

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082721\
 Data File : VV021988.D
 Acq On : 27 Aug 2021 20:06
 Operator : SY/MD
 Sample : M3552-03 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AH2

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: VV021988.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	75	82	94	rBV	184759	181259	14.14%	1.692%
2	1.561	155	162	177	rVB	143956	167262	13.04%	1.562%
3	2.105	321	331	345	rBV	287514	422473	32.95%	3.945%
4	2.507	446	456	468	rVV	20576	34635	2.70%	0.323%
5	2.609	486	488	495	rBV2	472	436	0.03%	0.004%
6	2.761	533	535	536	rBV2	403	186	0.01%	0.002%
7	2.905	578	580	585	rBV2	310	225	0.02%	0.002%
8	3.089	634	637	642	rVB2	376	321	0.03%	0.003%
9	3.169	655	662	664	rBV	764	704	0.05%	0.007%
10	3.269	688	693	695	rBV3	300	272	0.02%	0.003%
11	3.310	701	706	708	rBV2	465	421	0.03%	0.004%
12	3.394	729	732	737	rBV2	443	376	0.03%	0.004%
13	3.423	739	741	744	rVB	411	182	0.01%	0.002%
14	3.442	744	747	749	rBV2	316	144	0.01%	0.001%
15	3.648	808	811	814	rBV2	246	167	0.01%	0.002%
16	3.696	824	826	830	rVB3	240	139	0.01%	0.001%
17	3.744	838	841	844	rVB2	296	182	0.01%	0.002%
18	3.761	844	846	849	rBV2	241	161	0.01%	0.002%
19	3.873	872	881	922	rBV	105763	290393	22.65%	2.711%
20	4.349	1012	1029	1061	rBV	196344	502168	39.16%	4.689%
21	4.584	1100	1102	1104	rBV	394	219	0.02%	0.002%
22	4.629	1113	1116	1118	rBV2	274	218	0.02%	0.002%
23	4.744	1149	1152	1156	rBV3	398	276	0.02%	0.003%
24	4.873	1188	1192	1195	rBV2	468	398	0.03%	0.004%
25	4.963	1216	1220	1227	rBV3	248	282	0.02%	0.003%
26	5.047	1229	1246	1272	rBV2	505073	1282227	100.00%	11.972%
27	5.413	1358	1360	1363	rBV3	279	158	0.01%	0.001%
28	5.490	1381	1384	1386	rBV3	490	340	0.03%	0.003%
29	5.619	1412	1424	1454	rBV	382415	781425	60.94%	7.296%
30	5.905	1504	1513	1529	rBV4	17944	37267	2.91%	0.348%
31	6.072	1551	1565	1589	rBV	275182	572015	44.61%	5.341%
32	6.465	1678	1687	1711	rBV	106627	199347	15.55%	1.861%
33	6.793	1787	1789	1792	rBV2	423	233	0.02%	0.002%
34	6.895	1817	1821	1825	rBV2	479	483	0.04%	0.005%
35	6.915	1825	1827	1829	rBV	294	185	0.01%	0.002%
36	6.989	1839	1850	1874	rBV	154472	284344	22.18%	2.655%

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Integrator: RTE

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

37	7.191	1904	1913	1924	rBV	17404	29361	2.29%	0.274%
38	7.317	1940	1952	1971	rBV	621267	1078253	84.09%	10.067%
39	7.625	2037	2048	2076	rBV	102999	186844	14.57%	1.745%
40	7.873	2122	2125	2130	rVB4	598	425	0.03%	0.004%
41	7.931	2133	2143	2154	rBV3	4630	8140	0.63%	0.076%
42	8.040	2169	2177	2183	rBV2	13003	18844	1.47%	0.176%
43	8.088	2183	2192	2215	rVV	321115	590923	46.09%	5.517%
44	8.191	2217	2224	2254	rVB	192153	310322	24.20%	2.897%
45	8.535	2329	2331	2336	rVB3	674	314	0.02%	0.003%
46	8.683	2366	2377	2405	rBV	102437	168688	13.16%	1.575%
47	8.854	2418	2430	2454	rBV	590155	962231	75.04%	8.984%
48	9.101	2505	2507	2509	rBV2	494	248	0.02%	0.002%
49	9.207	2537	2540	2543	rVB3	436	258	0.02%	0.002%
50	9.243	2549	2551	2555	rVB2	504	279	0.02%	0.003%
51	9.268	2555	2559	2560	rBV2	463	352	0.03%	0.003%
52	9.317	2572	2574	2577	rVB2	533	213	0.02%	0.002%
53	9.333	2577	2579	2582	rBV	337	159	0.01%	0.001%
54	9.358	2584	2587	2591	rBV3	341	202	0.02%	0.002%
55	9.384	2592	2595	2598	rBV	298	219	0.02%	0.002%
56	9.481	2622	2625	2628	rVB3	362	223	0.02%	0.002%
57	9.497	2628	2630	2633	rVB2	312	137	0.01%	0.001%
58	9.555	2641	2648	2655	rBV5	3156	4819	0.38%	0.045%
59	9.628	2668	2671	2678	rVB3	587	434	0.03%	0.004%
60	9.683	2686	2688	2693	rBV2	465	282	0.02%	0.003%
61	9.702	2693	2694	2699	rVB2	263	165	0.01%	0.002%
62	9.738	2702	2705	2711	rBV2	539	428	0.03%	0.004%
63	9.792	2719	2722	2732	rVB2	314	293	0.02%	0.003%
64	9.866	2741	2745	2746	rBV	279	209	0.02%	0.002%
65	9.934	2763	2766	2772	rBV	652	410	0.03%	0.004%
66	10.130	2819	2827	2838	rVB5	2261	3917	0.31%	0.037%
67	10.217	2842	2854	2876	rBV	379643	603995	47.11%	5.639%
68	10.458	2926	2929	2930	rBV	463	288	0.02%	0.003%
69	10.487	2935	2938	2942	rVB2	346	253	0.02%	0.002%
70	10.513	2943	2946	2950	rVB2	216	152	0.01%	0.001%
71	10.551	2953	2958	2960	rBV4	649	469	0.04%	0.004%
72	10.638	2983	2985	2987	rBV	295	146	0.01%	0.001%
73	10.751	3016	3020	3023	rBV2	560	317	0.02%	0.003%
74	10.812	3036	3039	3041	rBV2	215	141	0.01%	0.001%
75	10.828	3042	3044	3048	rVB3	556	292	0.02%	0.003%
76	10.882	3059	3061	3066	rBV2	236	134	0.01%	0.001%

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Integration Parameters: LSCINT.P

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 Title : VOC Analysis

77	10.924	3066	3074	3085	rVV5	2922	4869	0.38%	0.045%
78	11.034	3106	3108	3117	rVB3	519	476	0.04%	0.004%
79	11.085	3121	3124	3127	rBV	349	224	0.02%	0.002%
80	11.149	3136	3144	3150	rBV5	1223	1824	0.14%	0.017%
81	11.188	3154	3156	3158	rBV	488	304	0.02%	0.003%
82	11.252	3165	3176	3196	rBV	630019	975064	76.04%	9.104%
83	11.500	3250	3253	3257	rVB2	405	260	0.02%	0.002%
84	11.522	3257	3260	3262	rBV	361	199	0.02%	0.002%
85	11.625	3280	3292	3313	rBV	625009	986466	76.93%	9.210%
86	11.950	3390	3393	3395	rBV	515	227	0.02%	0.002%
87	11.966	3395	3398	3401	rVB2	248	180	0.01%	0.002%
88	12.091	3434	3437	3438	rBV2	584	282	0.02%	0.003%
89	12.252	3485	3487	3490	rVB	420	227	0.02%	0.002%
90	12.281	3493	3496	3497	rBV	287	156	0.01%	0.001%
91	12.323	3505	3509	3510	rBV	360	219	0.02%	0.002%
92	12.397	3529	3532	3533	rBV	283	167	0.01%	0.002%
93	12.474	3551	3556	3557	rBV2	358	240	0.02%	0.002%
94	12.516	3566	3569	3572	rBV2	228	143	0.01%	0.001%
95	12.648	3607	3610	3615	rBV2	631	586	0.05%	0.005%
96	12.670	3615	3617	3619	rVV	361	139	0.01%	0.001%
97	12.821	3662	3664	3667	rBV	333	187	0.01%	0.002%
98	12.886	3681	3684	3689	rBV3	529	381	0.03%	0.004%
99	13.275	3800	3805	3809	rBV2	951	906	0.07%	0.008%
100	13.519	3875	3881	3886	rBV3	1072	1372	0.11%	0.013%

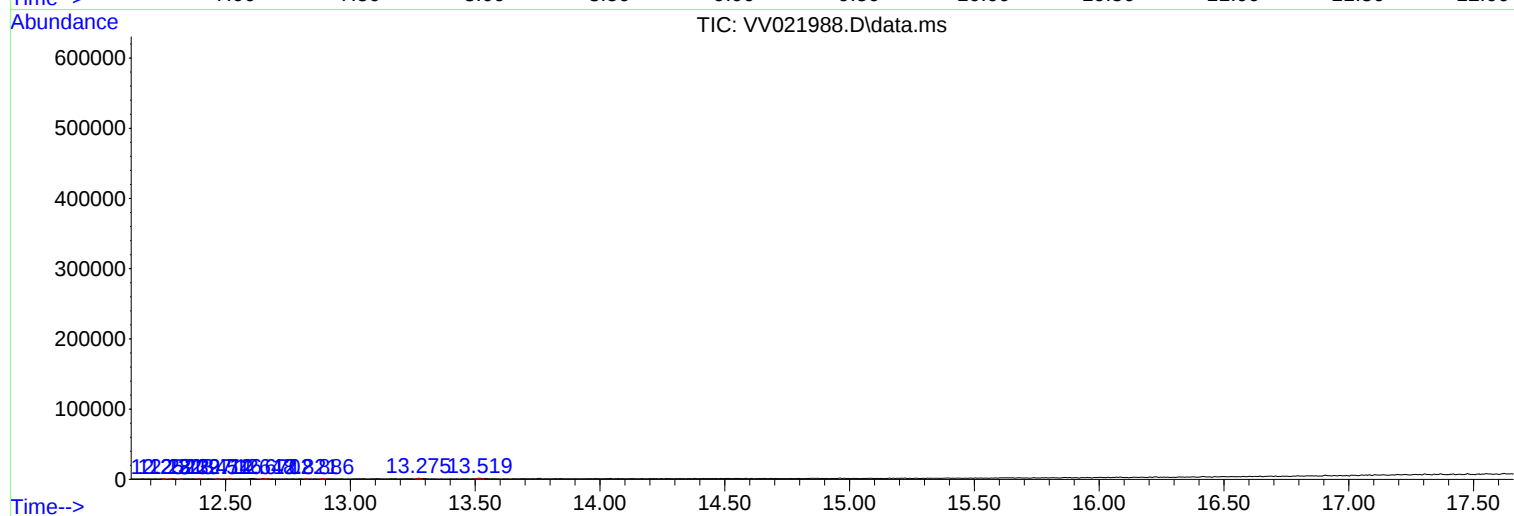
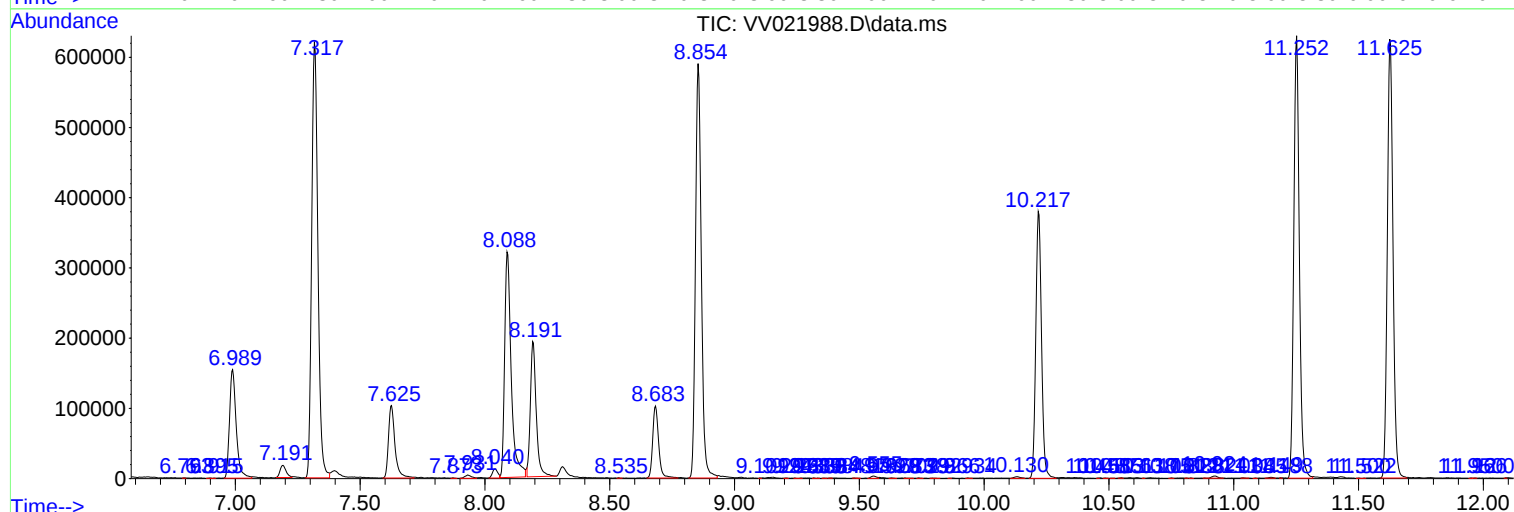
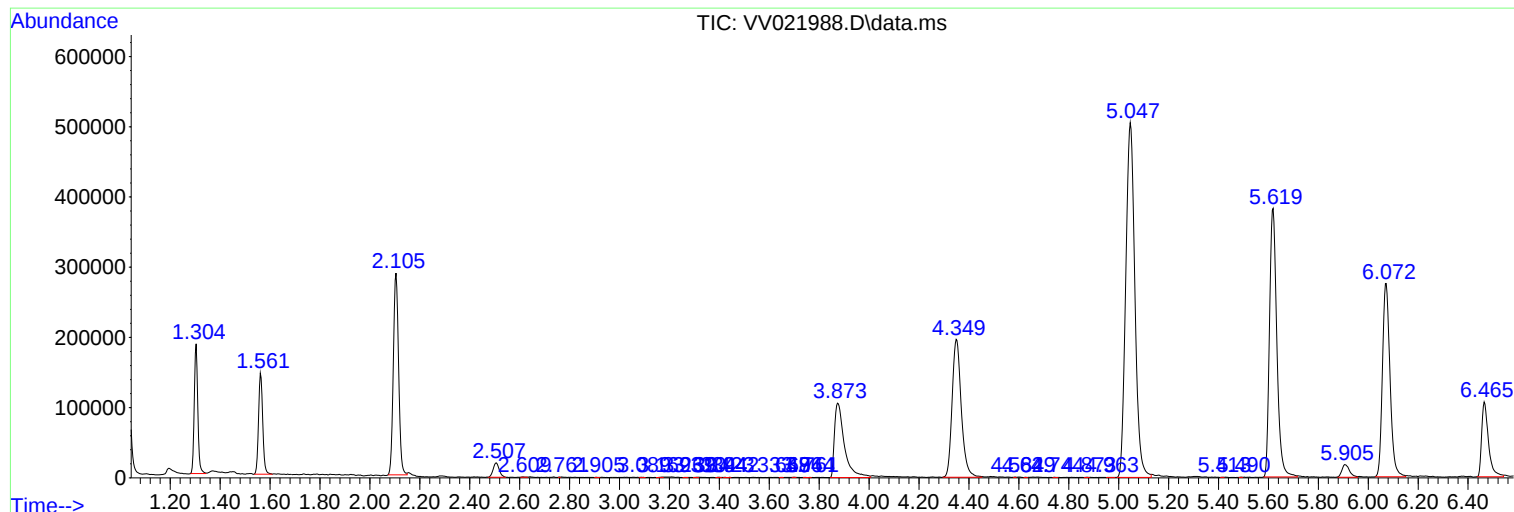
Sum of corrected areas: 10710400

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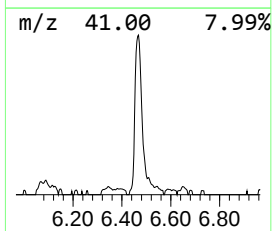
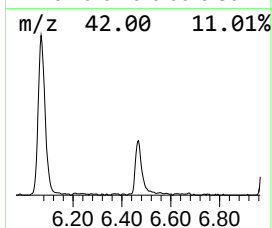
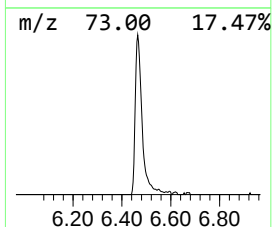
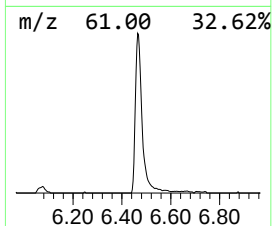
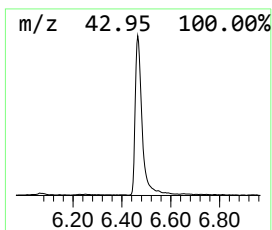
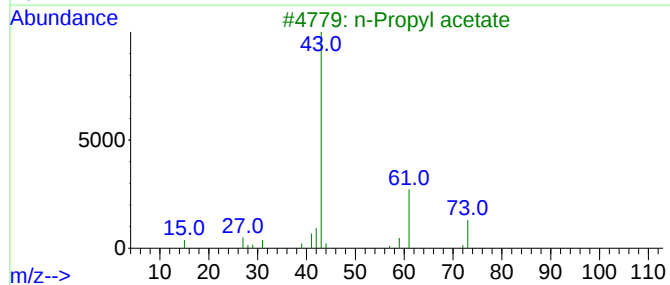
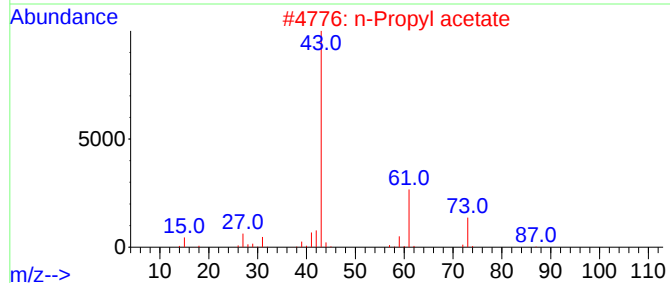
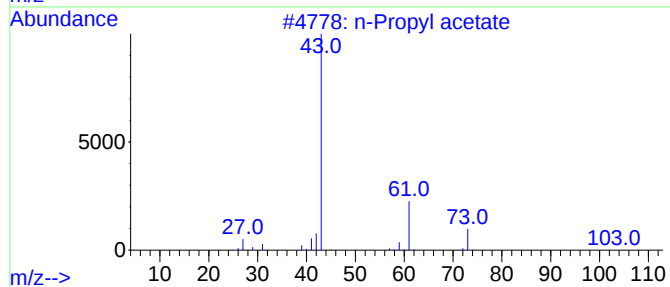
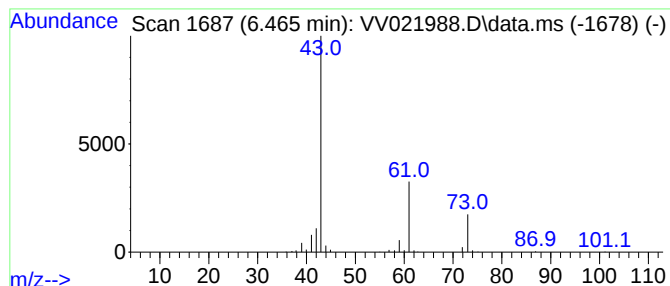
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.465	12.76 ug/L	199347	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	64
5	Propanal, 2,3-dihydroxy-, (S)-			90	C3H6O3	000497-09-6	36



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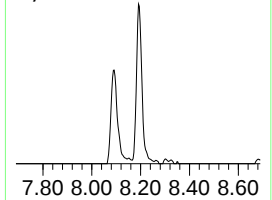
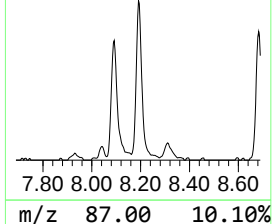
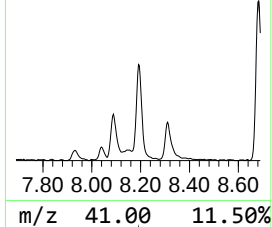
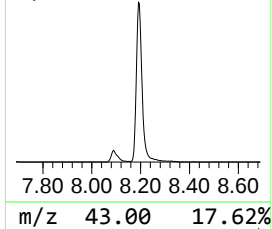
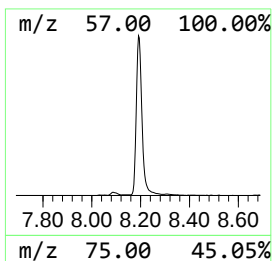
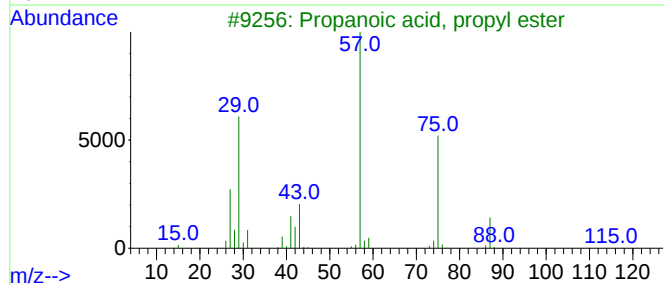
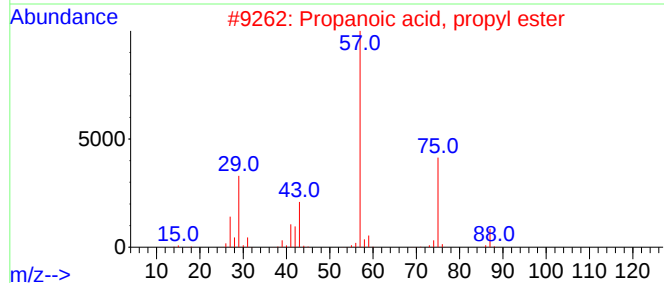
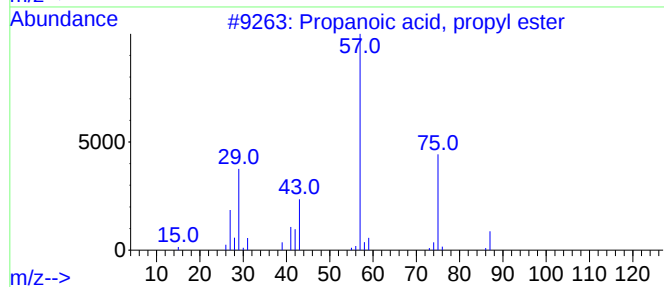
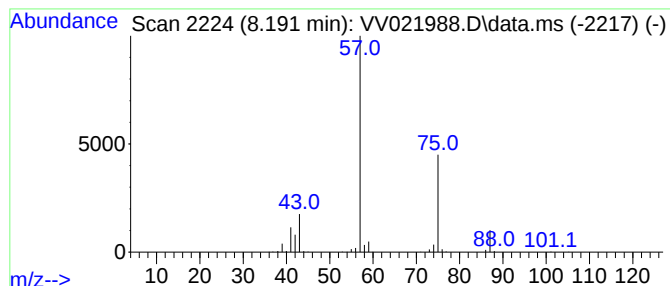
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.191	16.13 ug/L	310322	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



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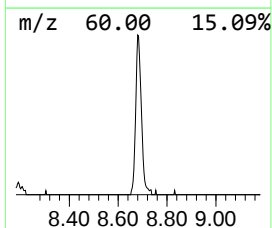
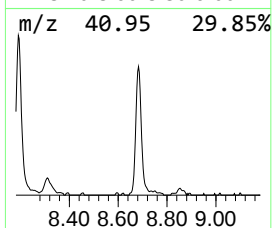
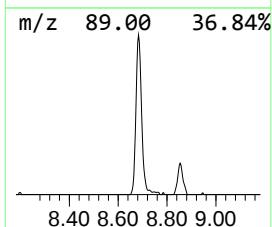
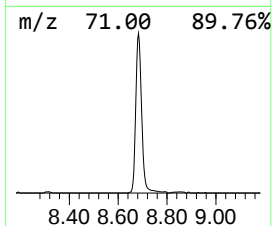
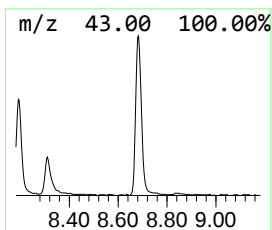
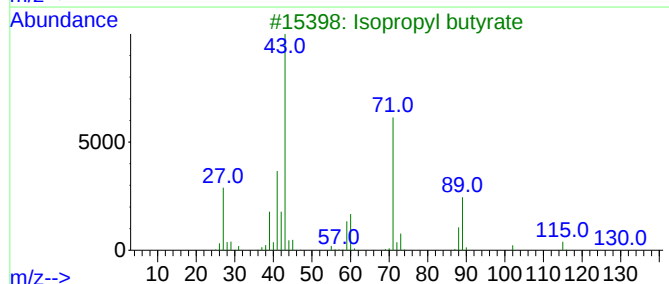
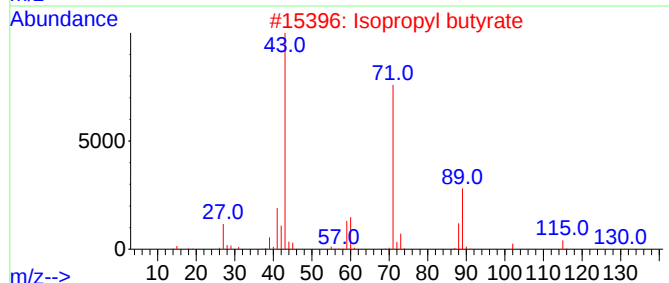
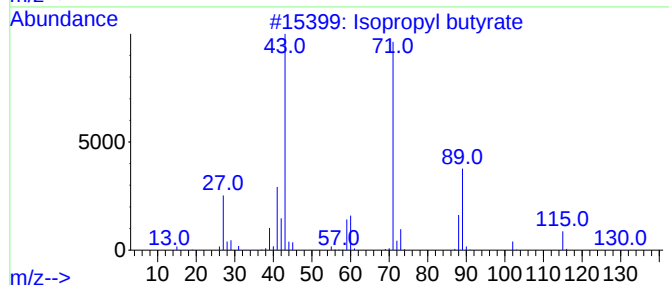
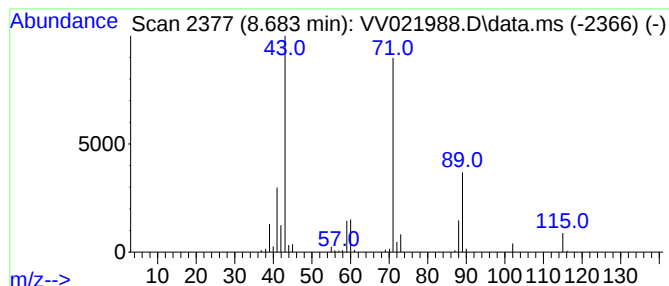
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.683	8.77 ug/L	168688	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			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082721\
Data File : VV021988.D
Acq On : 27 Aug 2021 20:06
Operator : SY/MD
Sample : M3552-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AH2

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
n-Propyl acetate	6.465	12.8	ug/L	199347	1	5.619	781425	50.0
Propanoic acid,...	8.191	16.1	ug/L	310322	2	8.854	962231	50.0
Isopropyl butyrate	8.683	8.8	ug/L	168688	2	8.854	962231	50.0