

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082721\
 Data File : VV021985.D
 Acq On : 27 Aug 2021 18:54
 Operator : SY/MD
 Sample : PB138768TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB768

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: VV021985.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	92	rBV	188468	185877	13.84%	1.631%
2	1.564	156	163	176	rVB	154668	173446	12.91%	1.522%
3	2.105	322	331	345	rBV	309987	452851	33.71%	3.973%
4	2.506	448	456	469	rVB2	14103	24018	1.79%	0.211%
5	2.725	523	524	528	rVV3	611	386	0.03%	0.003%
6	2.770	529	538	549	rVB8	2428	4969	0.37%	0.044%
7	2.844	556	561	566	rVB3	225	245	0.02%	0.002%
8	2.879	570	572	575	rVB3	362	184	0.01%	0.002%
9	2.899	576	578	583	rVB2	408	232	0.02%	0.002%
10	2.928	583	587	588	rBV2	306	211	0.02%	0.002%
11	2.966	597	599	601	rVB2	436	152	0.01%	0.001%
12	3.195	666	670	672	rBV2	617	412	0.03%	0.004%
13	3.330	710	712	716	rVB3	349	180	0.01%	0.002%
14	3.429	741	743	747	rVB2	351	208	0.02%	0.002%
15	3.545	775	779	782	rBV3	418	339	0.03%	0.003%
16	3.577	785	789	793	rBV2	373	339	0.03%	0.003%
17	3.641	806	809	815	rVB3	299	274	0.02%	0.002%
18	3.670	816	818	821	rVB2	323	162	0.01%	0.001%
19	3.696	821	826	830	rBV2	367	262	0.02%	0.002%
20	3.738	835	839	842	rBV2	404	340	0.03%	0.003%
21	3.844	866	872	873	rBV2	410	328	0.02%	0.003%
22	3.876	873	882	911	rBV	108022	292107	21.74%	2.562%
23	4.262	997	1002	1004	rBV4	871	676	0.05%	0.006%
24	4.352	1014	1030	1060	rBV	203148	520354	38.73%	4.565%
25	4.564	1094	1096	1098	rBV2	402	244	0.02%	0.002%
26	4.767	1156	1159	1162	rBV3	498	393	0.03%	0.003%
27	4.802	1167	1170	1173	rBV3	363	289	0.02%	0.003%
28	4.822	1173	1176	1177	rBV2	616	378	0.03%	0.003%
29	4.908	1199	1203	1206	rVB2	437	365	0.03%	0.003%
30	4.924	1206	1208	1209	rBV	468	151	0.01%	0.001%
31	5.047	1229	1246	1280	rBV2	528967	1343432	100.00%	11.785%
32	5.423	1360	1363	1365	rBV3	550	374	0.03%	0.003%
33	5.548	1400	1402	1404	rBV	476	248	0.02%	0.002%
34	5.619	1412	1424	1450	rBV	405442	814725	60.65%	7.147%
35	5.912	1505	1515	1532	rBV9	8756	20002	1.49%	0.175%
36	5.982	1535	1537	1540	rBV2	397	218	0.02%	0.002%

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 Title : VOC Analysis

37	6.072	1552	1565	1594	rBV	290828	602698	44.86%	5.287%
38	6.465	1678	1687	1717	rBV	112981	215526	16.04%	1.891%
39	6.764	1779	1780	1782	rBV	360	152	0.01%	0.001%
40	6.989	1839	1850	1873	rBV	162753	298784	22.24%	2.621%
41	7.188	1905	1912	1924	rBV2	17919	30130	2.24%	0.264%
42	7.317	1941	1952	1970	rBV	642548	1123189	83.61%	9.853%
43	7.625	2037	2048	2079	rBV	107938	198362	14.77%	1.740%
44	7.831	2108	2112	2113	rBV2	553	335	0.02%	0.003%
45	7.931	2132	2143	2152	rBV3	5529	10628	0.79%	0.093%
46	8.040	2169	2177	2183	rBV3	14632	20912	1.56%	0.183%
47	8.088	2184	2192	2215	rVV	351876	613054	45.63%	5.378%
48	8.191	2217	2224	2252	rVB	214418	353318	26.30%	3.099%
49	8.455	2304	2306	2308	rBV3	497	272	0.02%	0.002%
50	8.609	2348	2354	2357	rBV2	827	987	0.07%	0.009%
51	8.683	2366	2377	2400	rBV	131464	209024	15.56%	1.834%
52	8.854	2418	2430	2450	rBV	601270	1002428	74.62%	8.794%
53	9.024	2477	2483	2490	rBV4	3053	4097	0.30%	0.036%
54	9.149	2514	2522	2529	rBV5	3349	5870	0.44%	0.051%
55	9.268	2557	2559	2560	rBV	362	157	0.01%	0.001%
56	9.397	2597	2599	2601	rBV2	490	252	0.02%	0.002%
57	9.554	2639	2648	2667	rBV10	6751	16753	1.25%	0.147%
58	9.699	2690	2693	2695	rBV2	538	316	0.02%	0.003%
59	9.783	2714	2719	2722	rBV2	581	437	0.03%	0.004%
60	9.902	2754	2756	2759	rVB3	432	221	0.02%	0.002%
61	9.940	2759	2768	2775	rBV4	3346	4982	0.37%	0.044%
62	10.017	2790	2792	2802	rVB2	516	366	0.03%	0.003%
63	10.066	2803	2807	2809	rBV	205	155	0.01%	0.001%
64	10.130	2820	2827	2842	rVB8	2593	4473	0.33%	0.039%
65	10.220	2842	2855	2880	rBV	419164	667920	49.72%	5.859%
66	10.545	2948	2956	2965	rBV3	4630	7359	0.55%	0.065%
67	10.821	3039	3042	3043	rBV	273	164	0.01%	0.001%
68	10.837	3043	3047	3051	rVB4	601	518	0.04%	0.005%
69	10.921	3068	3073	3084	rVB3	7269	10485	0.78%	0.092%
70	10.998	3093	3097	3100	rVB2	586	414	0.03%	0.004%
71	11.117	3129	3134	3135	rBV	240	189	0.01%	0.002%
72	11.152	3135	3145	3150	rVV5	1319	2140	0.16%	0.019%
73	11.191	3150	3157	3165	rVV4	4760	6833	0.51%	0.060%
74	11.252	3165	3176	3205	rVV	661774	1030856	76.73%	9.043%
75	11.532	3262	3263	3266	rBV2	333	181	0.01%	0.002%
76	11.551	3266	3269	3274	rVB3	416	357	0.03%	0.003%

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Title : VOC Analysis

77	11.625	3280	3292	3317	rBV	642980	1036832	77.18%	9.095%
78	11.844	3357	3360	3363	rBV3	457	391	0.03%	0.003%
79	11.895	3373	3376	3377	rBV	373	155	0.01%	0.001%
80	11.953	3391	3394	3398	rVB2	425	291	0.02%	0.003%
81	11.976	3398	3401	3403	rBV2	441	247	0.02%	0.002%
82	11.992	3403	3406	3407	rBV2	332	198	0.01%	0.002%
83	12.030	3412	3418	3420	rBV2	424	373	0.03%	0.003%
84	12.230	3478	3480	3482	rBV2	371	217	0.02%	0.002%
85	12.435	3538	3544	3553	rVB5	1521	2040	0.15%	0.018%
86	12.477	3554	3557	3562	rBV3	379	353	0.03%	0.003%
87	12.577	3585	3588	3589	rBV3	420	180	0.01%	0.002%
88	12.654	3603	3612	3624	rVB4	7755	11589	0.86%	0.102%
89	12.882	3679	3683	3684	rBV2	506	311	0.02%	0.003%
90	12.982	3709	3714	3715	rBV2	288	226	0.02%	0.002%
91	13.140	3759	3763	3765	rBV	257	182	0.01%	0.002%
92	13.226	3787	3790	3795	rBV2	576	367	0.03%	0.003%
93	13.271	3796	3804	3818	rVB3	9304	14107	1.05%	0.124%
94	13.394	3838	3842	3845	rVB	439	314	0.02%	0.003%
95	13.458	3859	3862	3864	rVV	511	228	0.02%	0.002%
96	13.509	3870	3878	3892	rBV	17315	27514	2.05%	0.241%
97	13.603	3903	3907	3909	rBV	462	355	0.03%	0.003%
98	13.696	3933	3936	3939	rBV2	430	299	0.02%	0.003%
99	13.750	3943	3953	3967	rVB3	11275	17813	1.33%	0.156%
100	14.101	4060	4062	4066	rVB	638	300	0.02%	0.003%

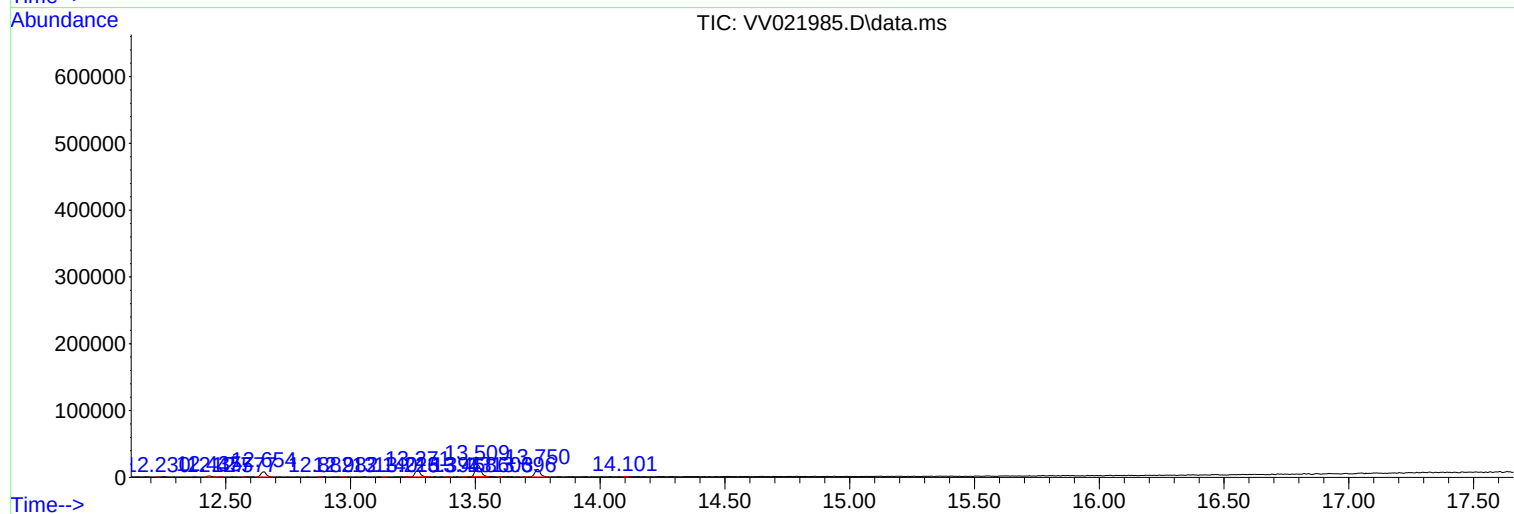
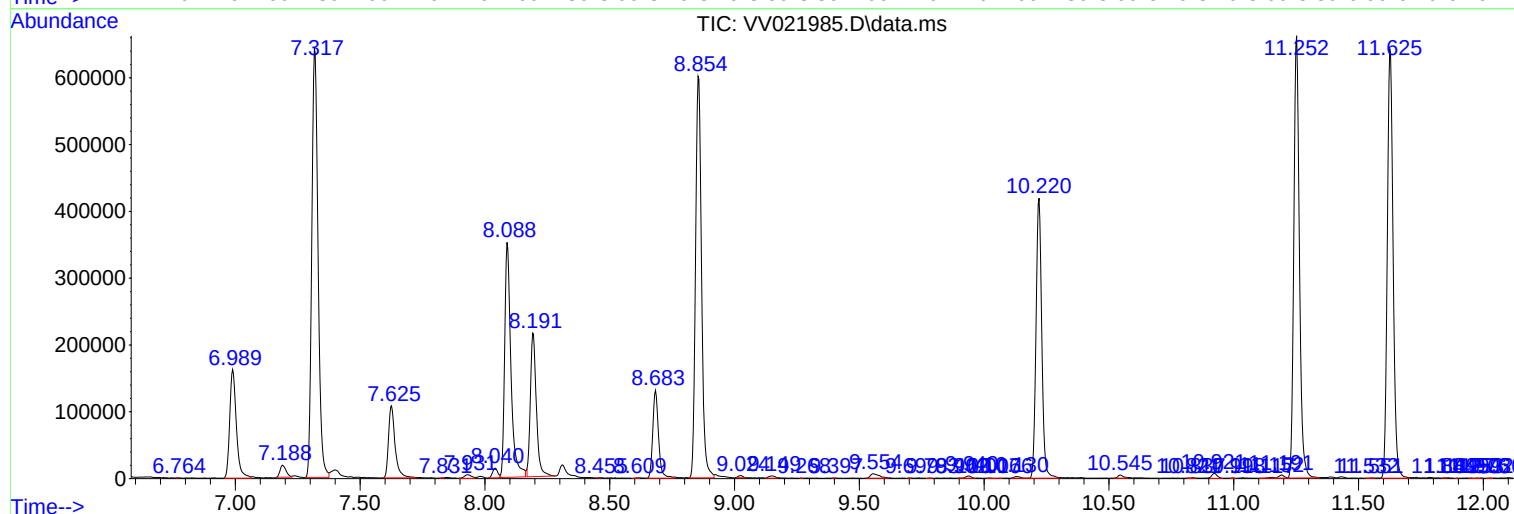
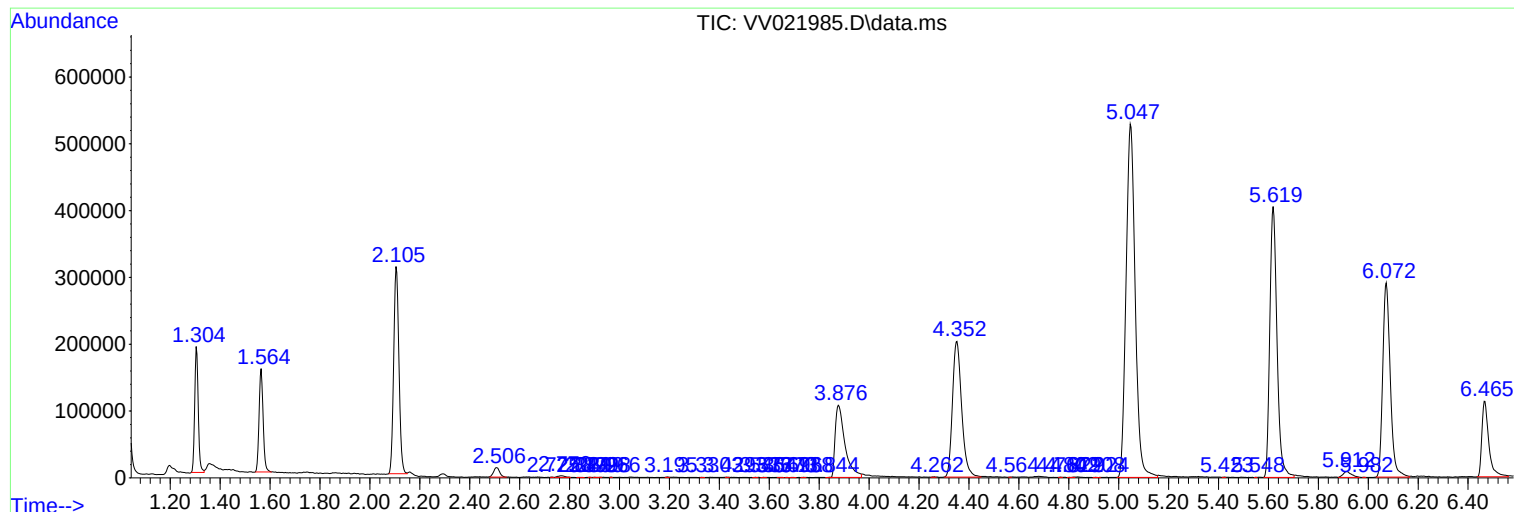
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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



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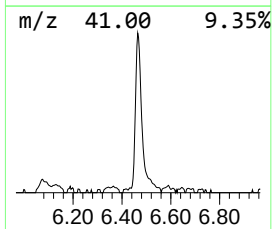
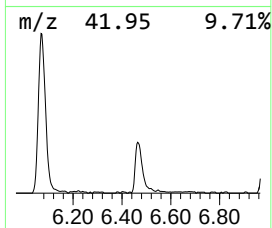
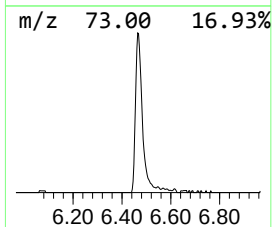
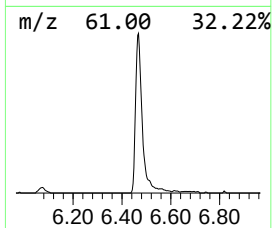
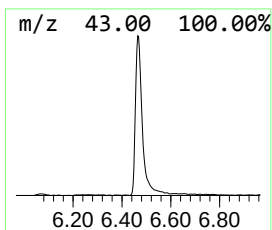
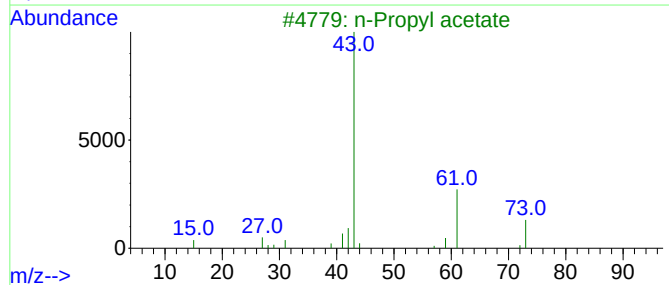
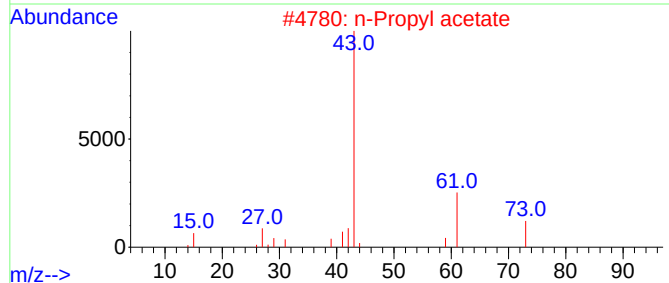
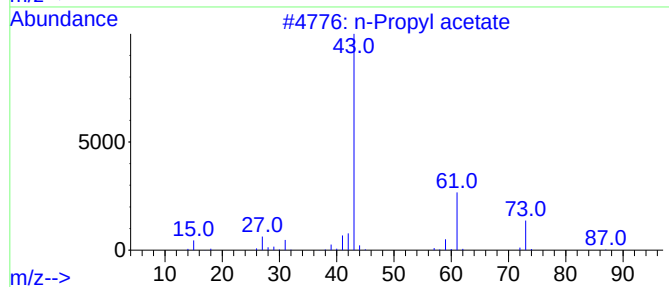
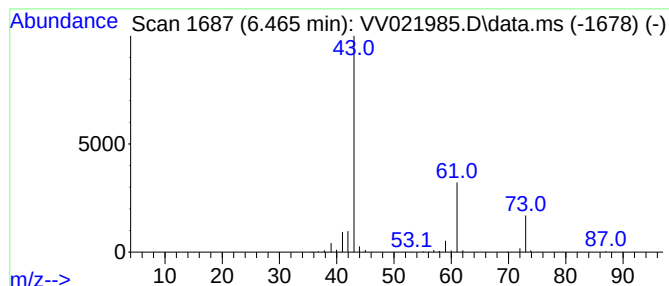
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.465	13.23 ug/L	215526	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	72
3	n-Propyl acetate			102	C5H10O2	000109-60-4	64
4	n-Propyl acetate			102	C5H10O2	000109-60-4	50
5	n-Propyl acetate			102	C5H10O2	000109-60-4	40



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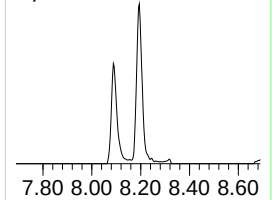
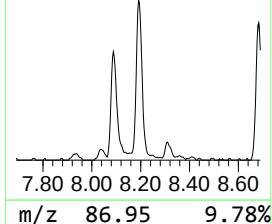
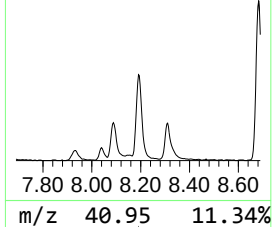
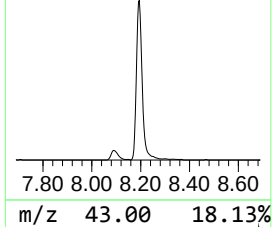
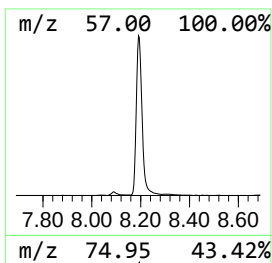
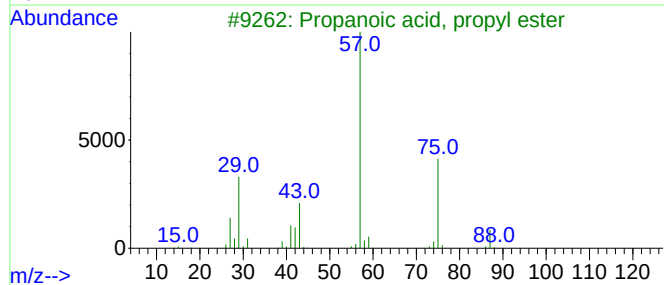
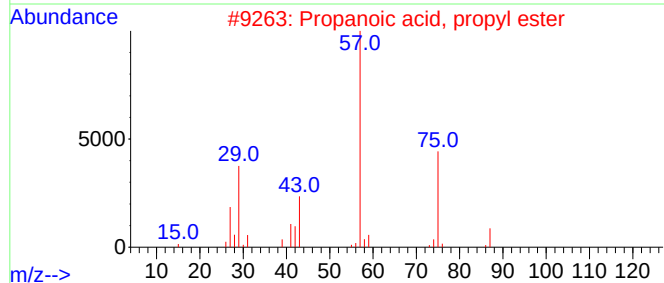
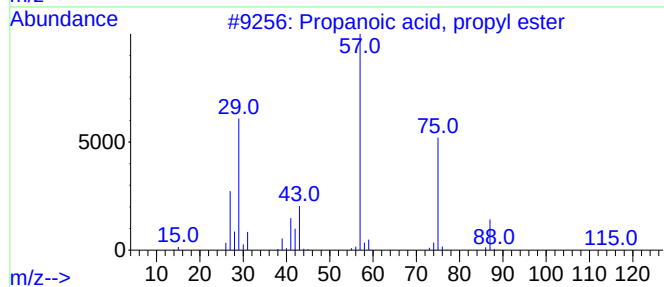
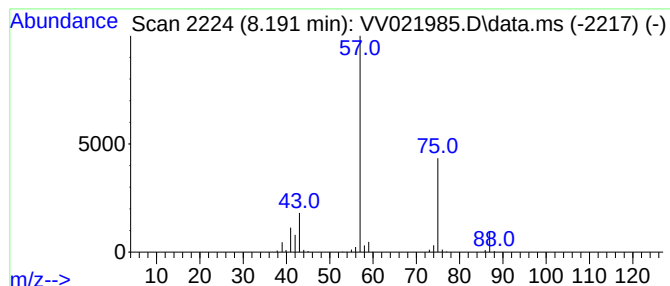
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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	17.62 ug/L	353318	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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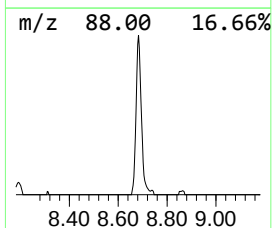
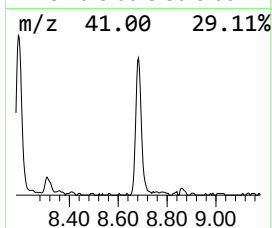
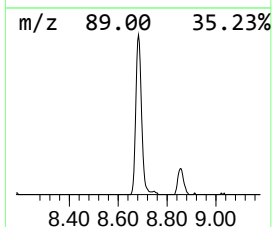
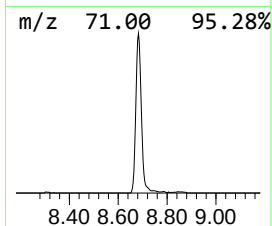
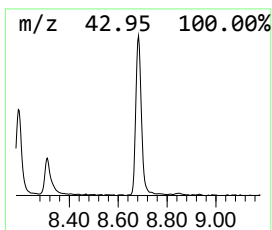
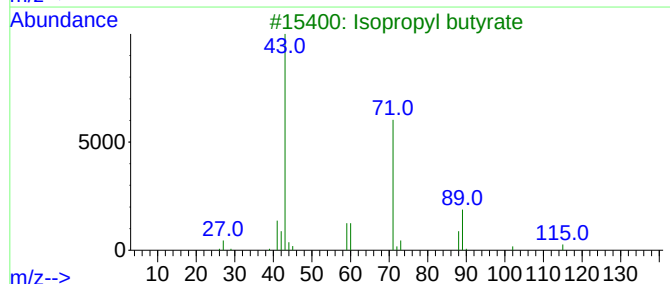
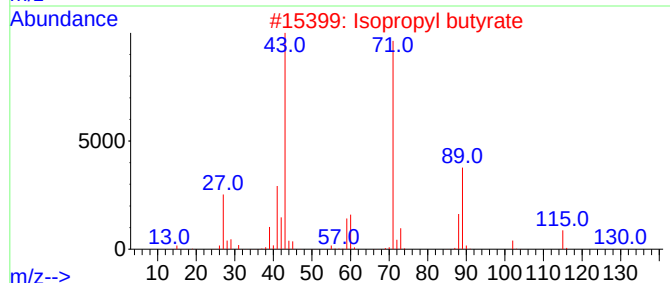
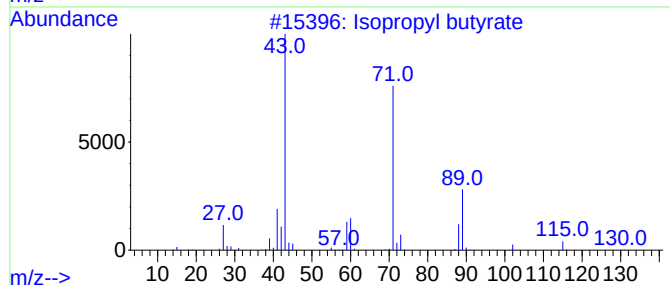
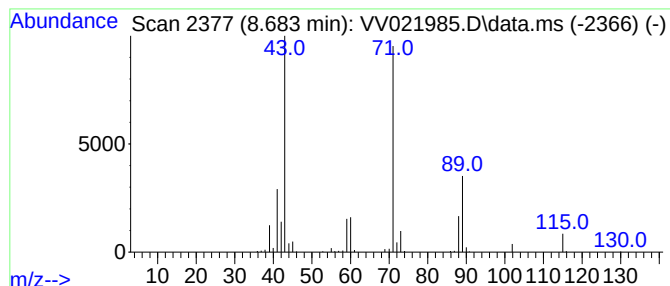
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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	10.43 ug/L	209024	Chlorobenzene-d5	8.854

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			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
5			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082721\
Data File : VV021985.D
Acq On : 27 Aug 2021 18:54
Operator : SY/MD
Sample : PB138768TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB768

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	13.2	ug/L	215526	1	5.619	814725	50.0
Propanoic acid,...	8.191	17.6	ug/L	353318	2	8.854	1002430	50.0
Isopropyl butyrate	8.683	10.4	ug/L	209024	2	8.854	1002430	50.0