

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083021\
 Data File : VV021993.D
 Acq On : 30 Aug 2021 10:37
 Operator : SY/MD
 Sample : M3552-04 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AH3

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\SFAMVLM082721WMA.M

Title : VOC Analysis

Signal : TIC: VV021993.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	94	rBV	166751	167370	13.78%	1.673%
2	1.565	156	163	180	rVB	139429	161159	13.27%	1.611%
3	2.105	321	331	343	rBV	262993	388578	32.00%	3.884%
4	2.507	446	456	469	rVB2	21216	34324	2.83%	0.343%
5	2.745	523	530	532	rBV3	496	514	0.04%	0.005%
6	2.761	532	535	542	rBV4	796	847	0.07%	0.008%
7	2.825	552	555	560	rVB2	421	318	0.03%	0.003%
8	2.864	560	567	568	rBV2	464	376	0.03%	0.004%
9	2.966	597	599	607	rVB2	468	407	0.03%	0.004%
10	3.005	607	611	613	rBV	220	177	0.01%	0.002%
11	3.047	620	624	626	rBV2	333	279	0.02%	0.003%
12	3.134	648	651	655	rVB	614	344	0.03%	0.003%
13	3.249	685	687	690	rBV	354	175	0.01%	0.002%
14	3.298	697	702	704	rBV2	281	204	0.02%	0.002%
15	3.372	722	725	728	rBV	261	168	0.01%	0.002%
16	3.407	733	736	740	rVV2	269	219	0.02%	0.002%
17	3.445	744	748	751	rBV2	586	455	0.04%	0.005%
18	3.481	755	759	761	rBV2	356	240	0.02%	0.002%
19	3.654	811	813	816	rBV2	244	148	0.01%	0.001%
20	3.799	855	858	860	rBV2	271	162	0.01%	0.002%
21	3.876	872	882	924	rBV	105682	297453	24.49%	2.973%
22	4.262	1000	1002	1005	rBV	542	304	0.03%	0.003%
23	4.349	1013	1029	1063	rBV	185596	485480	39.97%	4.853%
24	4.635	1114	1118	1120	rBV2	576	346	0.03%	0.003%
25	4.667	1126	1128	1132	rVB3	418	237	0.02%	0.002%
26	4.693	1132	1136	1138	rBV	257	194	0.02%	0.002%
27	4.764	1157	1158	1163	rVB2	538	432	0.04%	0.004%
28	4.802	1163	1170	1173	rBV2	416	427	0.04%	0.004%
29	4.896	1192	1199	1204	rBV2	323	421	0.03%	0.004%
30	4.957	1215	1218	1220	rBV2	333	192	0.02%	0.002%
31	5.047	1229	1246	1275	rBV2	470366	1214474	100.00%	12.140%
32	5.423	1359	1363	1367	rVV4	420	397	0.03%	0.004%
33	5.442	1368	1369	1372	rVB2	395	147	0.01%	0.001%
34	5.490	1378	1384	1388	rBV5	713	772	0.06%	0.008%
35	5.548	1399	1402	1406	rBV3	713	397	0.03%	0.004%
36	5.571	1406	1409	1411	rBV3	363	229	0.02%	0.002%

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 Title : VOC Analysis

37	5.619	1411	1424	1452	rBV	359119	731908	60.27%	7.316%
38	5.908	1503	1514	1530	rBV3	22728	48603	4.00%	0.486%
39	6.008	1543	1545	1547	rVB	572	227	0.02%	0.002%
40	6.069	1550	1564	1592	rVV	266016	549475	45.24%	5.493%
41	6.465	1678	1687	1715	rBV	84673	163661	13.48%	1.636%
42	6.725	1766	1768	1771	rVB2	704	386	0.03%	0.004%
43	6.757	1776	1778	1784	rVB3	706	562	0.05%	0.006%
44	6.908	1820	1825	1827	rBV2	424	377	0.03%	0.004%
45	6.989	1837	1850	1871	rBV	151492	276405	22.76%	2.763%
46	7.191	1903	1913	1926	rBV2	16970	30172	2.48%	0.302%
47	7.317	1940	1952	1971	rBV	541984	950536	78.27%	9.502%
48	7.622	2037	2047	2074	rBV	103324	185758	15.30%	1.857%
49	7.867	2120	2123	2125	rVV3	365	239	0.02%	0.002%
50	7.931	2132	2143	2152	rBV3	4852	8135	0.67%	0.081%
51	8.040	2169	2177	2183	rBV3	12487	17425	1.43%	0.174%
52	8.088	2183	2192	2216	rVV	309370	573763	47.24%	5.735%
53	8.191	2217	2224	2245	rVB	163827	265411	21.85%	2.653%
54	8.468	2308	2310	2313	rBV	369	170	0.01%	0.002%
55	8.683	2364	2377	2397	rBV2	102578	164399	13.54%	1.643%
56	8.854	2418	2430	2459	rBV	532285	875350	72.08%	8.750%
57	9.204	2535	2539	2541	rVB2	225	159	0.01%	0.002%
58	9.227	2542	2546	2552	rVB2	373	346	0.03%	0.003%
59	9.272	2557	2560	2561	rBV2	255	161	0.01%	0.002%
60	9.323	2573	2576	2579	rBV2	329	235	0.02%	0.002%
61	9.481	2622	2625	2626	rBV2	312	157	0.01%	0.002%
62	9.558	2641	2649	2655	rBV7	3199	4630	0.38%	0.046%
63	9.796	2720	2723	2728	rVB	273	197	0.02%	0.002%
64	9.828	2728	2733	2735	rBV2	210	180	0.01%	0.002%
65	9.886	2744	2751	2752	rBV2	386	300	0.02%	0.003%
66	9.895	2752	2754	2758	rVB2	435	251	0.02%	0.003%
67	9.966	2773	2776	2781	rVB	635	406	0.03%	0.004%
68	10.075	2808	2810	2815	rVB2	227	172	0.01%	0.002%
69	10.130	2820	2827	2836	rVB6	2303	3752	0.31%	0.038%
70	10.165	2836	2838	2842	rVB	407	184	0.02%	0.002%
71	10.217	2842	2854	2876	rBV	364791	581853	47.91%	5.816%
72	10.526	2945	2950	2952	rBV	351	298	0.02%	0.003%
73	10.545	2952	2956	2957	rBV2	548	357	0.03%	0.004%
74	10.587	2965	2969	2973	rBV4	910	900	0.07%	0.009%
75	10.625	2979	2981	2983	rBV	386	169	0.01%	0.002%
76	10.641	2983	2986	2989	rBV2	267	175	0.01%	0.002%

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 Title : VOC Analysis

77	10.747	3015	3019	3021	rBV	306	249	0.02%	0.002%
78	10.764	3021	3024	3027	rVV2	395	314	0.03%	0.003%
79	10.780	3027	3029	3035	rVB2	371	416	0.03%	0.004%
80	10.873	3056	3058	3062	rVB	409	261	0.02%	0.003%
81	10.924	3062	3074	3085	rBV6	2930	4729	0.39%	0.047%
82	11.024	3101	3105	3106	rBV	319	227	0.02%	0.002%
83	11.146	3138	3143	3144	rBV2	692	580	0.05%	0.006%
84	11.252	3164	3176	3198	rBV	564816	888958	73.20%	8.886%
85	11.426	3227	3230	3238	rVB5	1903	2459	0.20%	0.025%
86	11.625	3280	3292	3314	rBV	560031	903349	74.38%	9.030%
87	11.786	3340	3342	3351	rVB5	1016	1131	0.09%	0.011%
88	11.834	3355	3357	3359	rBV	341	190	0.02%	0.002%
89	12.098	3433	3439	3443	rBV4	832	921	0.08%	0.009%
90	12.207	3470	3473	3474	rBV3	668	323	0.03%	0.003%
91	12.461	3549	3552	3554	rVB2	400	211	0.02%	0.002%
92	12.474	3554	3556	3559	rBV	368	249	0.02%	0.002%
93	12.487	3559	3560	3565	rVB	434	180	0.01%	0.002%
94	12.648	3608	3610	3612	rBV2	546	229	0.02%	0.002%
95	12.796	3654	3656	3658	rBV2	308	148	0.01%	0.001%
96	12.886	3682	3684	3689	rVB3	447	302	0.02%	0.003%
97	12.905	3689	3690	3692	rBV	345	152	0.01%	0.002%
98	13.271	3799	3804	3809	rBV3	1106	1343	0.11%	0.013%
99	13.471	3862	3866	3868	rBV2	678	480	0.04%	0.005%
100	14.143	4071	4075	4076	rBV2	537	422	0.03%	0.004%

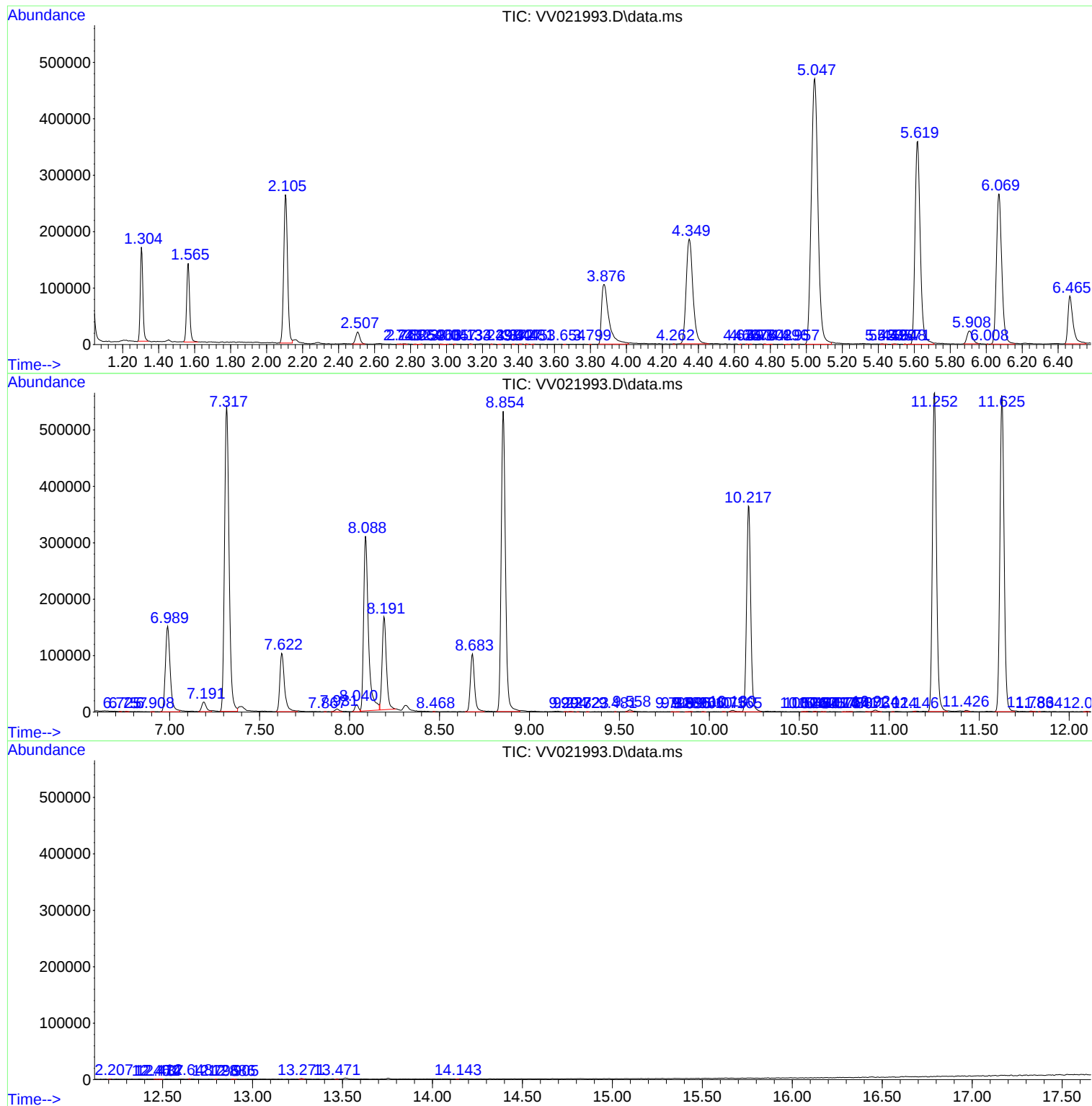
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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



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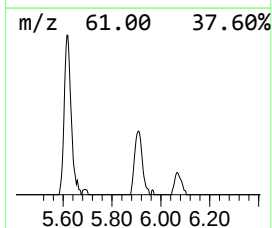
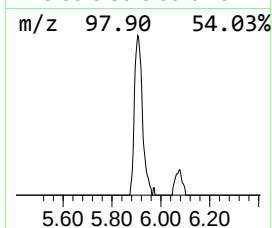
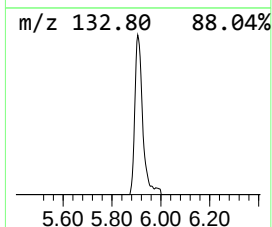
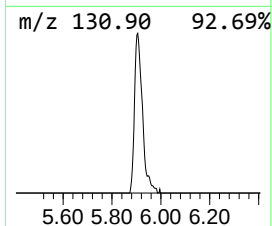
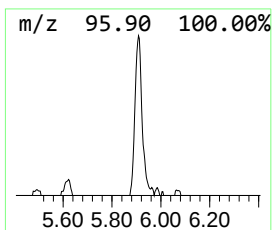
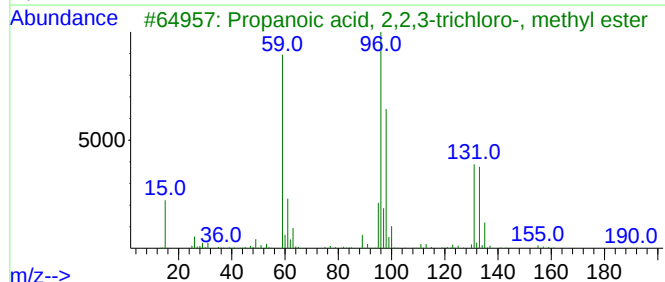
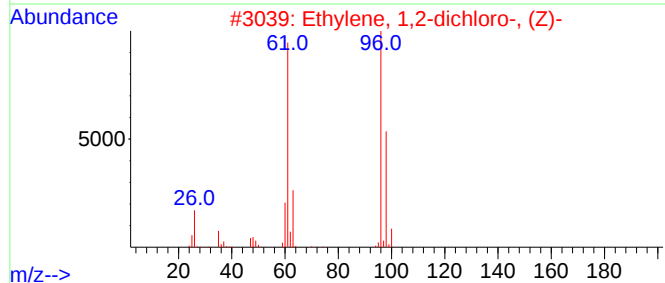
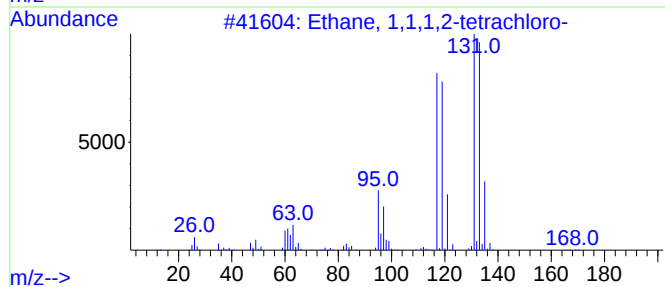
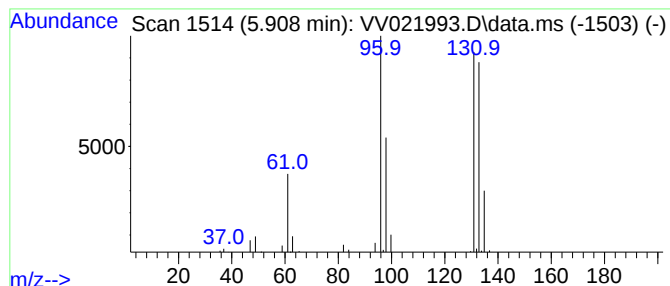
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	3.32 ug/L	48603	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	37
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	30
3			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	25
4			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	23
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	22



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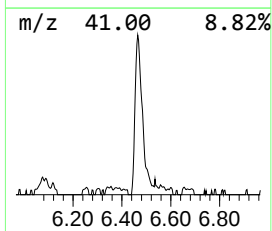
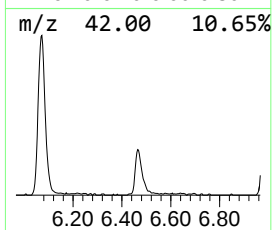
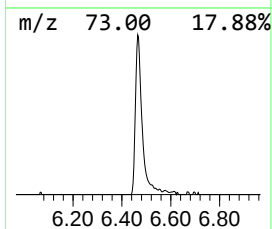
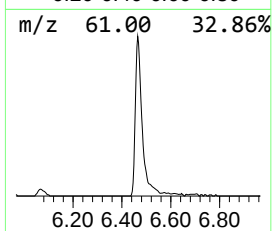
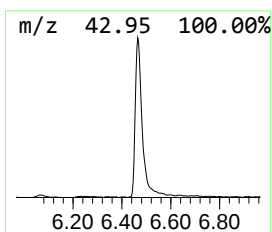
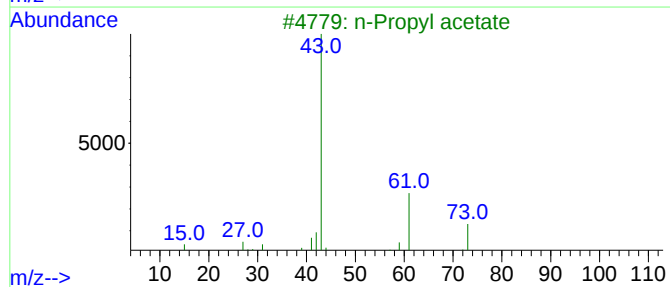
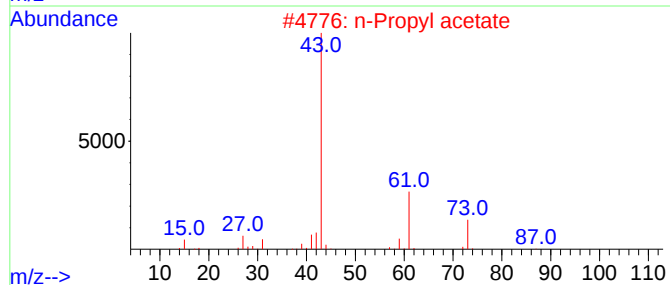
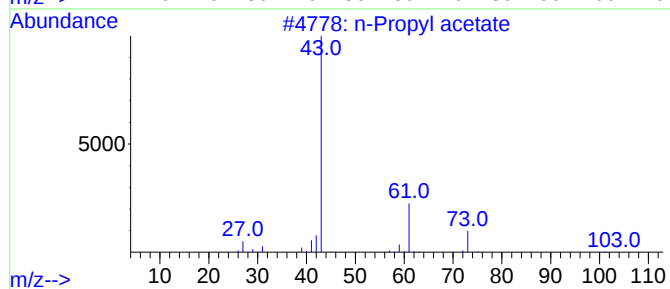
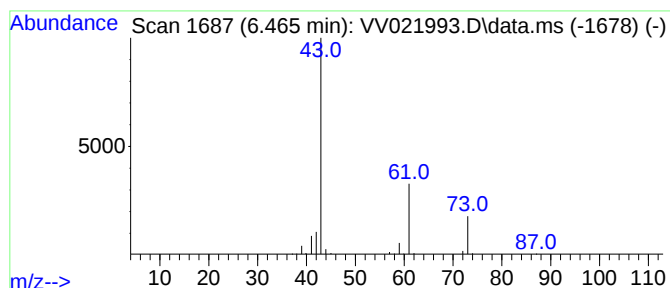
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.465	11.18 ug/L	163661	1,4-Difluorobenzene	5.619

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	83
3		n-Propyl acetate	102	C5H10O2	000109-60-4	78
4		n-Propyl acetate	102	C5H10O2	000109-60-4	78
5		n-Propyl acetate	102	C5H10O2	000109-60-4	64



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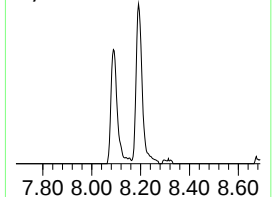
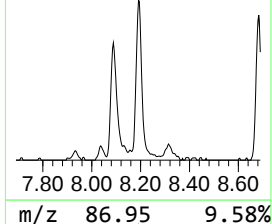
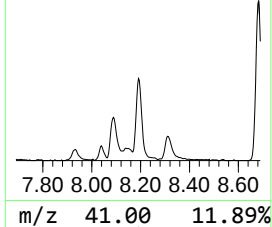
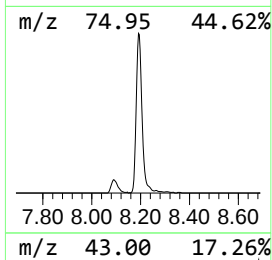
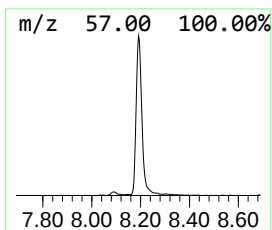
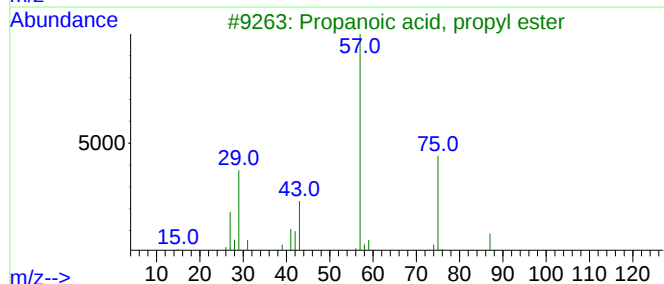
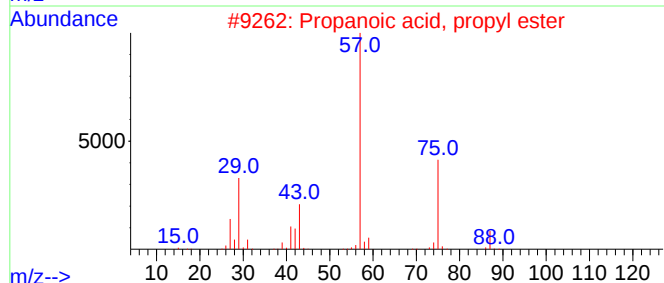
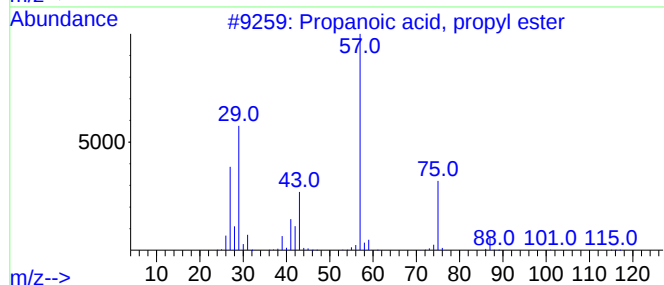
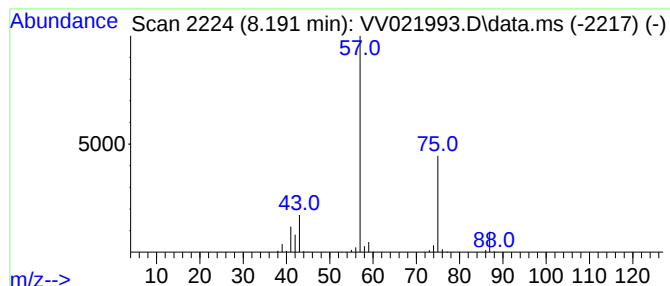
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.191	15.16 ug/L	265411	Chlorobenzene-d5	8.854

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	83
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083021\
Data File : VV021993.D
Acq On : 30 Aug 2021 10:37
Operator : SY/MD
Sample : M3552-04 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AH3

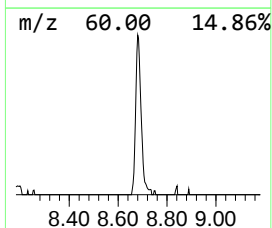
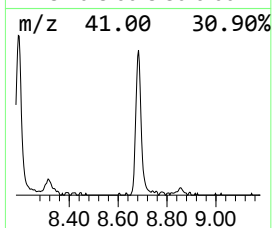
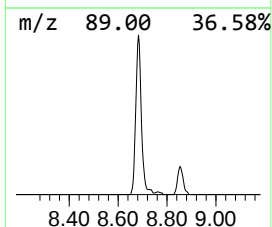
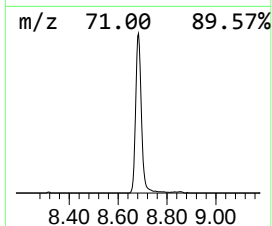
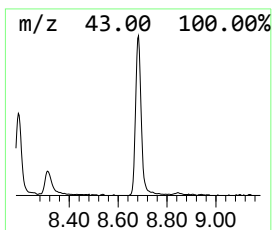
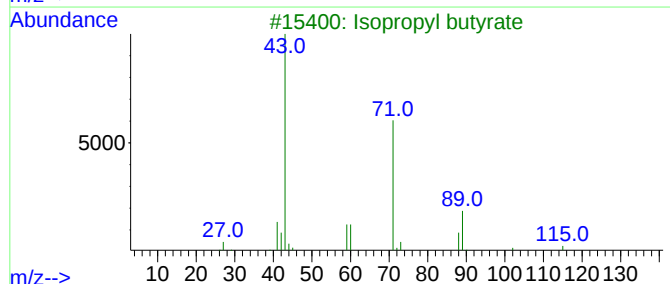
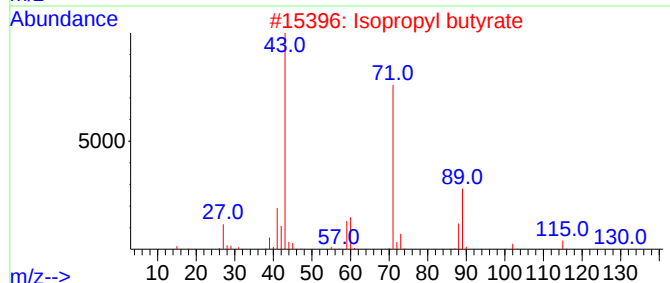
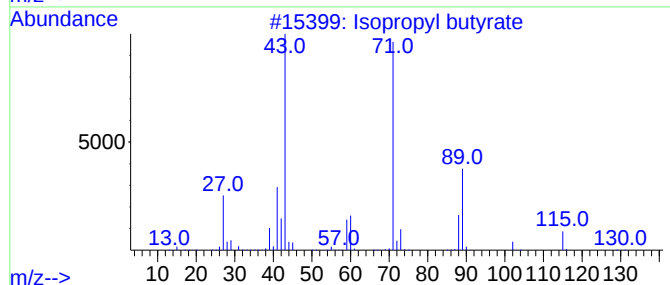
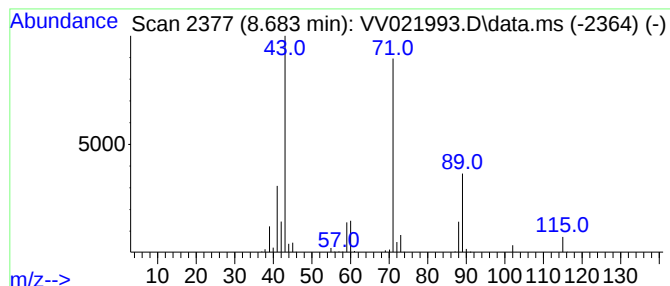
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Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.683	9.39 ug/L	164399	Chlorobenzene-d5	8.854

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			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083021\
Data File : VV021993.D
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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AH3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.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
unknown-01	5.908	3.3	ug/L	48603	1	5.619	731908	50.0
n-Propyl acetate	6.465	11.2	ug/L	163661	1	5.619	731908	50.0
Propanoic acid,...	8.191	15.2	ug/L	265411	2	8.854	875350	50.0
Isopropyl butyrate	8.683	9.4	ug/L	164399	2	8.854	875350	50.0