

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040924\
 Data File : VV035091.D
 Acq On : 09 Apr 2024 18:39
 Operator : SY/MD
 Sample : PB160098TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB098

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: VV035091.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	87	rVB	196508	199670	13.49%	1.753%
2	1.526	145	151	170	rVB	180221	217918	14.72%	1.913%
3	2.056	307	316	329	rBV	331518	474176	32.03%	4.163%
4	2.449	430	438	447	rVB2	6499	10077	0.68%	0.088%
5	2.555	465	471	472	rBV3	1613	1601	0.11%	0.014%
6	2.793	541	545	549	rBV2	328	315	0.02%	0.003%
7	2.931	585	588	591	rVB3	676	350	0.02%	0.003%
8	2.973	599	601	602	rBV	338	127	0.01%	0.001%
9	2.998	608	609	611	rVB	446	149	0.01%	0.001%
10	3.063	627	629	635	rVB	317	201	0.01%	0.002%
11	3.117	635	646	649	rBV8	2265	3738	0.25%	0.033%
12	3.233	680	682	683	rBV8	338	134	0.01%	0.001%
13	3.288	696	699	700	rBV2	199	75	0.01%	0.001%
14	3.304	700	704	709	rBV4	740	676	0.05%	0.006%
15	3.349	716	718	720	rBV2	377	163	0.01%	0.001%
16	3.368	722	724	725	rVV	350	109	0.01%	0.001%
17	3.410	734	737	742	rBV2	356	285	0.02%	0.003%
18	3.436	742	745	748	rBV2	403	283	0.02%	0.002%
19	3.497	762	764	771	rVB2	442	309	0.02%	0.003%
20	3.526	771	773	783	rBV4	368	509	0.03%	0.004%
21	3.580	786	790	795	rVB3	372	405	0.03%	0.004%
22	3.603	795	797	799	rVB	339	114	0.01%	0.001%
23	3.622	799	803	804	rBV2	292	190	0.01%	0.002%
24	3.654	810	813	814	rBV2	247	112	0.01%	0.001%
25	3.664	814	816	818	rBV2	169	96	0.01%	0.001%
26	3.680	818	821	823	rVB2	277	137	0.01%	0.001%
27	3.693	823	825	826	rBV	144	56	0.00%	0.000%
28	3.741	838	840	842	rBV	278	121	0.01%	0.001%
29	3.786	842	854	887	rBV	112725	328019	22.16%	2.880%
30	4.246	983	997	1026	rBV	230476	596133	40.27%	5.233%
31	4.490	1070	1073	1076	rVB3	854	449	0.03%	0.004%
32	4.764	1155	1158	1159	rBV	285	103	0.01%	0.001%
33	4.783	1162	1164	1166	rBV	303	174	0.01%	0.002%
34	4.825	1175	1177	1179	rBV2	336	138	0.01%	0.001%
35	4.953	1200	1217	1247	rBV2	557723	1480223	100.00%	12.995%
36	5.217	1290	1299	1317	rBV2	8042	23354	1.58%	0.205%

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

37	5.381	1348	1350	1352	rBV2	610	300	0.02%	0.003%
38	5.416	1358	1361	1368	rVB5	902	767	0.05%	0.007%
39	5.445	1368	1370	1373	rBV3	371	204	0.01%	0.002%
40	5.465	1373	1376	1378	rBV2	358	233	0.02%	0.002%
41	5.532	1387	1397	1444	rBV	390196	824263	55.69%	7.236%
42	5.834	1482	1491	1504	rBV4	9327	21337	1.44%	0.187%
43	5.989	1525	1539	1563	rBV	334047	699323	47.24%	6.139%
44	6.394	1658	1665	1700	rBV	118046	238343	16.10%	2.092%
45	6.780	1783	1785	1789	rBV2	527	501	0.03%	0.004%
46	6.847	1803	1806	1808	rBV	713	388	0.03%	0.003%
47	6.912	1816	1826	1860	rBV	163892	313799	21.20%	2.755%
48	7.124	1884	1892	1911	rBV	26913	48847	3.30%	0.429%
49	7.243	1918	1929	1953	rBV	610264	1083364	73.19%	9.511%
50	7.555	2017	2026	2064	rBV	143157	271479	18.34%	2.383%
51	7.863	2112	2122	2141	rBV	37289	66588	4.50%	0.585%
52	7.976	2151	2157	2163	rBV5	7683	12058	0.81%	0.106%
53	8.024	2163	2172	2198	rBV2	348856	695875	47.01%	6.109%
54	8.249	2235	2242	2267	rVB	32541	64701	4.37%	0.568%
55	8.619	2347	2357	2380	rBV	105868	181965	12.29%	1.597%
56	8.783	2398	2408	2431	rBV	598419	1002111	67.70%	8.797%
57	9.217	2540	2543	2545	rBV3	666	343	0.02%	0.003%
58	9.268	2556	2559	2560	rBV	491	299	0.02%	0.003%
59	9.310	2569	2572	2573	rBV2	367	213	0.01%	0.002%
60	9.500	2623	2631	2644	rBV5	5456	10742	0.73%	0.094%
61	9.744	2705	2707	2711	rVB2	396	234	0.02%	0.002%
62	9.844	2734	2738	2741	rBV3	477	395	0.03%	0.003%
63	9.873	2744	2747	2753	rBV4	553	671	0.05%	0.006%
64	9.944	2766	2769	2772	rBV	476	349	0.02%	0.003%
65	9.985	2780	2782	2785	rBB	317	150	0.01%	0.001%
66	10.001	2785	2787	2792	rBV3	454	244	0.02%	0.002%
67	10.108	2817	2820	2822	rBV2	581	411	0.03%	0.004%
68	10.153	2822	2834	2858	rVV	460127	739147	49.93%	6.489%
69	10.320	2883	2886	2895	rBV5	801	1031	0.07%	0.009%
70	10.538	2951	2954	2955	rBV2	402	234	0.02%	0.002%
71	10.599	2970	2973	2976	rBV2	552	364	0.02%	0.003%
72	10.683	2996	2999	3003	rBV3	648	570	0.04%	0.005%
73	10.712	3006	3008	3010	rBV	349	188	0.01%	0.002%
74	10.725	3010	3012	3015	rVB2	582	281	0.02%	0.002%
75	10.751	3015	3020	3022	rBV2	485	400	0.03%	0.004%
76	10.808	3034	3038	3040	rBV	519	355	0.02%	0.003%

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77	10.818	3040	3041	3042	rBV	343	120	0.01%	0.001%
78	10.860	3051	3054	3056	rVB2	607	258	0.02%	0.002%
79	10.876	3056	3059	3061	rBV2	467	244	0.02%	0.002%
80	10.918	3071	3072	3073	rBV2	378	124	0.01%	0.001%
81	10.934	3073	3077	3078	rVV	462	291	0.02%	0.003%
82	11.066	3114	3118	3119	rBV	357	233	0.02%	0.002%
83	11.185	3144	3155	3178	rBV	512801	824177	55.68%	7.235%
84	11.445	3229	3236	3237	rBV2	515	547	0.04%	0.005%
85	11.561	3259	3272	3296	rBV	576322	929409	62.79%	8.159%
86	11.934	3386	3388	3393	rBV4	547	463	0.03%	0.004%
87	12.188	3463	3467	3471	rBV4	605	669	0.05%	0.006%
88	12.255	3486	3488	3489	rBV	271	96	0.01%	0.001%
89	12.265	3489	3491	3492	rBV2	331	109	0.01%	0.001%
90	12.342	3512	3515	3516	rBV2	283	157	0.01%	0.001%
91	12.567	3582	3585	3588	rVB3	347	205	0.01%	0.002%
92	12.593	3590	3593	3594	rBV3	363	227	0.02%	0.002%
93	12.622	3599	3602	3604	rBV	268	157	0.01%	0.001%
94	12.635	3604	3606	3608	rBV2	326	139	0.01%	0.001%
95	12.670	3614	3617	3619	rVB2	420	217	0.01%	0.002%
96	12.754	3640	3643	3645	rBV2	323	208	0.01%	0.002%
97	13.210	3777	3785	3795	rBV4	4951	8183	0.55%	0.072%
98	13.316	3815	3818	3821	rBV4	527	364	0.02%	0.003%
99	13.570	3895	3897	3900	rBV	500	333	0.02%	0.003%
100	14.066	4049	4051	4054	rVB2	517	176	0.01%	0.002%

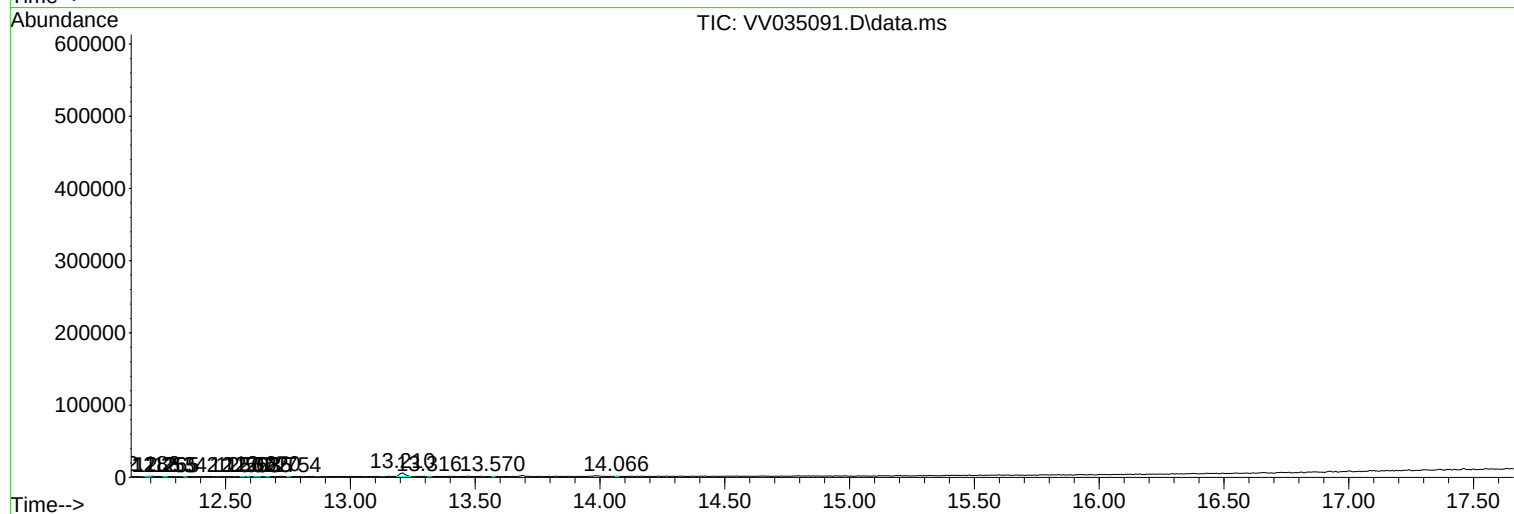
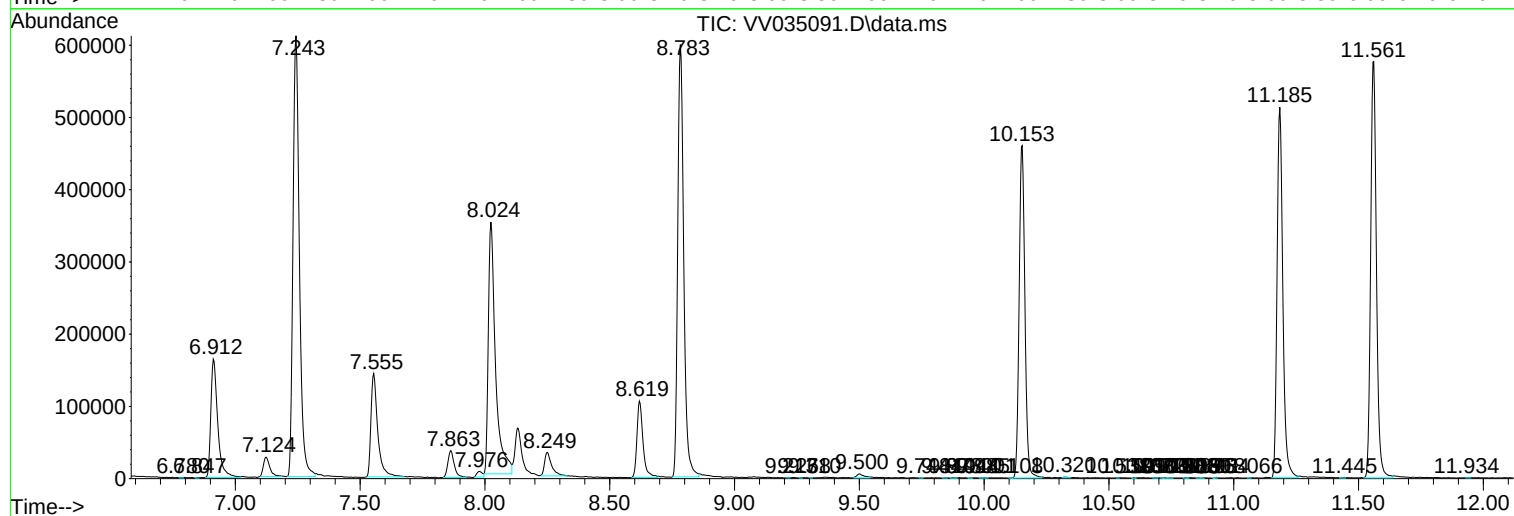
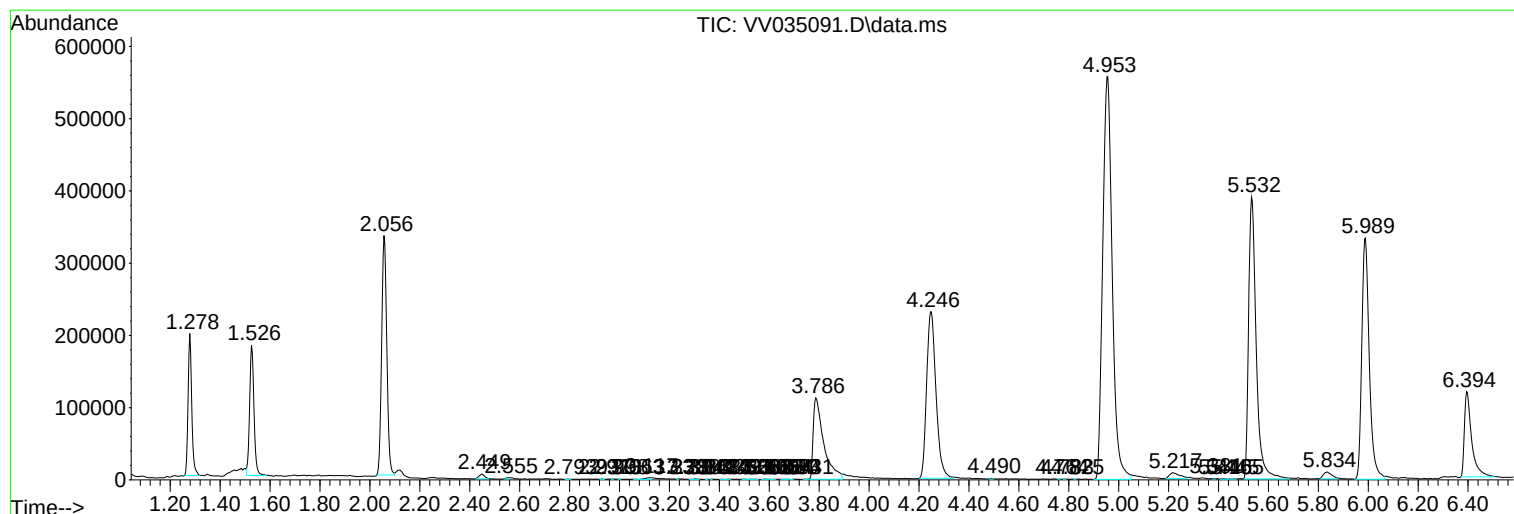
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MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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



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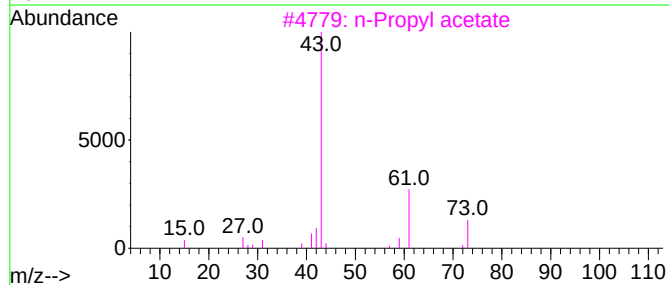
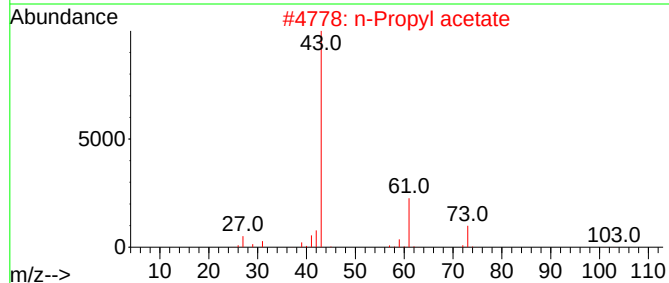
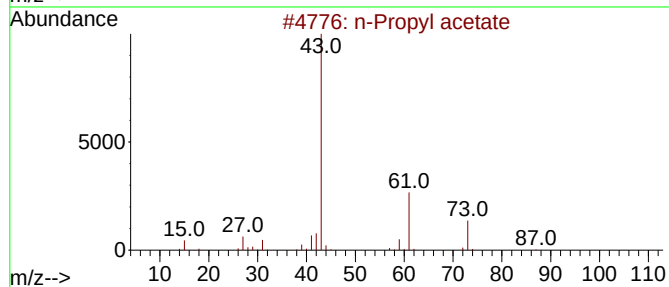
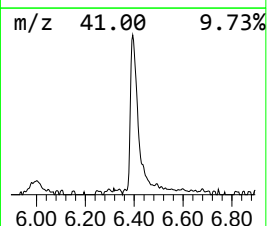
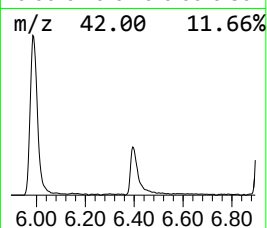
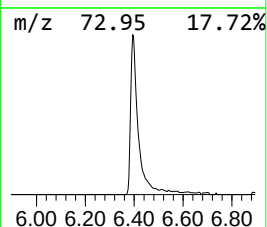
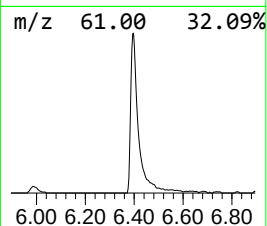
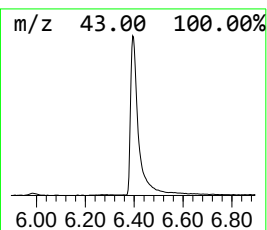
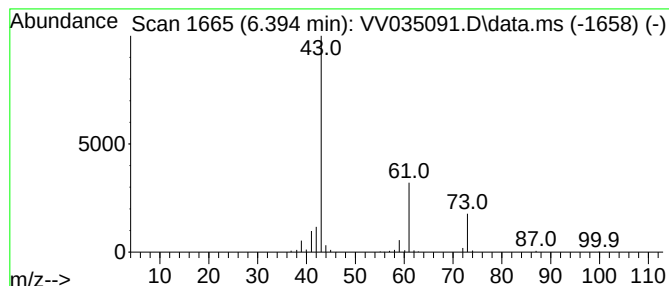
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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.
6.394	14.46 ug/L	238343	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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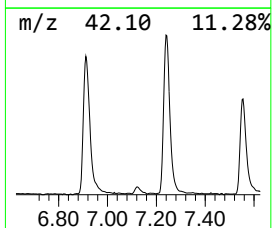
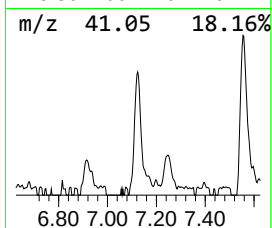
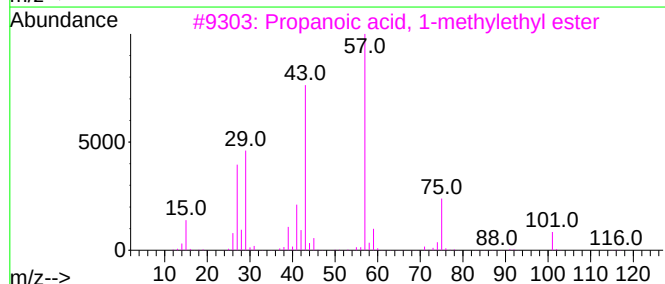
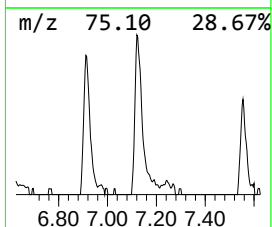
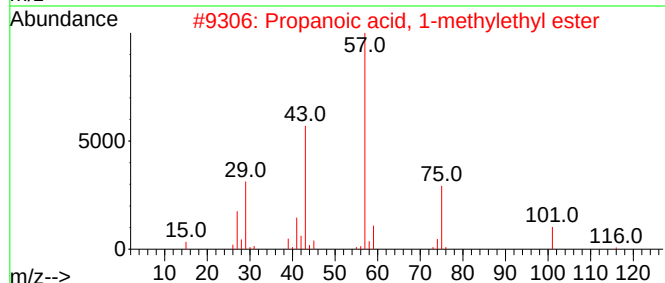
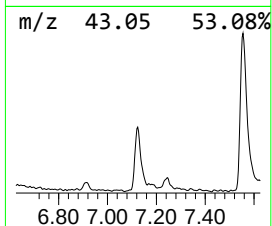
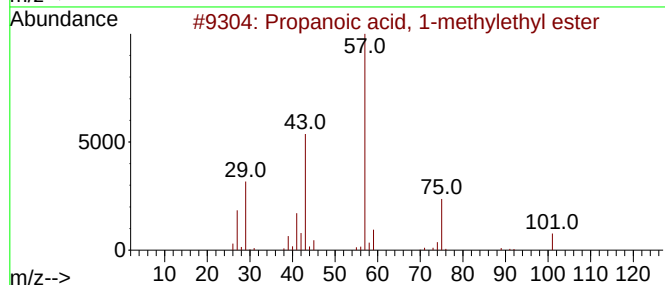
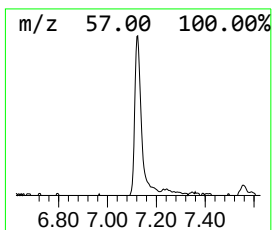
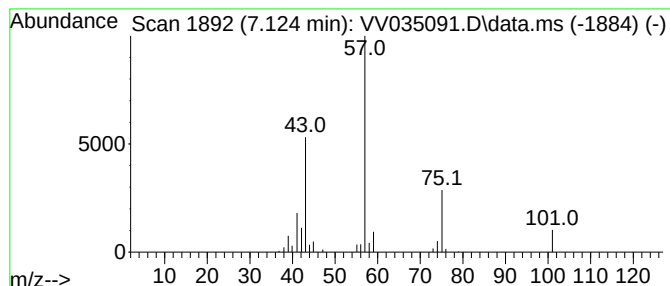
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.124	2.96 ug/L	48847	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	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



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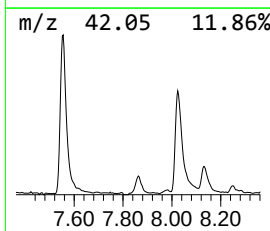
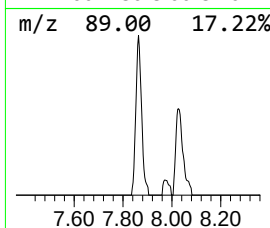
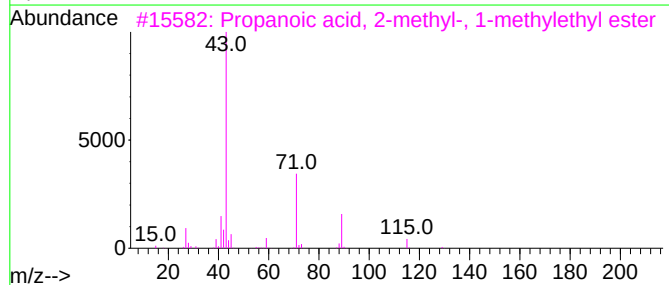
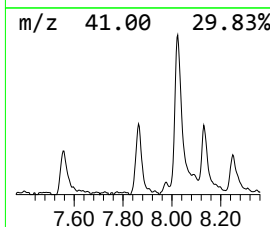
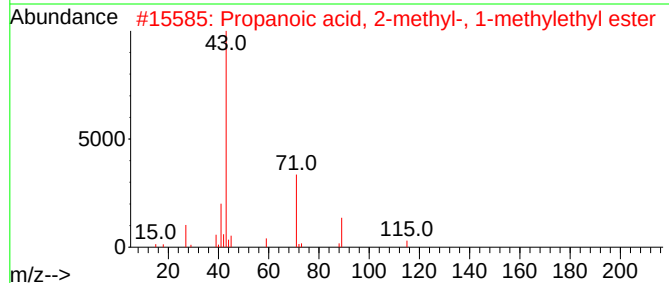
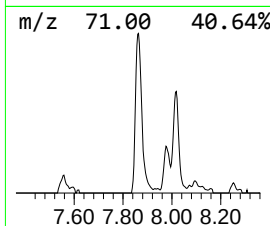
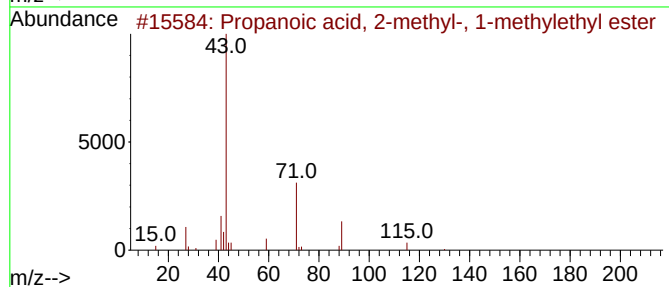
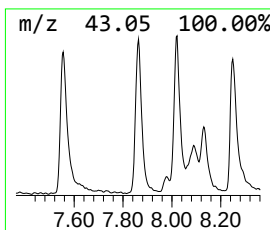
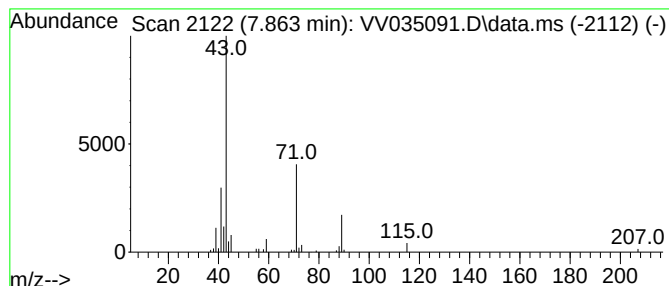
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	3.32 ug/L	66588	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	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\VV040924\
Data File : VV035091.D
Acq On : 09 Apr 2024 18:39
Operator : SY/MD
Sample : PB160098TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB098

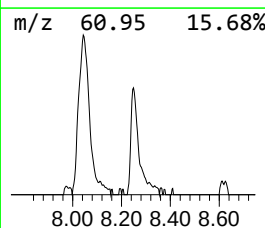
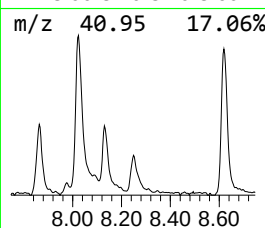
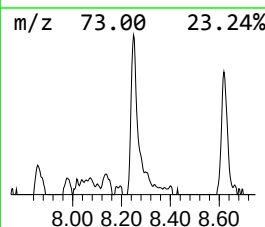
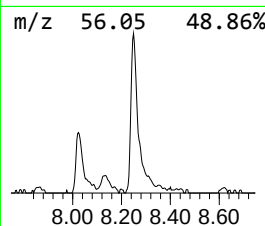
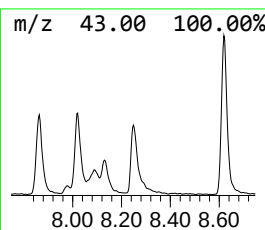
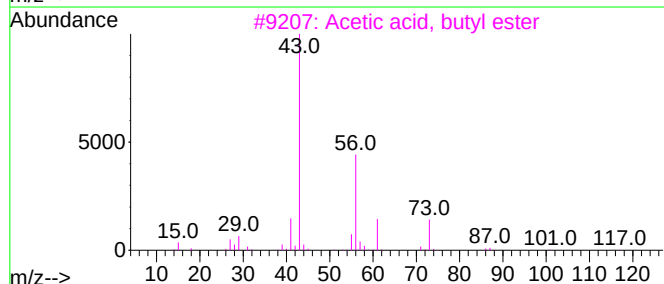
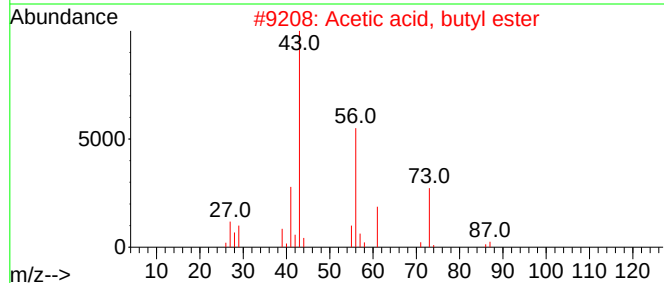
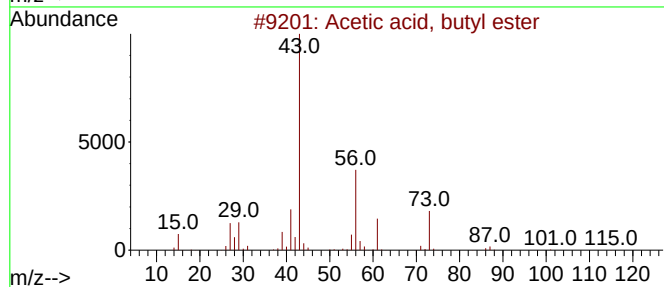
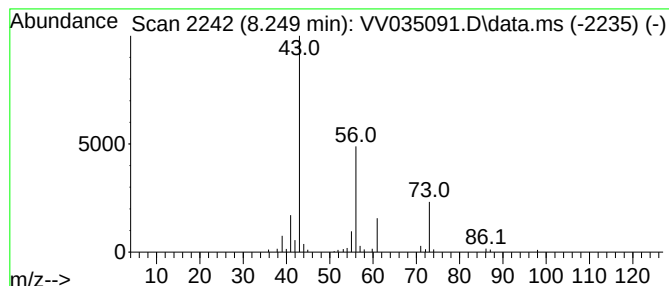
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Quant Title : VOC Analysis

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

Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.249	3.23 ug/L	64701	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	42
5			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040924\
Data File : VV035091.D
Acq On : 09 Apr 2024 18:39
Operator : SY/MD
Sample : PB160098TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB098

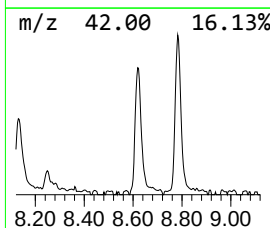
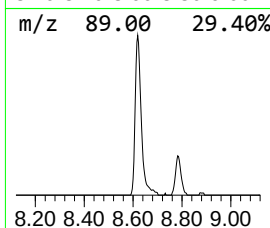
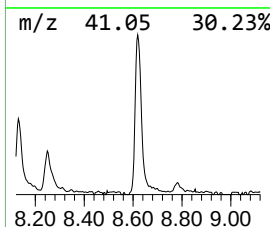
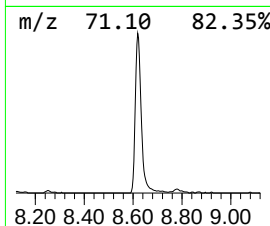
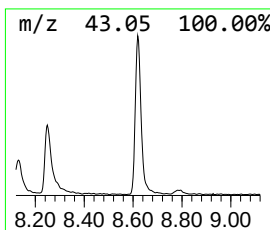
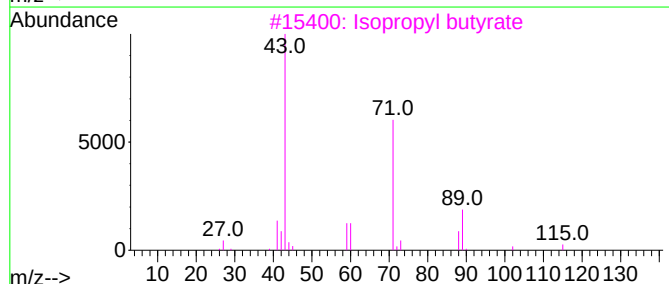
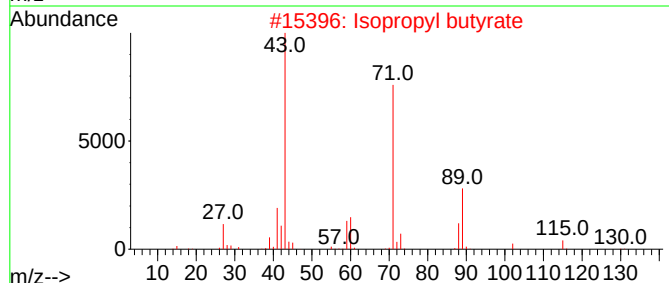
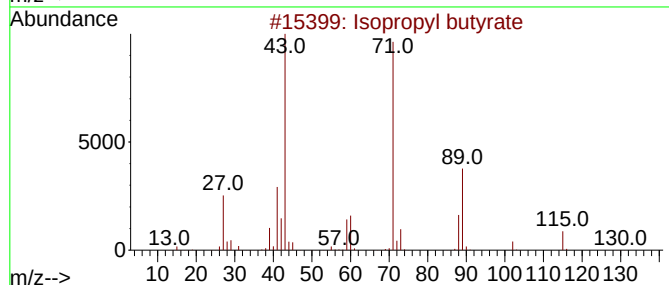
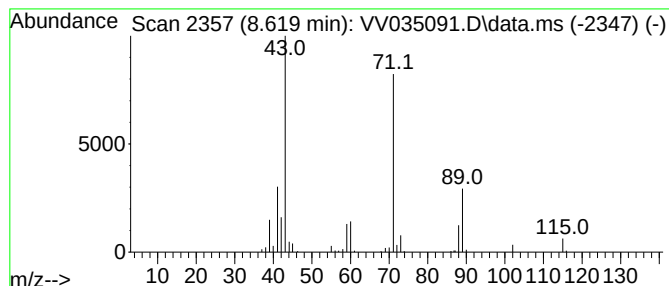
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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.
8.619	9.08 ug/L	181965	Chlorobenzene-d5	8.783

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040924\
Data File : VV035091.D
Acq On : 09 Apr 2024 18:39
Operator : SY/MD
Sample : PB160098TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB098

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	6.394	14.5	ug/L	238343	1	5.532	824263	50.0
Propanoic acid,...	7.124	3.0	ug/L	48847	1	5.532	824263	50.0
Propanoic acid,...	7.863	3.3	ug/L	66588	2	8.783	1002110	50.0
Acetic acid, bu...	8.249	3.2	ug/L	64701	2	8.783	1002110	50.0
Isopropyl butyrate	8.619	9.1	ug/L	181965	2	8.783	1002110	50.0