

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW122022\
 Data File : VW029745.D
 Acq On : 20 Dec 2022 12:49
 Operator : SY/MD
 Sample : PB149759TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB759

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\SFAMVLM120722WMA.M
 Title : VOC Analysis

Signal : TIC: VW029745.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	99	rVB	254848	254023	14.04%	1.740%
2	1.564	155	163	174	rBV	218193	248378	13.73%	1.702%
3	2.105	321	331	343	rBV	420555	600265	33.18%	4.112%
4	2.503	446	455	470	rBV2	10876	18118	1.00%	0.124%
5	2.613	487	489	491	rBV2	409	191	0.01%	0.001%
6	2.760	530	535	539	rBV3	527	596	0.03%	0.004%
7	2.995	604	608	613	rVB2	354	280	0.02%	0.002%
8	3.037	619	621	626	rVB2	375	284	0.02%	0.002%
9	3.092	633	638	640	rBV	232	182	0.01%	0.001%
10	3.108	640	643	648	rVB	156	121	0.01%	0.001%
11	3.166	652	661	662	rBV4	1055	1374	0.08%	0.009%
12	3.236	681	683	689	rVB2	354	215	0.01%	0.001%
13	3.291	697	700	703	rBV3	199	152	0.01%	0.001%
14	3.349	716	718	721	rBV2	184	108	0.01%	0.001%
15	3.371	721	725	728	rVB2	233	220	0.01%	0.002%
16	3.555	778	782	786	rVB2	164	167	0.01%	0.001%
17	3.638	804	808	810	rBV	188	116	0.01%	0.001%
18	3.680	818	821	822	rBV	218	105	0.01%	0.001%
19	3.693	823	825	829	rVB	280	139	0.01%	0.001%
20	3.757	841	845	847	rBV2	211	145	0.01%	0.001%
21	3.789	851	855	856	rBV	428	279	0.02%	0.002%
22	3.873	870	881	932	rBV	110808	356490	19.71%	2.442%
23	4.336	1008	1025	1062	rBV	280594	709718	39.23%	4.862%
24	4.600	1105	1107	1110	rBV2	391	165	0.01%	0.001%
25	4.690	1132	1135	1141	rVB3	486	437	0.02%	0.003%
26	4.725	1141	1146	1150	rBV2	359	392	0.02%	0.003%
27	4.780	1159	1163	1166	rBV2	296	245	0.01%	0.002%
28	4.821	1170	1176	1179	rBV3	238	215	0.01%	0.001%
29	4.969	1220	1222	1224	rBV	176	89	0.00%	0.001%
30	5.037	1224	1243	1284	rBV2	686483	1809059	100.00%	12.394%
31	5.278	1308	1318	1338	rBV2	13571	32943	1.82%	0.226%
32	5.487	1380	1383	1386	rBV2	611	457	0.03%	0.003%
33	5.545	1392	1401	1406	rBV4	498	832	0.05%	0.006%
34	5.606	1406	1420	1447	rBV	472543	964556	53.32%	6.608%
35	5.899	1503	1511	1528	rVB6	4653	9440	0.52%	0.065%
36	5.998	1538	1542	1544	rVB2	292	159	0.01%	0.001%

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37	6.059	1544	1561	1594	rBV	403383	831382	45.96%	5.696%
38	6.346	1641	1650	1657	rBV2	5925	11879	0.66%	0.081%
39	6.458	1675	1685	1725	rBV	165474	338593	18.72%	2.320%
40	6.825	1797	1799	1802	rBV2	322	166	0.01%	0.001%
41	6.899	1819	1822	1824	rBV	318	212	0.01%	0.001%
42	6.976	1834	1846	1878	rBV	206666	385715	21.32%	2.643%
43	7.178	1897	1909	1922	rBV	40125	72242	3.99%	0.495%
44	7.307	1937	1949	1976	rBV	833647	1470411	81.28%	10.074%
45	7.571	2029	2031	2032	rBV	552	233	0.01%	0.002%
46	7.609	2032	2043	2065	rVV2	189556	342438	18.93%	2.346%
47	7.870	2122	2124	2126	rBV2	589	245	0.01%	0.002%
48	7.918	2129	2139	2156	rVV2	54497	93746	5.18%	0.642%
49	8.082	2180	2190	2214	rBV	440870	829897	45.87%	5.686%
50	8.185	2216	2222	2245	rVV	96183	160940	8.90%	1.103%
51	8.297	2249	2257	2278	rVB	55399	96135	5.31%	0.659%
52	8.599	2348	2351	2354	rBV4	510	475	0.03%	0.003%
53	8.673	2359	2374	2392	rBV	169175	271697	15.02%	1.861%
54	8.841	2414	2426	2456	rBV	709788	1175158	64.96%	8.051%
55	9.085	2500	2502	2503	rBV2	509	214	0.01%	0.001%
56	9.207	2538	2540	2541	rBV2	231	113	0.01%	0.001%
57	9.336	2577	2580	2581	rBV	258	123	0.01%	0.001%
58	9.381	2587	2594	2604	rBV4	2395	3447	0.19%	0.024%
59	9.461	2617	2619	2620	rBV4	232	97	0.01%	0.001%
60	9.542	2632	2644	2656	rBV2	15166	23886	1.32%	0.164%
61	9.619	2665	2668	2674	rBV2	330	379	0.02%	0.003%
62	9.648	2675	2677	2679	rBV2	210	100	0.01%	0.001%
63	9.696	2688	2692	2694	rBV	409	223	0.01%	0.002%
64	9.718	2698	2699	2703	rVV2	205	134	0.01%	0.001%
65	9.808	2725	2727	2729	rBB	187	86	0.00%	0.001%
66	9.821	2729	2731	2732	rBV	266	118	0.01%	0.001%
67	9.873	2744	2747	2750	rVV2	322	192	0.01%	0.001%
68	9.924	2755	2763	2768	rBV3	621	725	0.04%	0.005%
69	9.947	2768	2770	2775	rBV3	283	305	0.02%	0.002%
70	9.995	2782	2785	2787	rBV	404	216	0.01%	0.001%
71	10.027	2793	2795	2798	rBV	342	236	0.01%	0.002%
72	10.056	2801	2804	2806	rVB2	225	129	0.01%	0.001%
73	10.117	2820	2823	2825	rBV2	218	155	0.01%	0.001%
74	10.162	2825	2837	2839	rVV2	8904	11268	0.62%	0.077%
75	10.204	2840	2850	2874	rVB	588399	925015	51.13%	6.337%
76	10.371	2896	2902	2915	rVB6	2317	3654	0.20%	0.025%

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77	10.448	2922	2926	2928	rBV	368	228	0.01%	0.002%
78	10.474	2932	2934	2935	rBV	161	88	0.00%	0.001%
79	10.567	2953	2963	2976	rVB	4187	7288	0.40%	0.050%
80	10.619	2976	2979	2981	rBV2	240	173	0.01%	0.001%
81	10.651	2986	2989	2992	rBV3	234	164	0.01%	0.001%
82	10.712	3005	3008	3010	rBV2	351	220	0.01%	0.002%
83	10.760	3020	3023	3025	rBV	275	166	0.01%	0.001%
84	10.866	3053	3056	3058	rVB2	632	369	0.02%	0.003%
85	10.895	3058	3065	3066	rBV3	536	426	0.02%	0.003%
86	11.030	3105	3107	3110	rBV	235	192	0.01%	0.001%
87	11.091	3122	3126	3127	rBV2	238	190	0.01%	0.001%
88	11.236	3159	3171	3203	rBV	741286	1149753	63.56%	7.877%
89	11.480	3245	3247	3251	rVB2	421	255	0.01%	0.002%
90	11.513	3255	3257	3259	rBV	348	201	0.01%	0.001%
91	11.541	3263	3266	3268	rBV2	1057	818	0.05%	0.006%
92	11.612	3275	3288	3316	rBV	870673	1365617	75.49%	9.356%
93	11.818	3350	3352	3357	rVB3	522	317	0.02%	0.002%
94	11.927	3384	3386	3389	rVB2	273	158	0.01%	0.001%
95	12.021	3411	3415	3417	rBV	386	295	0.02%	0.002%
96	12.152	3453	3456	3457	rBV	316	174	0.01%	0.001%
97	12.181	3464	3465	3468	rBV	265	136	0.01%	0.001%
98	12.239	3479	3483	3493	rVB4	1521	1931	0.11%	0.013%
99	12.947	3697	3703	3708	rBV5	3060	3649	0.20%	0.025%
100	13.114	3751	3755	3762	rBV4	552	747	0.04%	0.005%

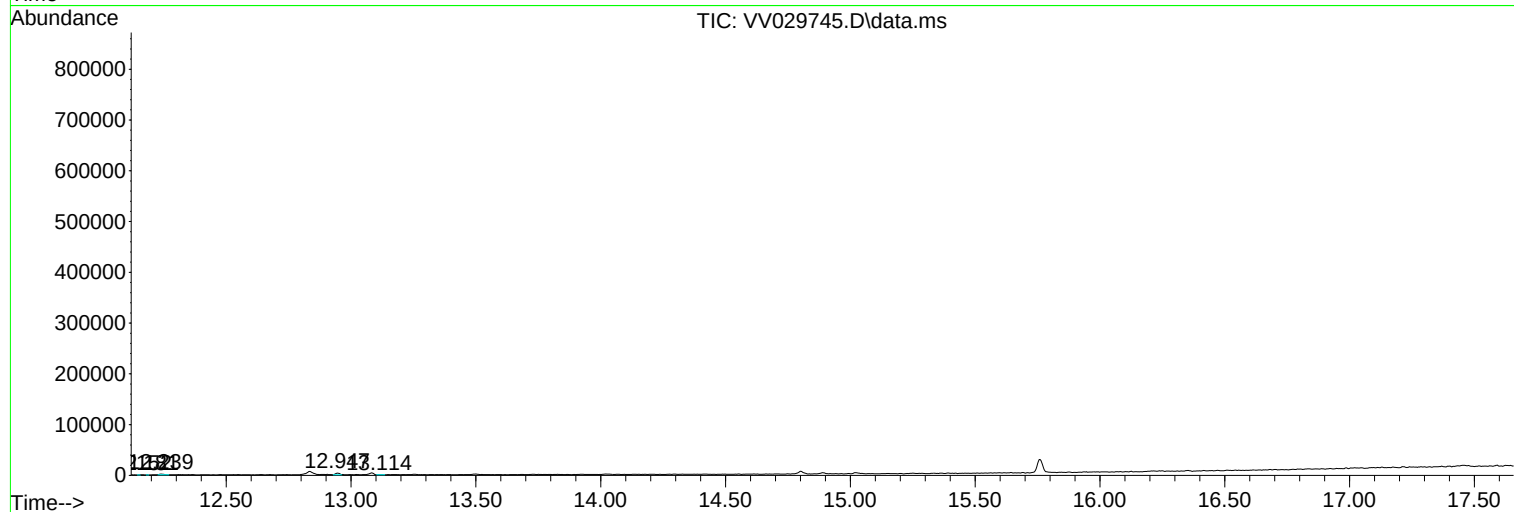
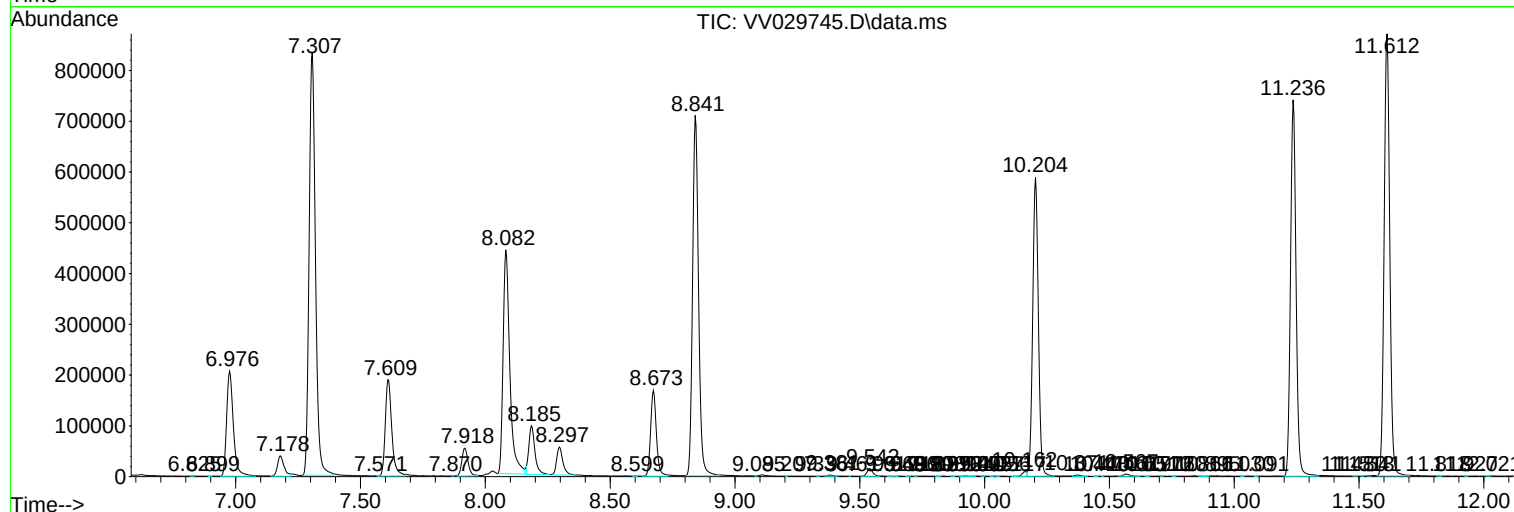
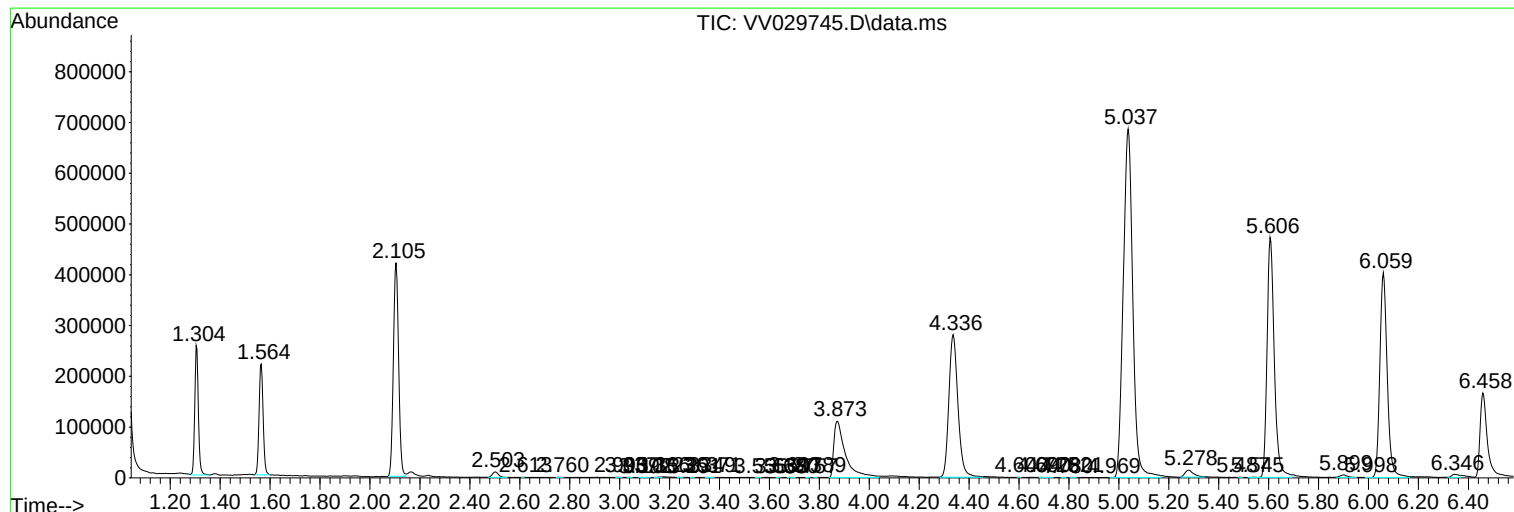
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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



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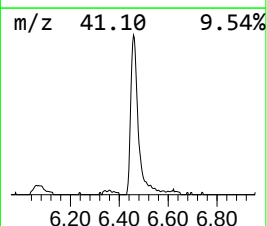
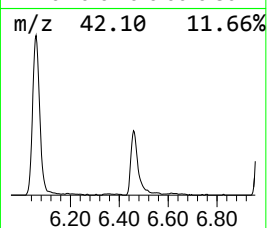
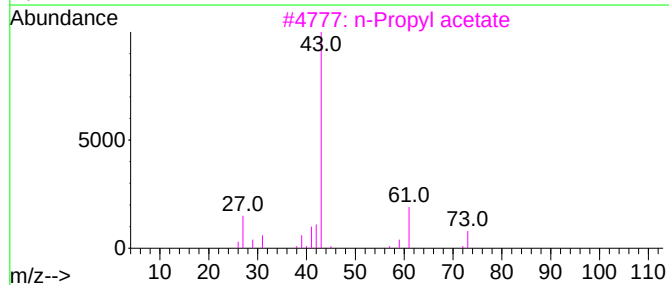
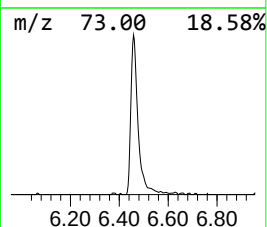
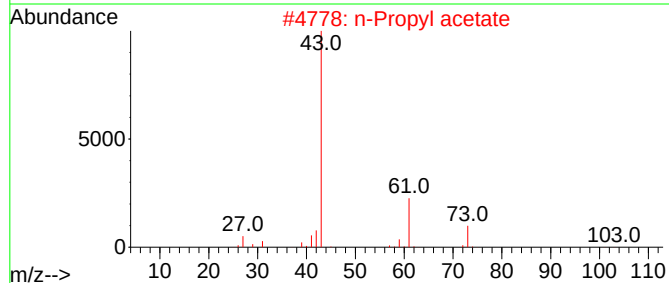
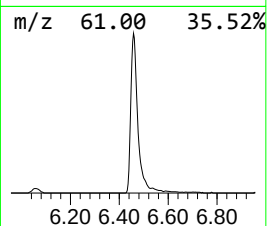
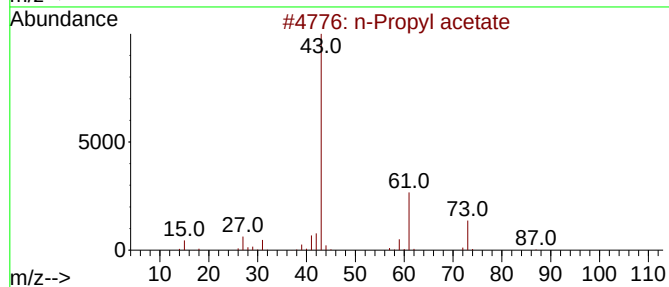
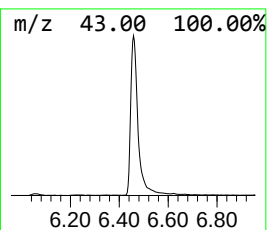
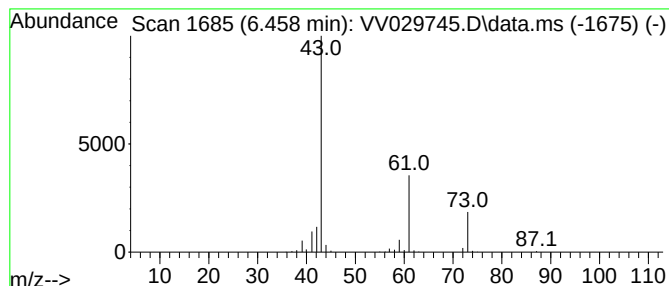
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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.
6.458	17.55 ug/L	338593	1,4-Difluorobenzene	5.606

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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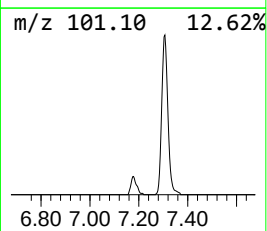
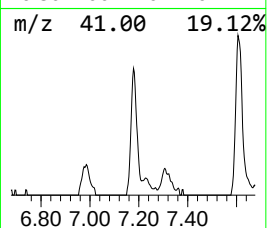
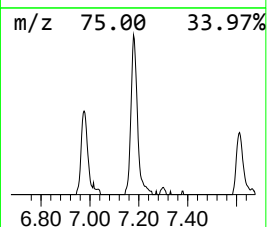
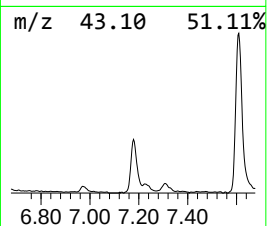
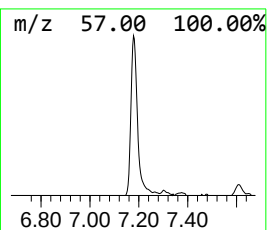
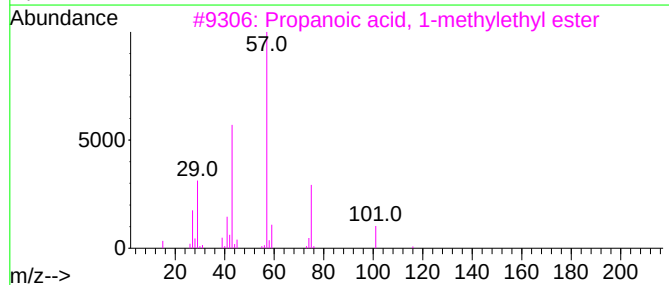
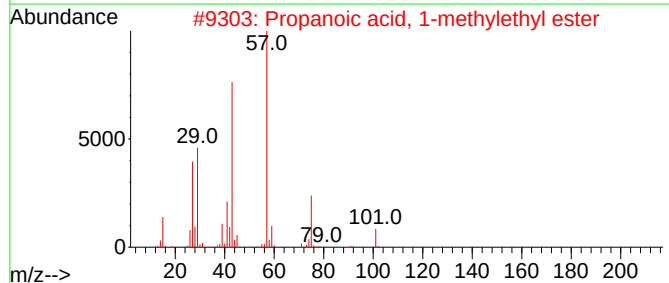
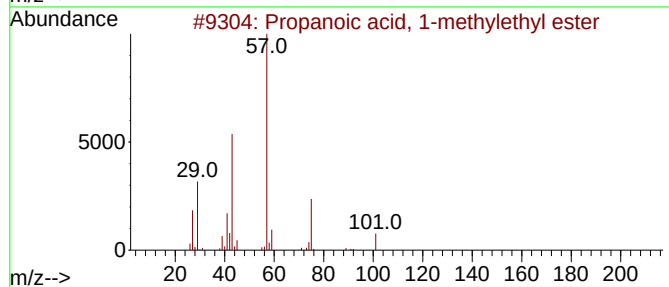
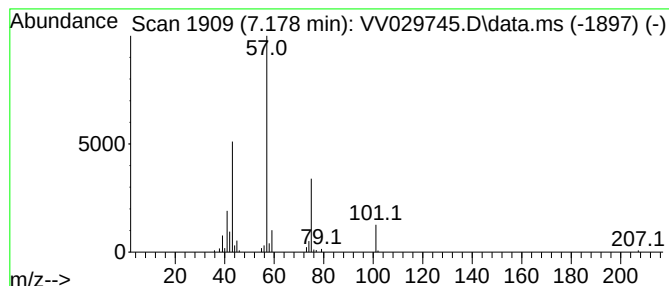
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.178	3.74 ug/L	72242	1,4-Difluorobenzene	5.606

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	74
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
4			Propionic acid, 4-hydroxy-3-hexy...	174	C9H18O3	1000151-16-9	59
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56



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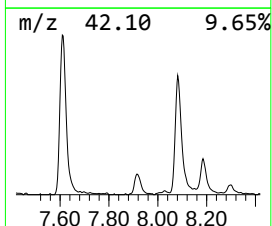
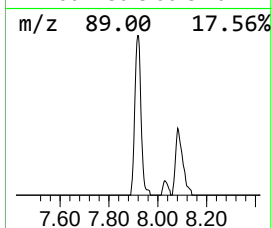
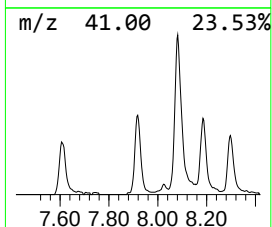
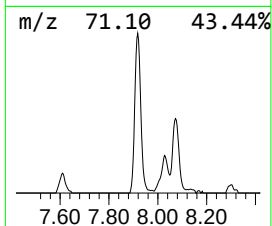
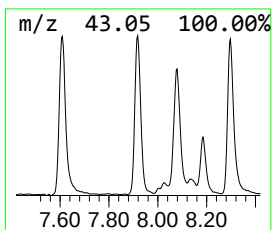
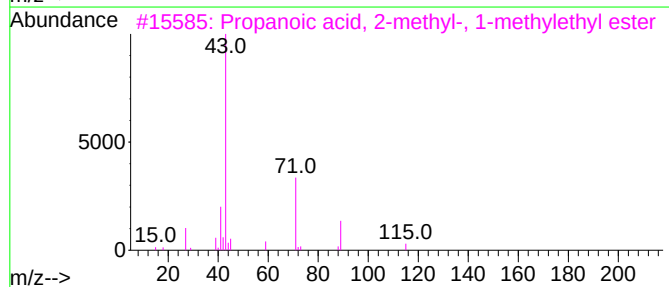
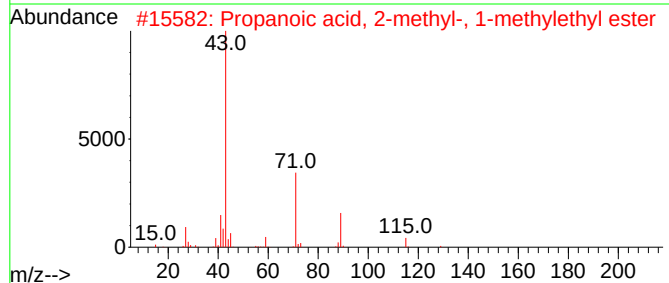
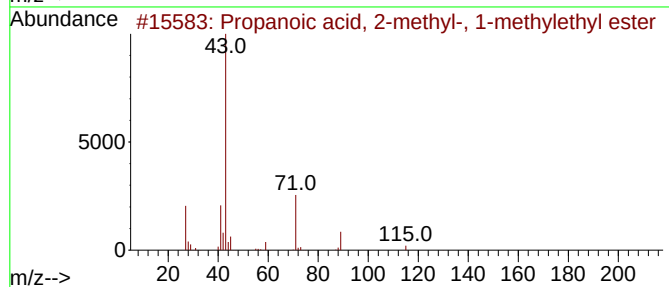
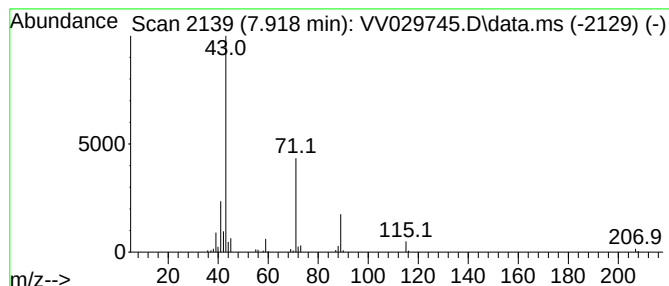
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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.918	3.99 ug/L	93746	Chlorobenzene-d5	8.841

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	78
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122022\
Data File : VV029745.D
Acq On : 20 Dec 2022 12:49
Operator : SY/MD
Sample : PB149759TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB759

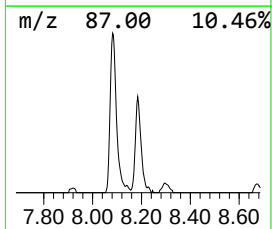
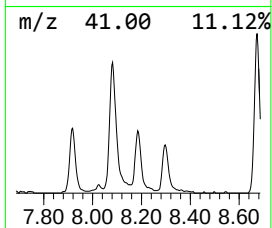
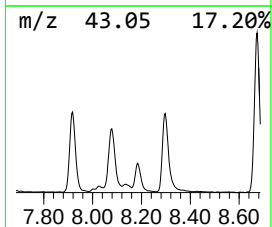
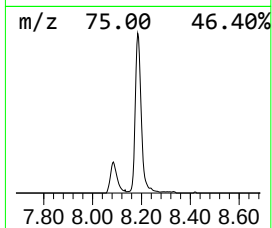
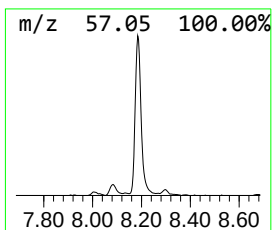
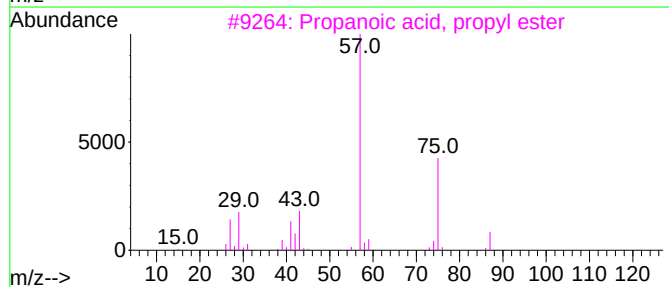
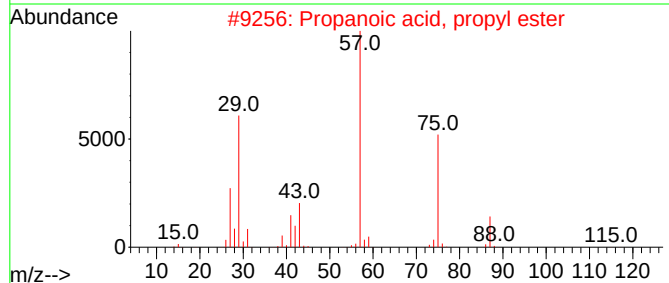
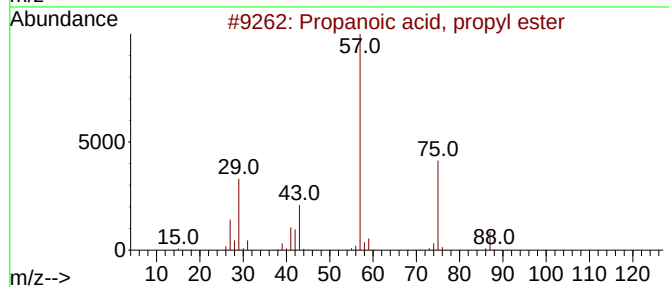
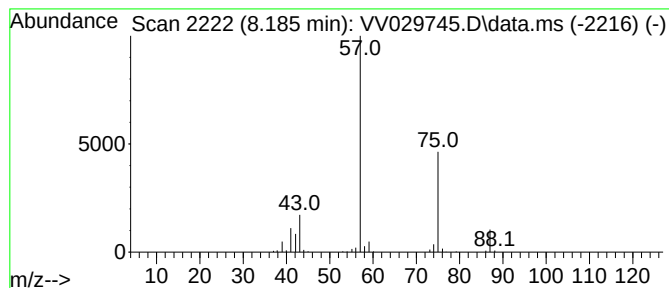
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Quant Title : VOC Analysis

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.
8.185	6.85 ug/L	160940	Chlorobenzene-d5	8.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	47
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122022\
Data File : VV029745.D
Acq On : 20 Dec 2022 12:49
Operator : SY/MD
Sample : PB149759TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB759

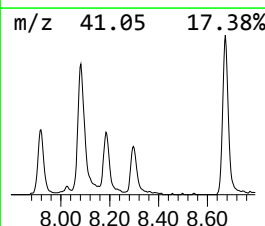
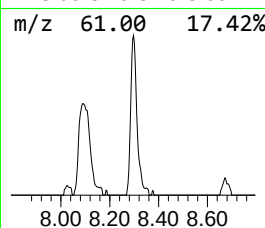
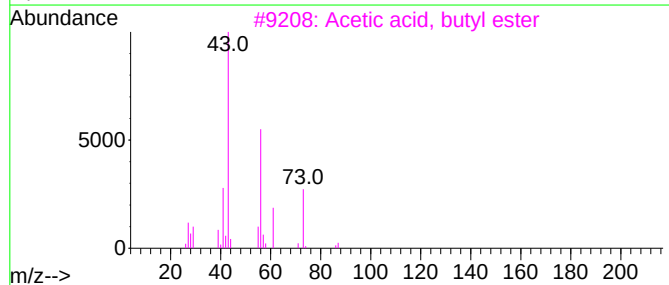
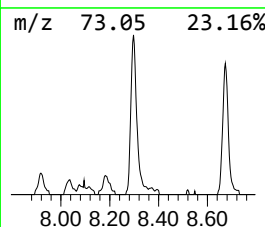
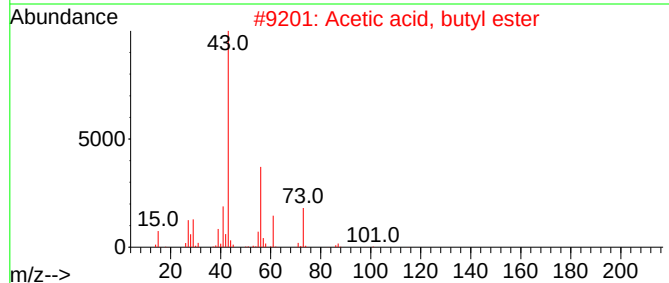
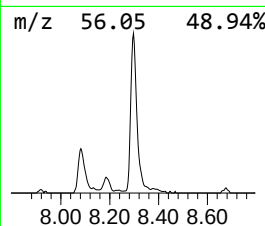
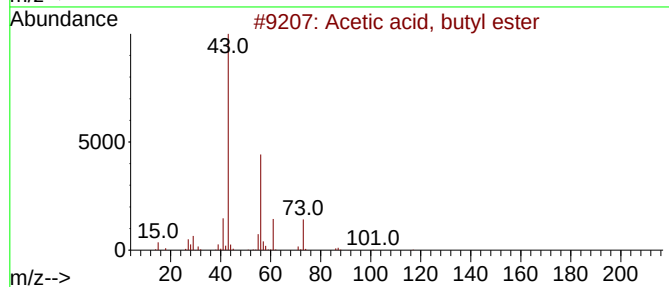
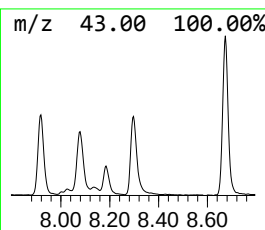
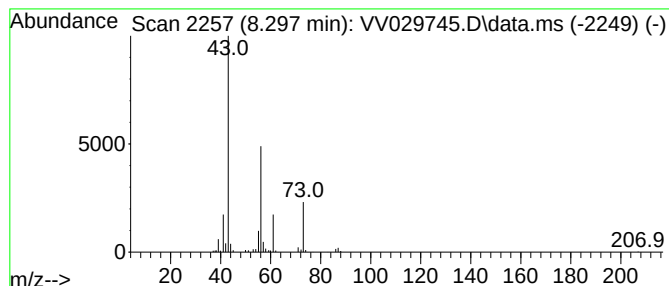
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.297	4.09 ug/L	96135	Chlorobenzene-d5	8.841

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	78
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
5			Isobutyl acetate	116	C6H12O2	000110-19-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122022\
Data File : VV029745.D
Acq On : 20 Dec 2022 12:49
Operator : SY/MD
Sample : PB149759TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB759

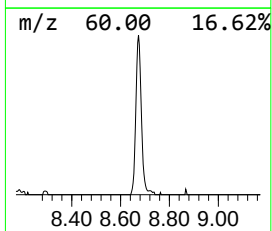
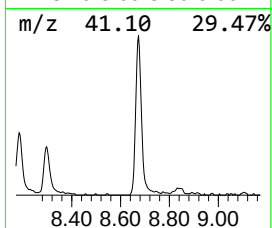
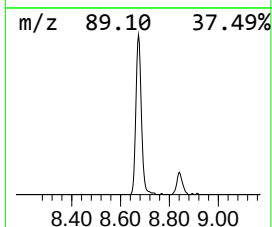
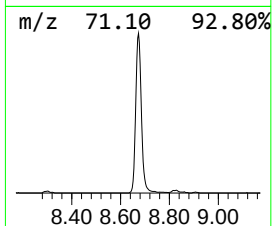
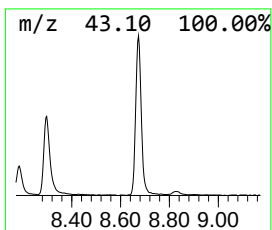
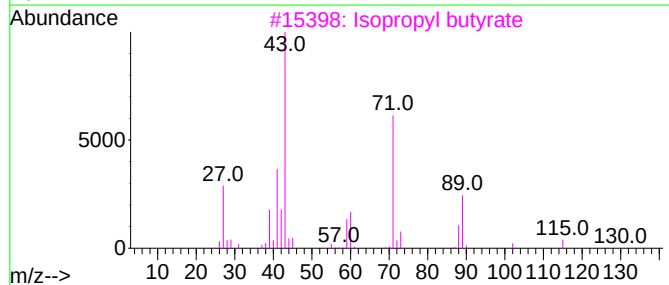
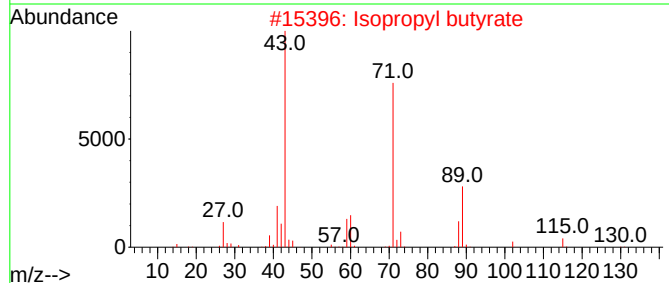
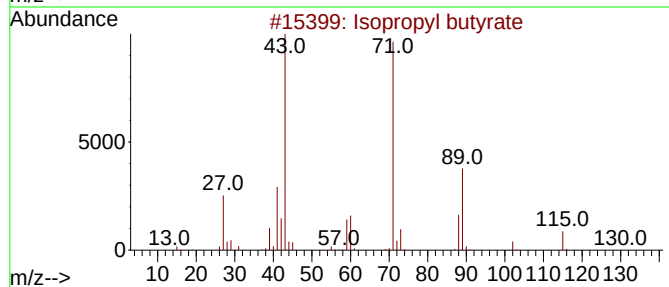
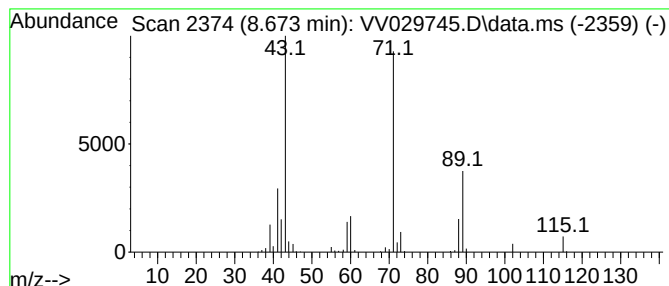
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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.
8.673	11.56 ug/L	271697	Chlorobenzene-d5	8.841

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	83
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW122022\
Data File : VW029745.D
Acq On : 20 Dec 2022 12:49
Operator : SY/MD
Sample : PB149759TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB759

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.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	6.458	17.6	ug/L	338593	1	5.606	964556	50.0
Propanoic acid,...	7.178	3.7	ug/L	72242	1	5.606	964556	50.0
Propanoic acid,...	7.918	4.0	ug/L	93746	2	8.841	1175160	50.0
Propanoic acid,...	8.185	6.8	ug/L	160940	2	8.841	1175160	50.0
Acetic acid, bu...	8.297	4.1	ug/L	96135	2	8.841	1175160	50.0
Isopropyl butyrate	8.673	11.6	ug/L	271697	2	8.841	1175160	50.0