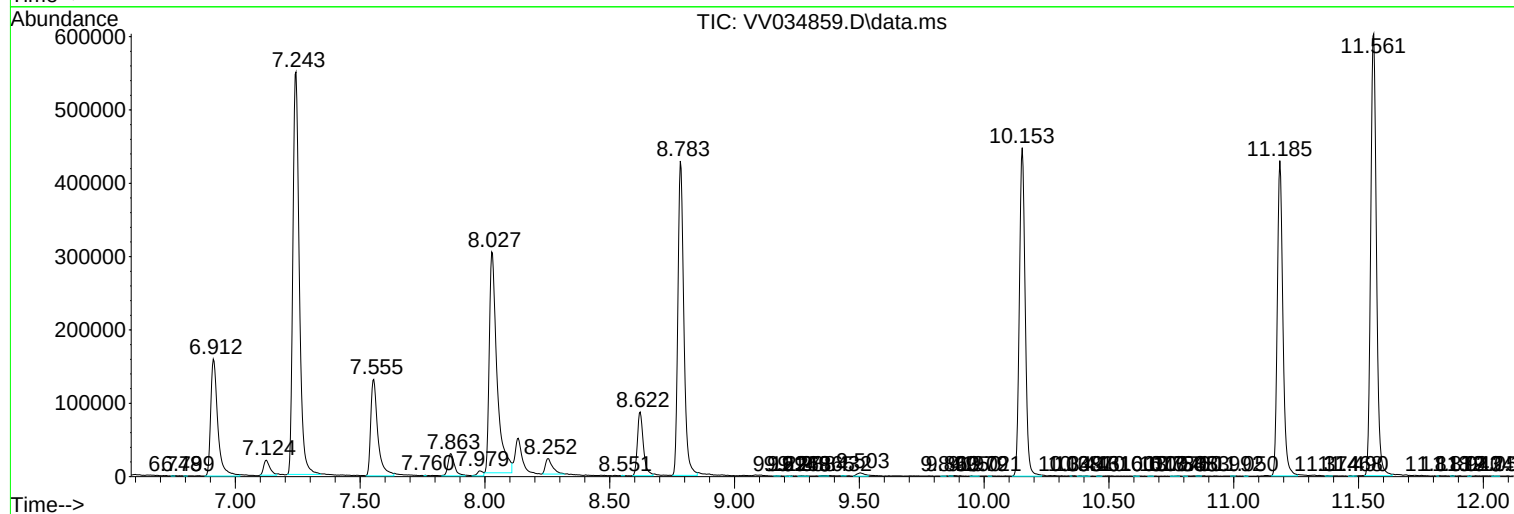
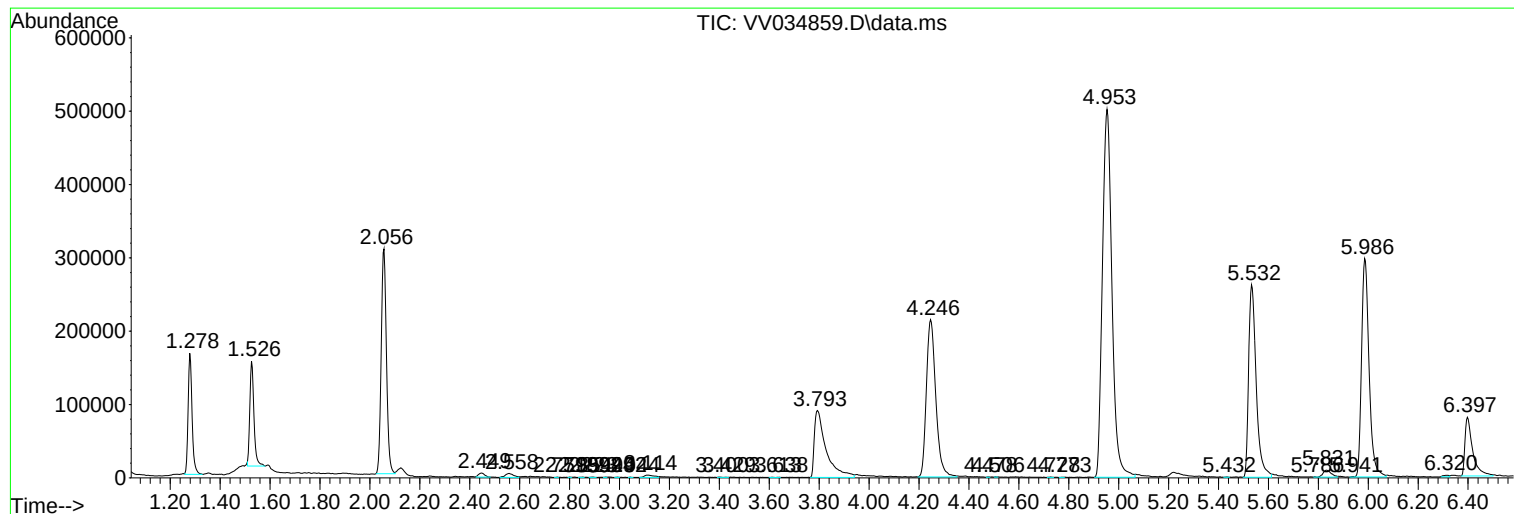
77	11.561	3260	3272	3295	rBV	602535	964070	72.08%	9.683%
78	11.818	3350	3352	3353	rBV	492	245	0.02%	0.002%
79	11.879	3367	3371	3373	rBV4	508	364	0.03%	0.004%
80	11.943	3389	3391	3394	rVB2	457	202	0.02%	0.002%
81	12.040	3419	3421	3423	rVB	473	178	0.01%	0.002%
82	12.056	3423	3426	3429	rBV2	282	234	0.02%	0.002%
83	12.120	3443	3446	3449	rBV3	318	281	0.02%	0.003%
84	12.281	3494	3496	3500	rBV	504	372	0.03%	0.004%
85	12.336	3510	3513	3517	rBV2	278	207	0.02%	0.002%
86	12.358	3518	3520	3524	rVB2	367	214	0.02%	0.002%
87	12.403	3531	3534	3536	rBV	401	232	0.02%	0.002%
88	12.471	3552	3555	3557	rBV2	526	263	0.02%	0.003%
89	12.506	3563	3566	3569	rBV2	324	198	0.01%	0.002%
90	12.686	3617	3622	3625	rBV3	634	531	0.04%	0.005%
91	12.763	3643	3646	3647	rBV2	719	348	0.03%	0.003%
92	12.860	3674	3676	3679	rBV	359	246	0.02%	0.002%
93	12.905	3687	3690	3691	rBV2	319	186	0.01%	0.002%
94	13.037	3728	3731	3733	rBV2	306	174	0.01%	0.002%
95	13.111	3752	3754	3759	rVB2	484	265	0.02%	0.003%
96	13.201	3778	3782	3783	rBV	1241	673	0.05%	0.007%
97	13.455	3855	3861	3865	rBV6	1827	2264	0.17%	0.023%
98	13.532	3883	3885	3887	rBV2	490	284	0.02%	0.003%
99	13.754	3949	3954	3956	rBV2	417	440	0.03%	0.004%
100	13.815	3970	3973	3976	rBV2	321	311	0.02%	0.003%

Sum of corrected areas: 9956425

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ALS Vial : 8 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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



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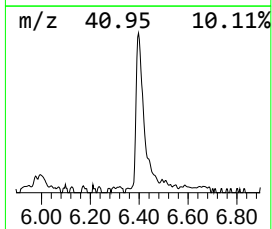
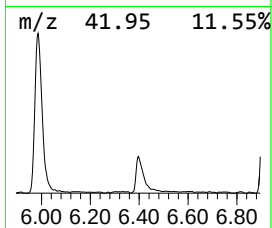
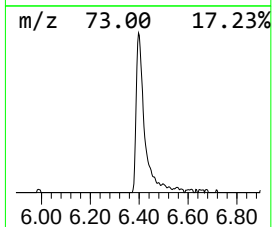
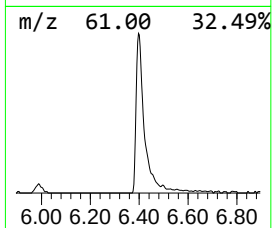
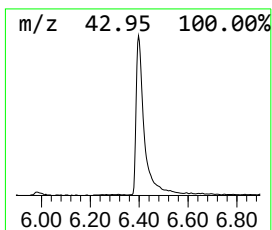
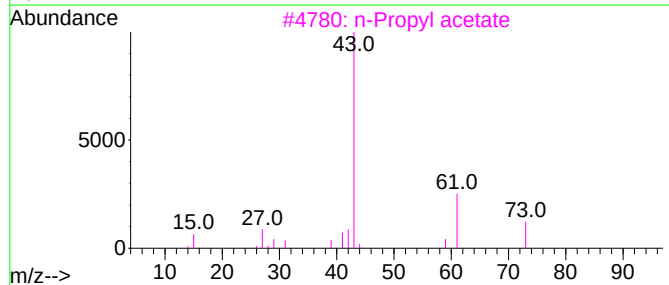
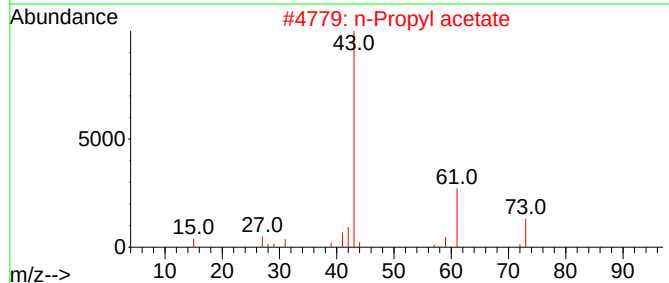
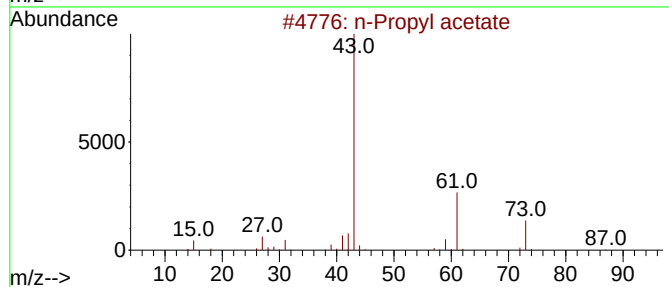
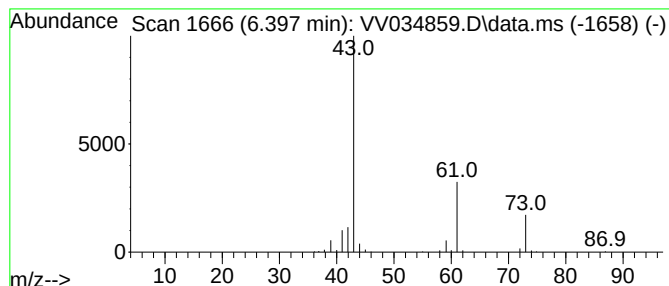
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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	15.71 ug/L	173193	1,4-Difluorobenzene	5.532

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	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

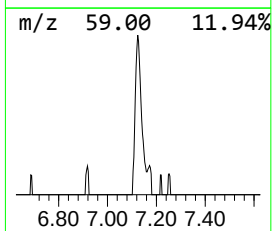
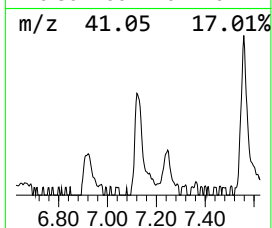
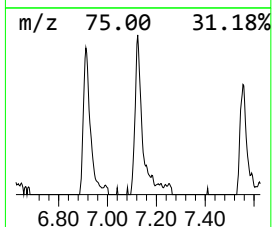
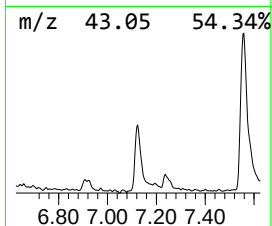
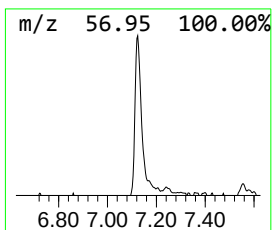
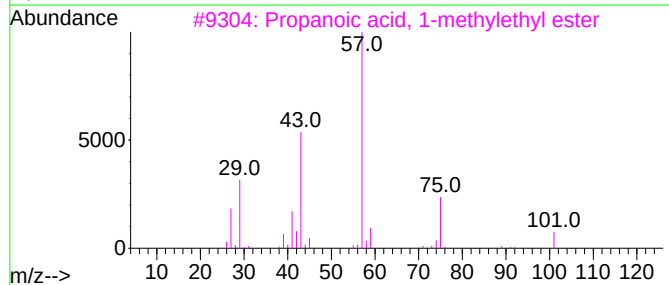
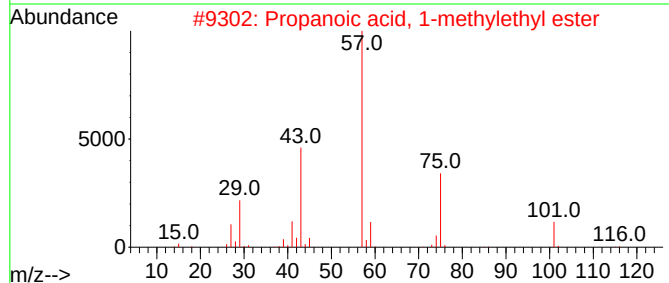
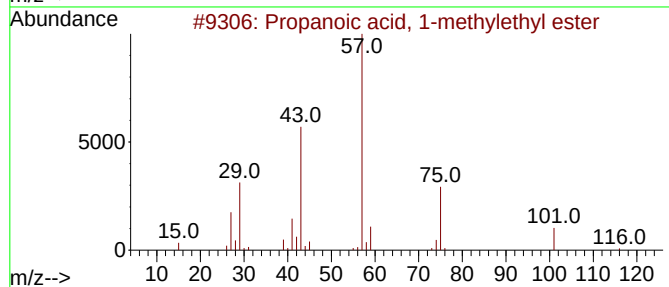
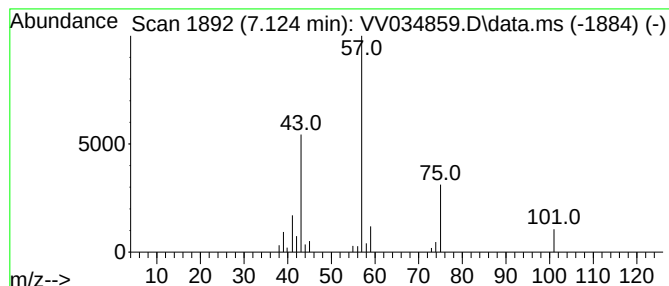
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.124	3.28 ug/L	36187	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
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	72
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64



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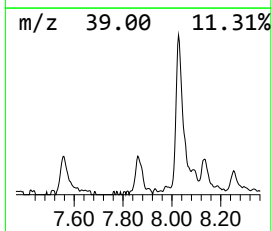
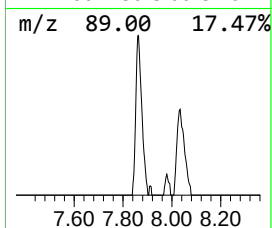
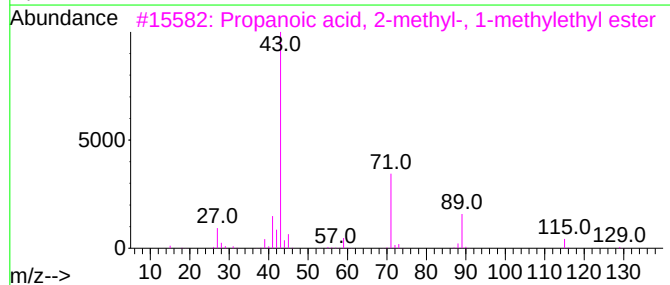
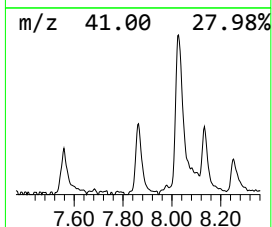
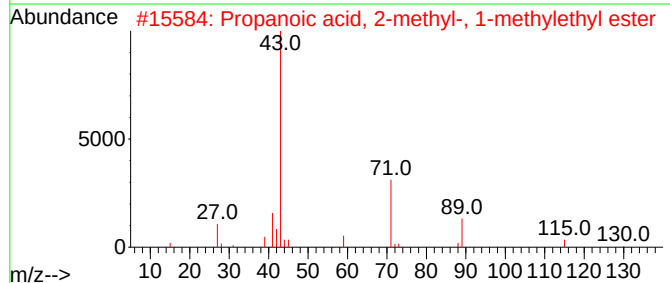
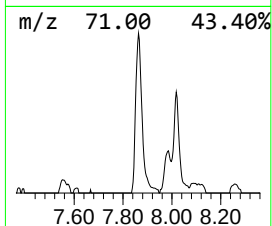
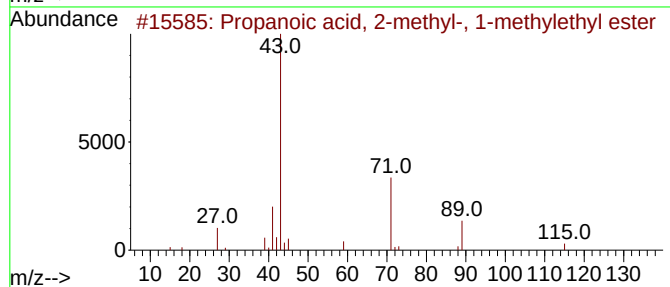
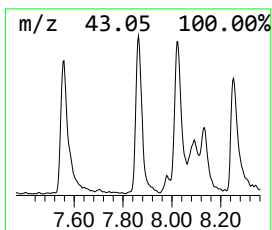
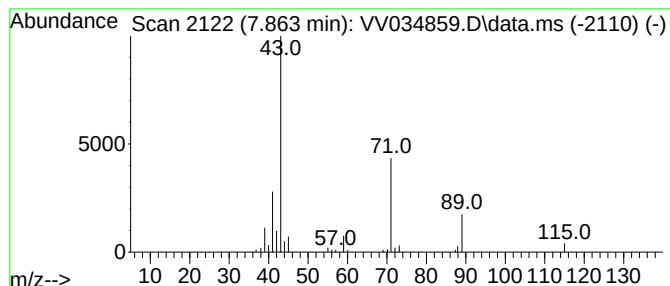
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	3.86 ug/L	54439	Chlorobenzene-d5	8.783

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	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	74
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032724\
Data File : VV034859.D
Acq On : 27 Mar 2024 12:53
Operator : SY/MD
Sample : PB159796TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

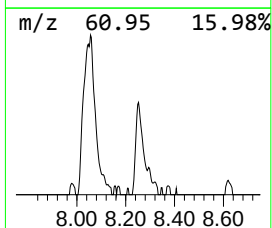
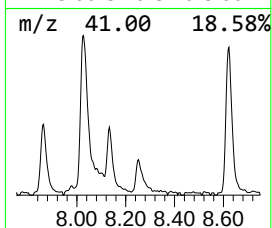
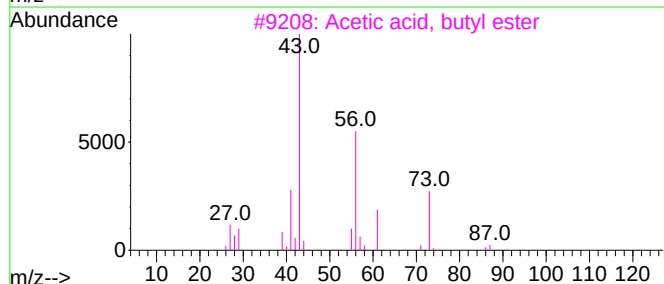
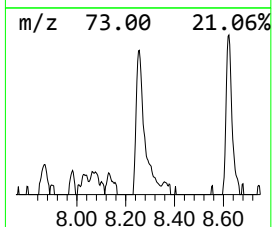
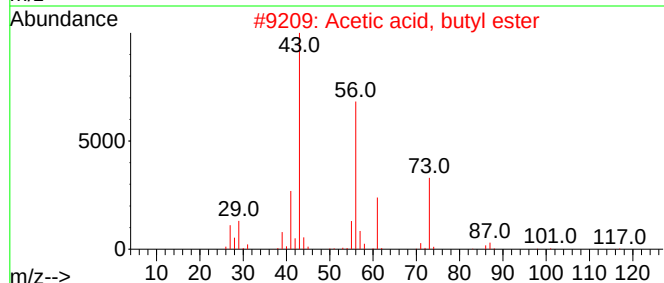
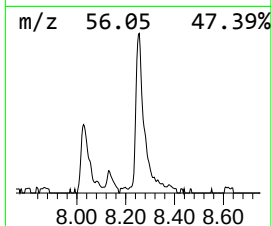
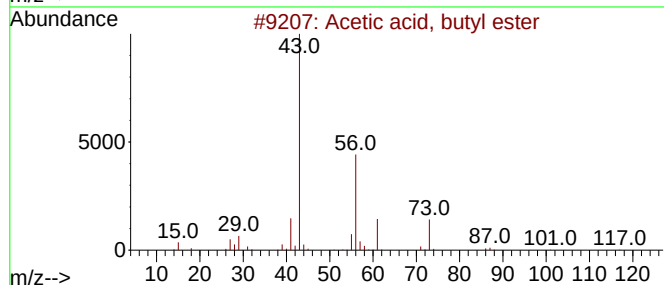
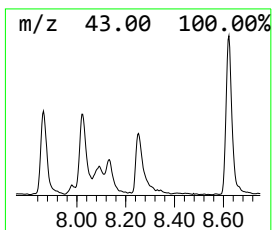
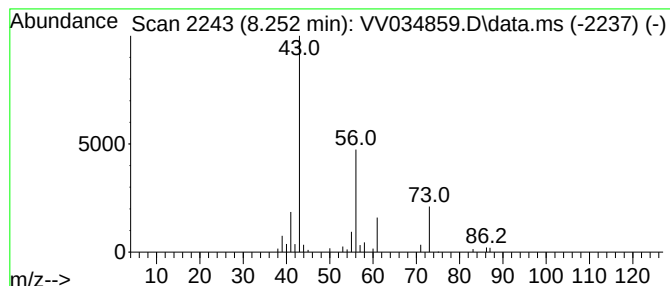
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Quant Title : VOC Analysis

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

Peak Number 5 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.252	2.98 ug/L	41979	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
5			Isobutyl acetate	116	C6H12O2	000110-19-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032724\
Data File : VV034859.D
Acq On : 27 Mar 2024 12:53
Operator : SY/MD
Sample : PB159796TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

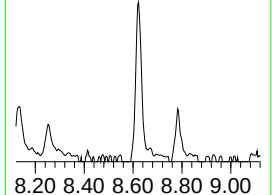
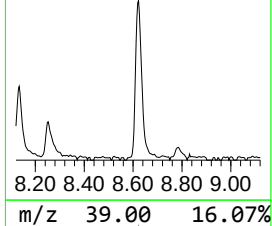
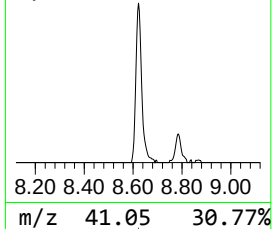
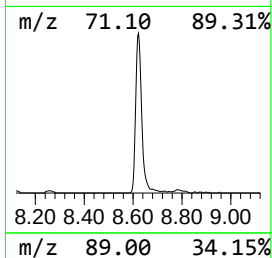
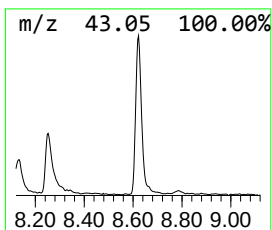
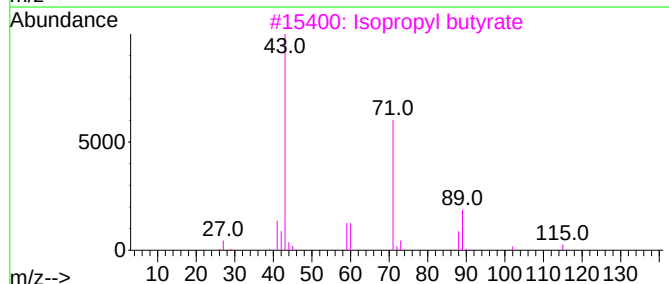
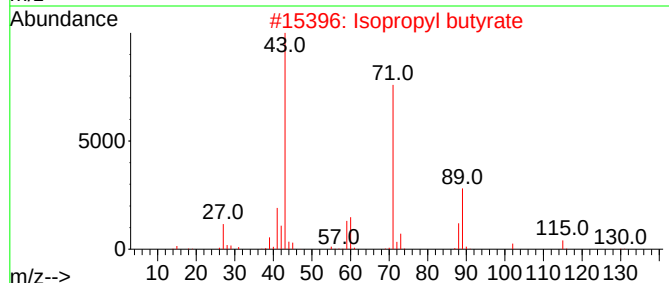
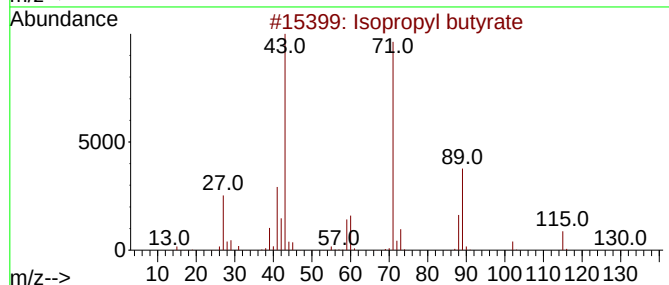
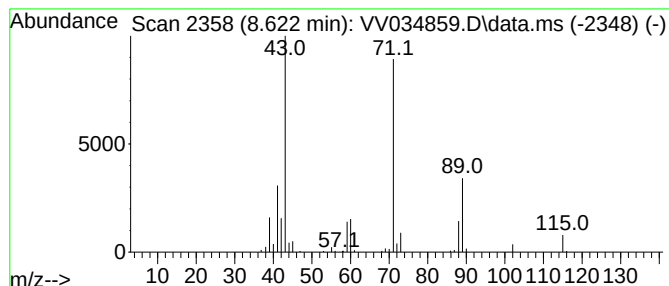
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.622	10.35 ug/L	145755	Chlorobenzene-d5	8.783

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, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032724\
Data File : VV034859.D
Acq On : 27 Mar 2024 12:53
Operator : SY/MD
Sample : PB159796TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.397	15.7	ug/L	173193	1	5.532	551157	50.0
Propanoic acid,...	7.124	3.3	ug/L	36187	1	5.532	551157	50.0
Propanoic acid,...	7.863	3.9	ug/L	54439	2	8.783	704429	50.0
Acetic acid, bu...	8.252	3.0	ug/L	41979	2	8.783	704429	50.0
Isopropyl butyrate	8.622	10.4	ug/L	145755	2	8.783	704429	50.0