

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW121922\
 Data File : VW029710.D
 Acq On : 19 Dec 2022 10:45
 Operator : SY/MD
 Sample : PB149722TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB722

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: VW029710.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	76	83	98	rVB	231294	234131	14.91%	1.705%
2	1.564	155	163	180	rVB	188034	213629	13.61%	1.555%
3	2.005	297	300	301	rBV2	571	310	0.02%	0.002%
4	2.105	319	331	344	rBV	378955	546767	34.82%	3.981%
5	2.294	384	390	399	rVB4	1374	2114	0.13%	0.015%
6	2.368	409	413	417	rVB2	327	294	0.02%	0.002%
7	2.420	425	429	430	rBV3	324	224	0.01%	0.002%
8	2.503	445	455	467	rVB2	7955	12960	0.83%	0.094%
9	2.744	526	530	532	rBV2	326	253	0.02%	0.002%
10	2.793	541	545	548	rBV	256	223	0.01%	0.002%
11	3.159	655	659	663	rBV2	242	253	0.02%	0.002%
12	3.175	663	664	670	rVB2	382	297	0.02%	0.002%
13	3.211	670	675	678	rBV2	308	284	0.02%	0.002%
14	3.773	844	850	855	rBV2	143	190	0.01%	0.001%
15	3.870	869	880	917	rBV	94874	287467	18.31%	2.093%
16	4.230	989	992	996	rVB2	297	227	0.01%	0.002%
17	4.256	999	1000	1004	rVB3	639	308	0.02%	0.002%
18	4.336	1004	1025	1057	rBV	240167	604566	38.51%	4.402%
19	4.571	1095	1098	1103	rVB4	380	333	0.02%	0.002%
20	4.609	1107	1110	1113	rVB2	402	257	0.02%	0.002%
21	4.658	1124	1125	1128	rVB2	470	187	0.01%	0.001%
22	4.950	1213	1216	1220	rVB	320	189	0.01%	0.001%
23	5.037	1223	1243	1295	rBV2	594385	1570071	100.00%	11.431%
24	5.278	1308	1318	1339	rVB	12991	30192	1.92%	0.220%
25	5.449	1366	1371	1373	rBV3	302	279	0.02%	0.002%
26	5.487	1381	1383	1386	rVB	438	261	0.02%	0.002%
27	5.606	1406	1420	1462	rBV	566972	1161743	73.99%	8.458%
28	5.828	1487	1489	1493	rVB2	501	239	0.02%	0.002%
29	5.899	1500	1511	1524	rVV3	5546	12225	0.78%	0.089%
30	6.059	1546	1561	1598	rBV	335327	696652	44.37%	5.072%
31	6.342	1641	1649	1654	rBV2	5081	8498	0.54%	0.062%
32	6.455	1674	1684	1725	rBV	156268	310048	19.75%	2.257%
33	6.690	1755	1757	1762	rVB2	246	210	0.01%	0.002%
34	6.844	1802	1805	1808	rBV2	312	236	0.02%	0.002%
35	6.911	1822	1826	1830	rVB2	414	381	0.02%	0.003%
36	6.976	1834	1846	1875	rBV	169622	317551	20.23%	2.312%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
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37	7.104	1884	1886	1889	rVB	402	187	0.01%	0.001%
38	7.178	1897	1909	1920	rBV2	38506	67414	4.29%	0.491%
39	7.307	1936	1949	1988	rBV	728199	1314811	83.74%	9.572%
40	7.609	2032	2043	2072	rBV2	164424	296107	18.86%	2.156%
41	7.786	2096	2098	2103	rVB4	322	223	0.01%	0.002%
42	7.828	2109	2111	2114	rVB2	434	237	0.02%	0.002%
43	7.918	2127	2139	2153	rBV	54773	93062	5.93%	0.678%
44	8.030	2160	2174	2179	rBV5	8537	15987	1.02%	0.116%
45	8.082	2179	2190	2213	rVV2	346617	643256	40.97%	4.683%
46	8.185	2214	2222	2242	rVB	87460	148749	9.47%	1.083%
47	8.297	2248	2257	2281	rVB	50056	87382	5.57%	0.636%
48	8.484	2311	2315	2317	rBV2	614	415	0.03%	0.003%
49	8.503	2318	2321	2323	rVV2	307	210	0.01%	0.002%
50	8.545	2331	2334	2338	rBV2	557	494	0.03%	0.004%
51	8.564	2338	2340	2344	rVB3	602	460	0.03%	0.003%
52	8.593	2347	2349	2354	rBV3	323	244	0.02%	0.002%
53	8.673	2362	2374	2392	rBV	166242	264785	16.86%	1.928%
54	8.841	2413	2426	2456	rVV	847225	1409249	89.76%	10.260%
55	9.104	2502	2508	2511	rBV2	1889	2220	0.14%	0.016%
56	9.381	2588	2594	2608	rVV5	1447	2942	0.19%	0.021%
57	9.435	2608	2611	2613	rVV	369	198	0.01%	0.001%
58	9.542	2635	2644	2658	rVV2	13530	22163	1.41%	0.161%
59	9.593	2658	2660	2662	rVV3	825	400	0.03%	0.003%
60	9.606	2662	2664	2668	rVV2	376	281	0.02%	0.002%
61	9.670	2680	2684	2688	rVB2	356	239	0.02%	0.002%
62	9.702	2688	2694	2696	rBV	285	220	0.01%	0.002%
63	9.712	2696	2697	2703	rVV2	321	243	0.02%	0.002%
64	9.751	2704	2709	2711	rVV	719	600	0.04%	0.004%
65	9.921	2756	2762	2769	rBV2	443	756	0.05%	0.006%
66	10.162	2825	2837	2840	rVV2	19405	27179	1.73%	0.198%
67	10.204	2841	2850	2875	rVB	445931	698696	44.50%	5.087%
68	10.371	2897	2902	2913	rVB3	1345	2003	0.13%	0.015%
69	10.532	2944	2952	2953	rBV3	699	684	0.04%	0.005%
70	10.564	2954	2962	2977	rVV	9598	15845	1.01%	0.115%
71	10.905	3061	3068	3075	rBV4	664	1219	0.08%	0.009%
72	11.169	3145	3150	3153	rBV4	1044	1170	0.07%	0.009%
73	11.236	3159	3171	3191	rBV	916467	1399429	89.13%	10.188%
74	11.455	3236	3239	3243	rBV3	390	224	0.01%	0.002%
75	11.612	3274	3288	3311	rBV	749601	1160283	73.90%	8.447%
76	11.886	3370	3373	3378	rBV2	383	435	0.03%	0.003%

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 Title : VOC Analysis

77	12.082	3431	3434	3436	rVB2	290	196	0.01%	0.001%
78	12.172	3456	3462	3464	rBV2	205	229	0.01%	0.002%
79	12.239	3477	3483	3490	rVV2	1525	1895	0.12%	0.014%
80	12.332	3509	3512	3515	rVV3	478	402	0.03%	0.003%
81	12.361	3519	3521	3527	rVV3	260	191	0.01%	0.001%
82	12.387	3527	3529	3532	rVV2	299	221	0.01%	0.002%
83	12.419	3536	3539	3542	rVB3	719	550	0.04%	0.004%
84	12.448	3542	3548	3551	rBV2	381	507	0.03%	0.004%
85	12.468	3551	3554	3559	rVB3	417	331	0.02%	0.002%
86	12.493	3559	3562	3566	rBV	316	246	0.02%	0.002%
87	12.593	3591	3593	3596	rBV2	438	323	0.02%	0.002%
88	12.635	3600	3606	3614	rVV5	1428	2165	0.14%	0.016%
89	12.705	3625	3628	3631	rVB2	409	278	0.02%	0.002%
90	12.722	3631	3633	3636	rBV2	367	194	0.01%	0.001%
91	12.776	3647	3650	3654	rVV3	399	372	0.02%	0.003%
92	12.824	3663	3665	3670	rVV2	302	206	0.01%	0.001%
93	12.950	3701	3704	3708	rBV2	238	197	0.01%	0.001%
94	13.008	3719	3722	3725	rBV2	632	536	0.03%	0.004%
95	13.101	3750	3751	3755	rBV2	250	189	0.01%	0.001%
96	13.246	3791	3796	3806	rVB7	2848	4550	0.29%	0.033%
97	13.291	3806	3810	3812	rBV3	585	355	0.02%	0.003%
98	13.493	3864	3873	3883	rBV2	12843	20637	1.31%	0.150%
99	13.731	3940	3947	3958	rVV5	3205	5588	0.36%	0.041%
100	13.934	4007	4010	4012	rBV3	424	319	0.02%	0.002%

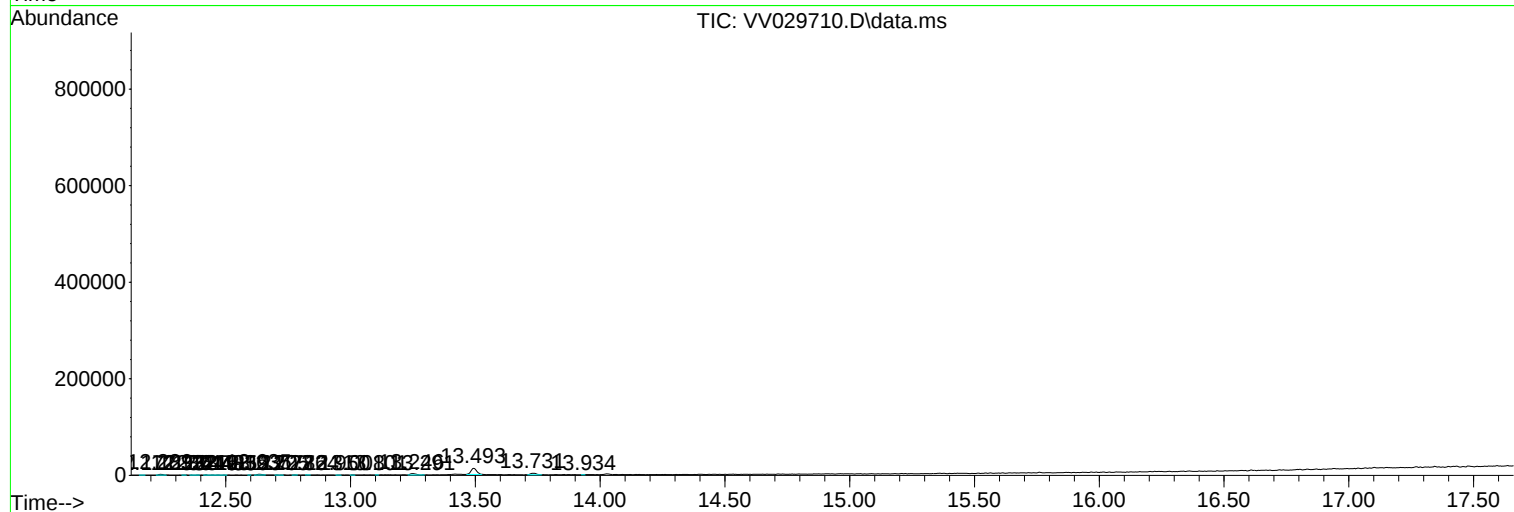
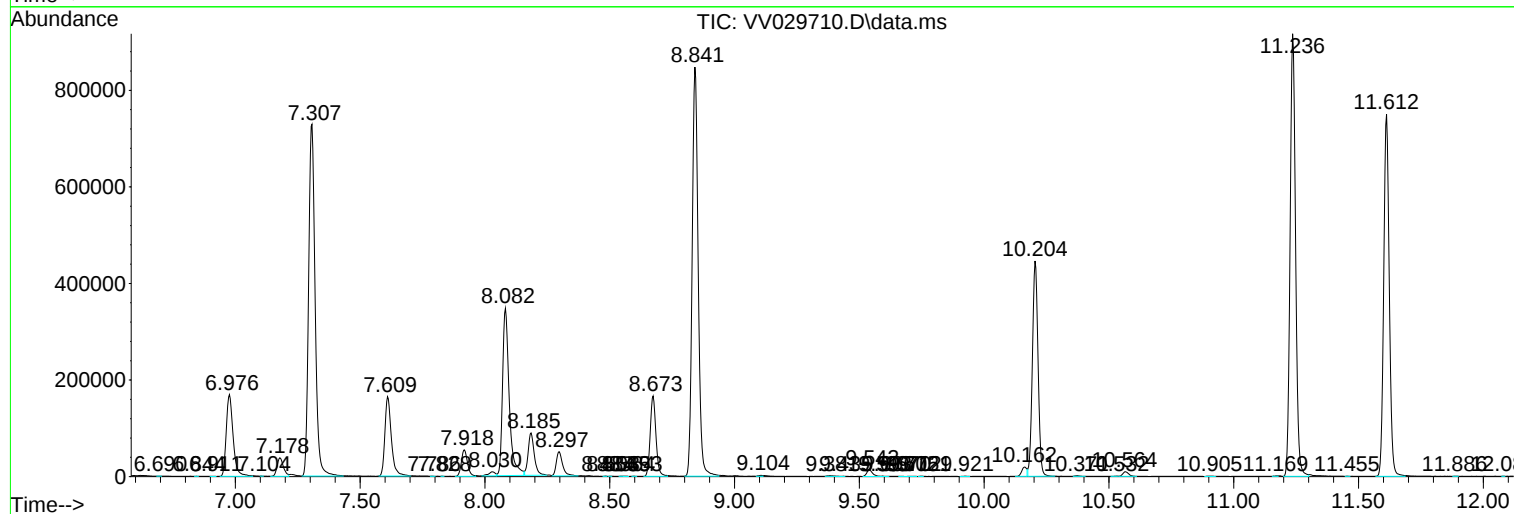
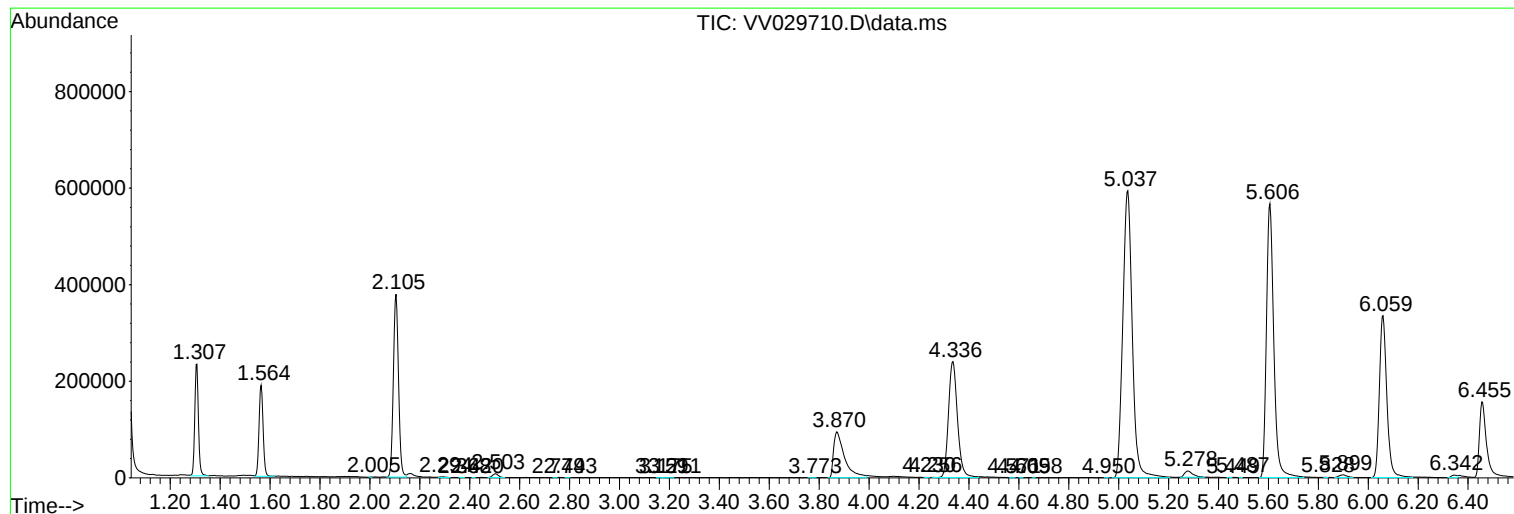
Sum of corrected areas: 13735427

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Instrument :
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VLEB722

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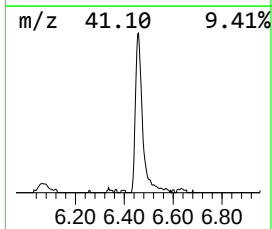
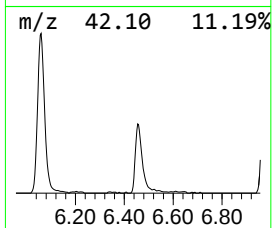
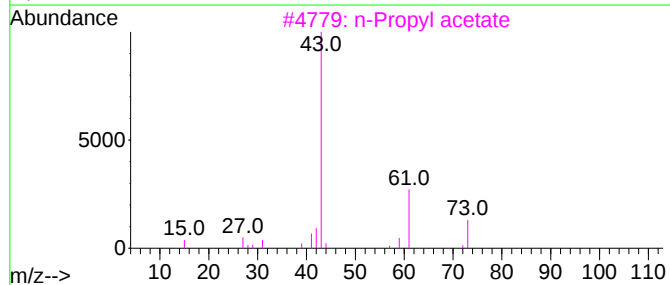
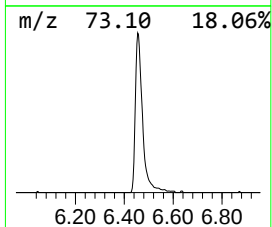
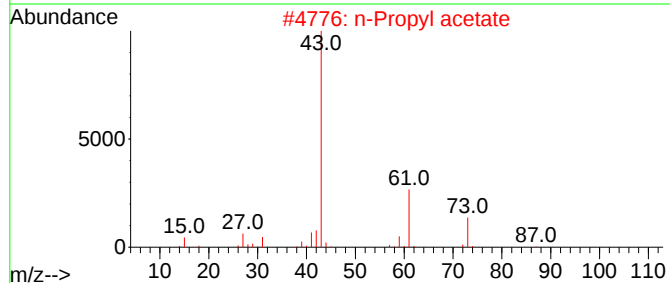
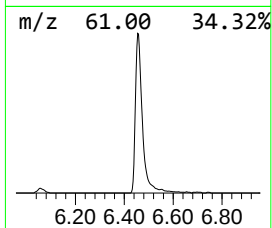
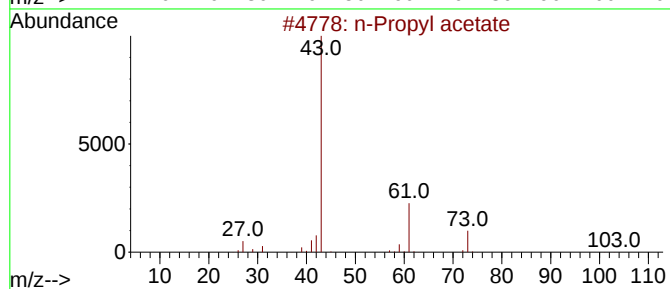
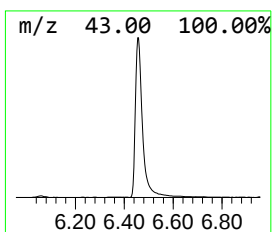
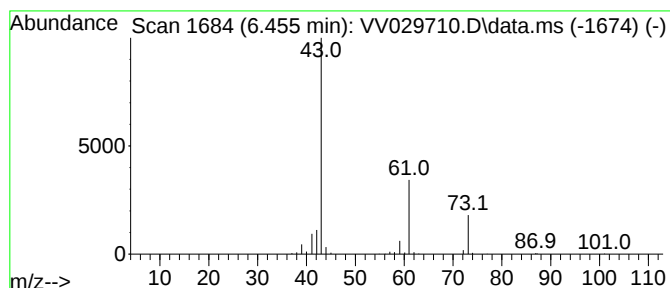
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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.
6.455	13.34 ug/L	310048	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	78
4	n-Propyl acetate		102	C5H10O2	000109-60-4	64
5	Propanal, 2,3-dihydroxy-, (S)-		90	C3H6O3	000497-09-6	36



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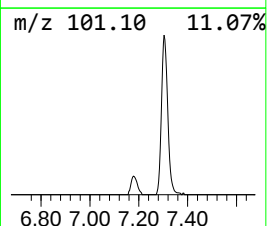
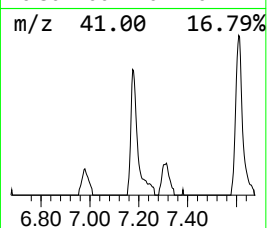
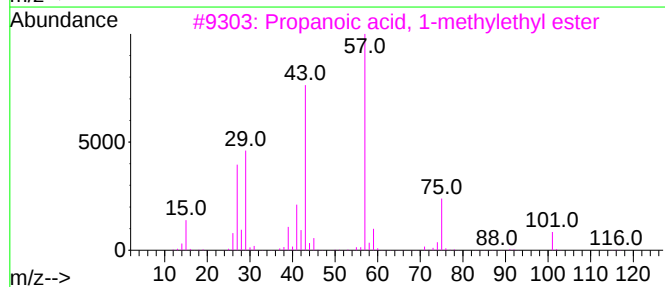
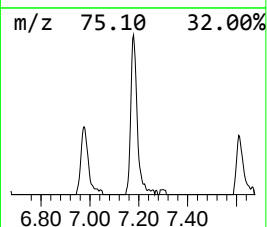
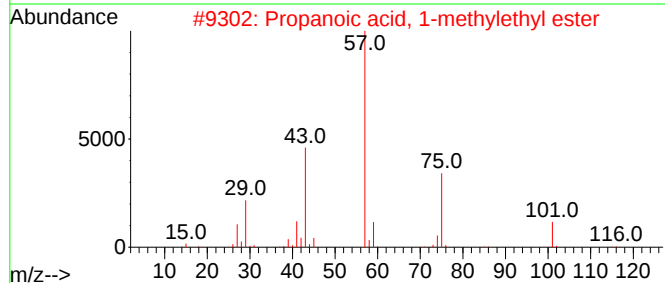
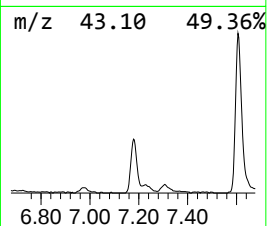
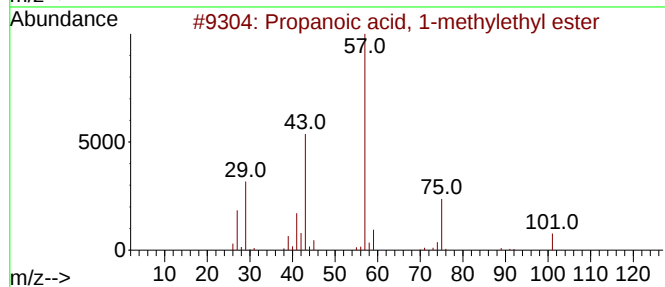
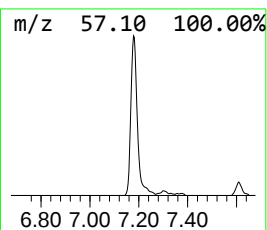
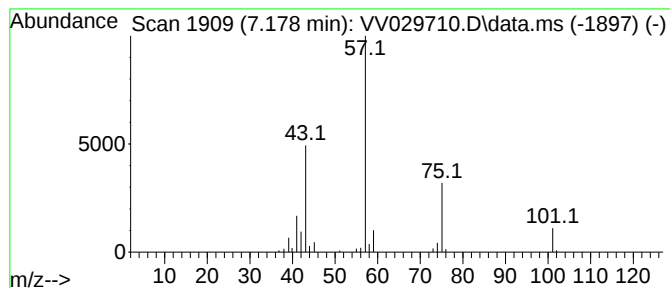
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.178	2.90 ug/L	67414	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	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59



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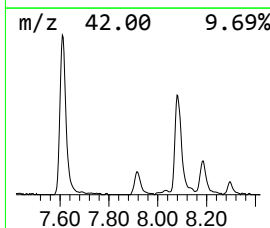
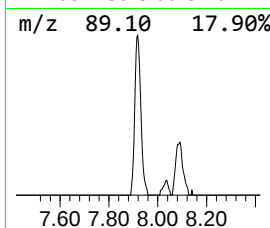
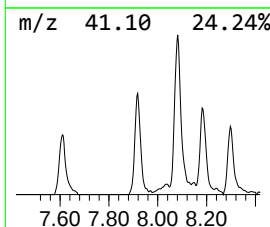
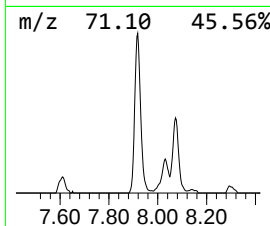
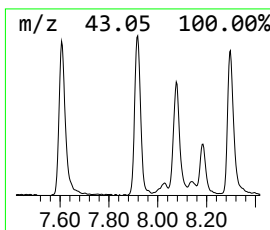
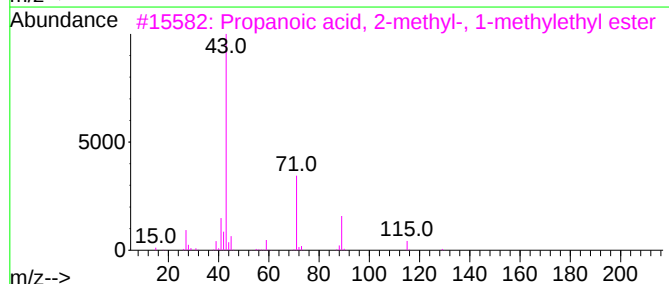
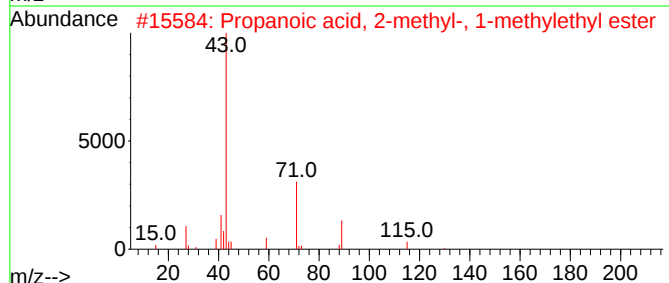
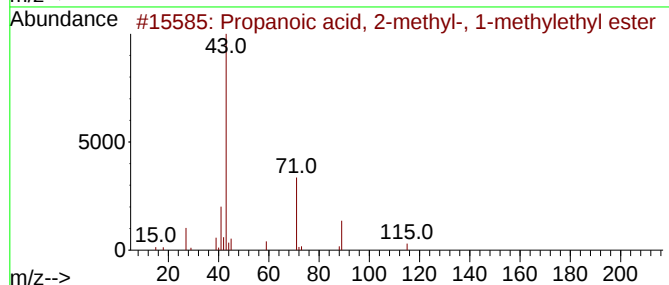
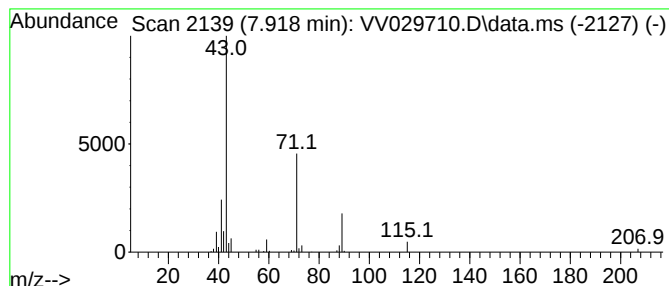
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.918	3.30 ug/L	93062	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-, propy...	130	C7H14O2	000644-49-5	78
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029710.D
Acq On : 19 Dec 2022 10:45
Operator : SY/MD
Sample : PB149722TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB722

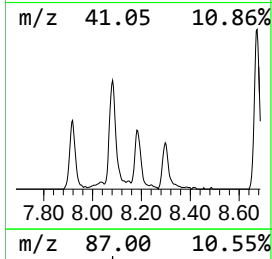
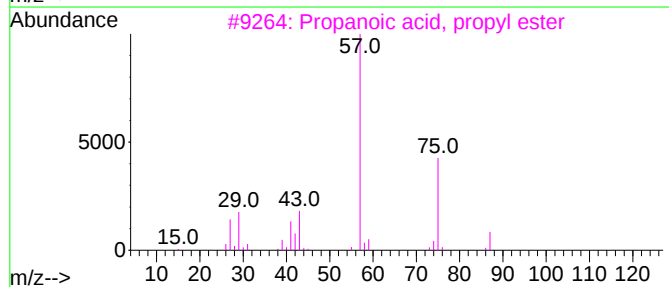
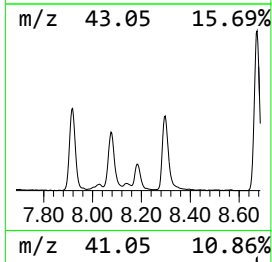
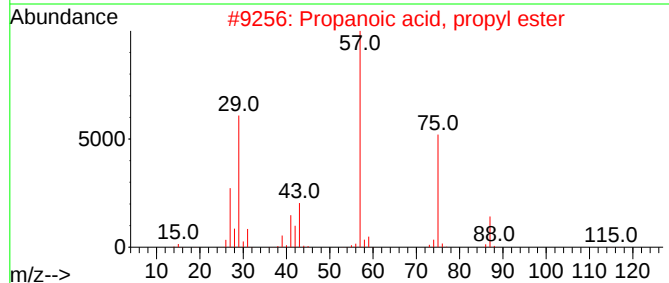
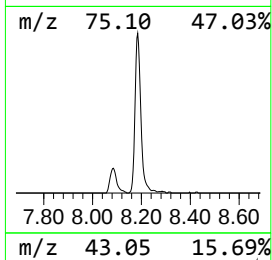
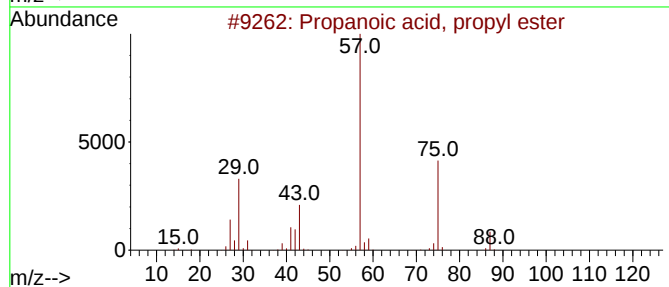
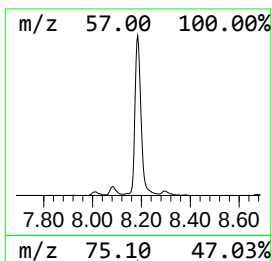
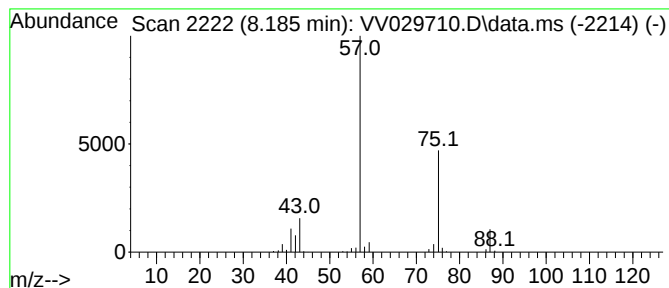
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Quant Title : VOC Analysis

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	5.28 ug/L	148749	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	83
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
5			1-Penten-3-ol	86	C5H10O	000616-25-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029710.D
Acq On : 19 Dec 2022 10:45
Operator : SY/MD
Sample : PB149722TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB722

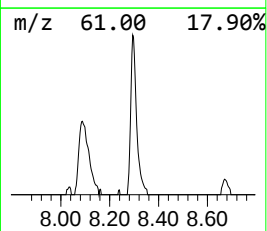
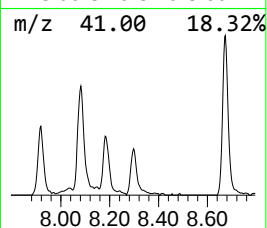
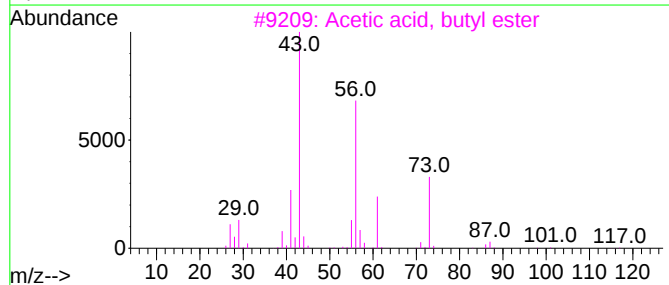
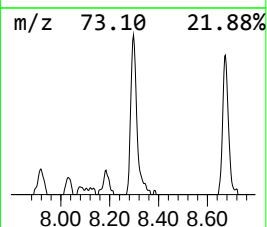
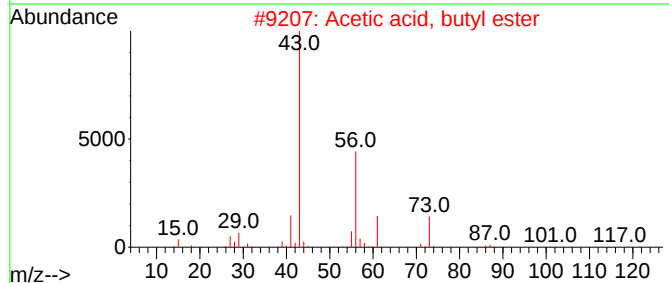
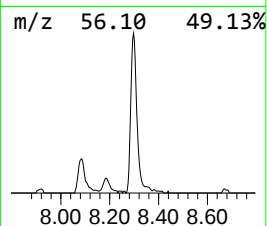
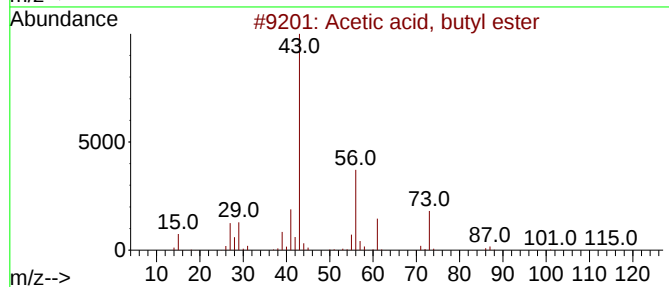
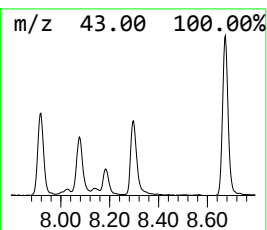
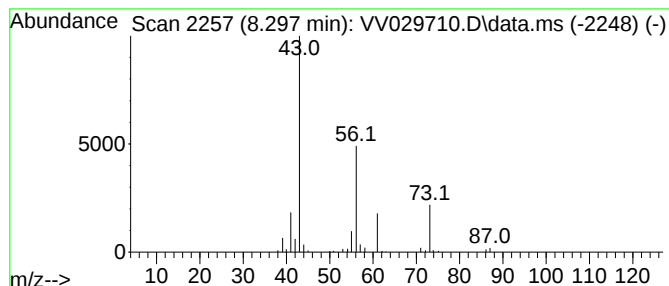
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.297	3.10 ug/L	87382	Chlorobenzene-d5	8.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	42
5			Isobutyl acetate	116	C6H12O2	000110-19-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029710.D
Acq On : 19 Dec 2022 10:45
Operator : SY/MD
Sample : PB149722TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB722

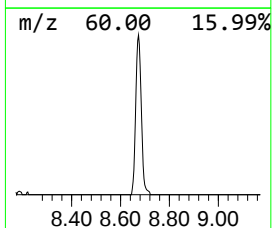
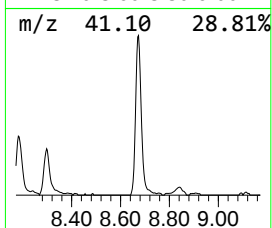
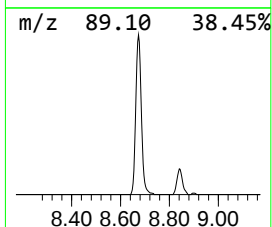
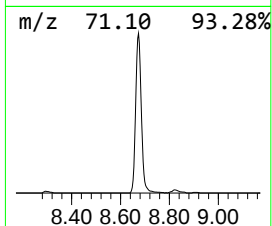
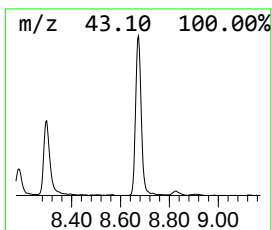
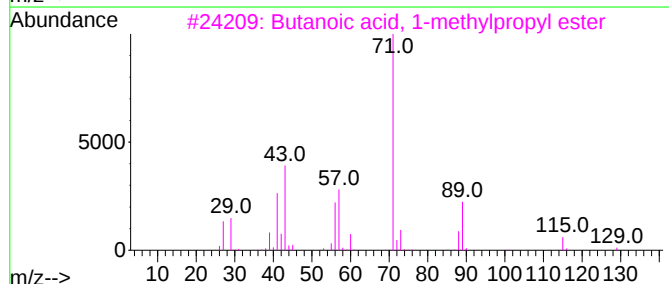
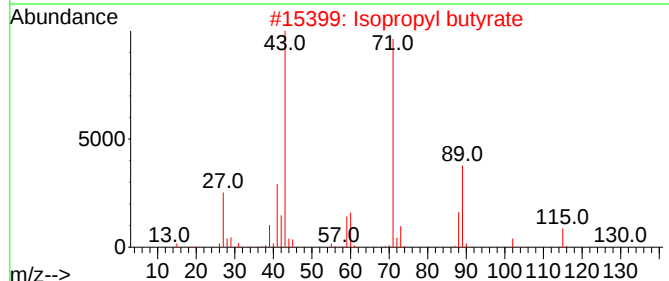
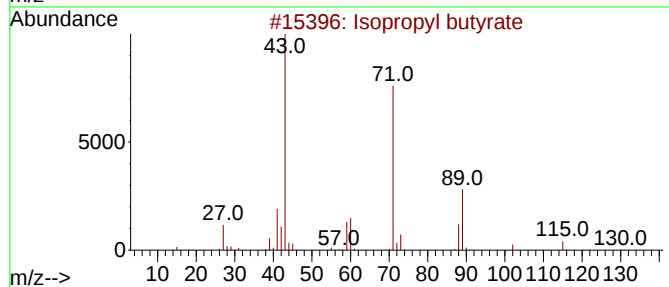
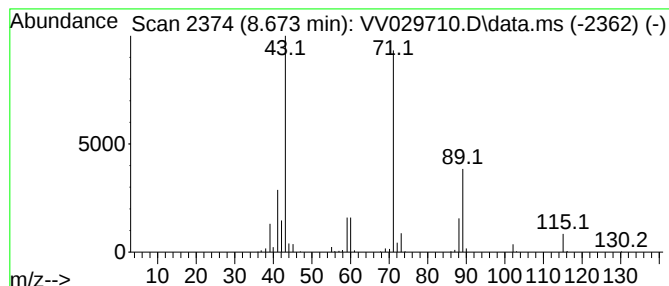
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Quant Title : VOC Analysis

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	9.39 ug/L	264785	Chlorobenzene-d5	8.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	97
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
3			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029710.D
Acq On : 19 Dec 2022 10:45
Operator : SY/MD
Sample : PB149722TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB722

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
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Propanoic acid,...	7.178	2.9	ug/L	67414	1	5.606	1161740	50.0
Propanoic acid,...	7.918	3.3	ug/L	93062	2	8.841	1409250	50.0
Propanoic acid,...	8.185	5.3	ug/L	148749	2	8.841	1409250	50.0
Acetic acid, bu...	8.297	3.1	ug/L	87382	2	8.841	1409250	50.0
Isopropyl butyrate	8.673	9.4	ug/L	264785	2	8.841	1409250	50.0