

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082721\
 Data File : VV021986.D
 Acq On : 27 Aug 2021 19:18
 Operator : SY/MD
 Sample : M3552-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 COAH0

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: VV021986.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	93	rVB	179431	177276	13.67%	1.623%
2	1.561	156	162	177	rVB	142052	165322	12.74%	1.513%
3	2.105	321	331	344	rBV	300666	431978	33.30%	3.955%
4	2.507	446	456	470	rVB	20558	33525	2.58%	0.307%
5	2.603	483	486	487	rBV2	295	157	0.01%	0.001%
6	2.770	530	538	543	rBV5	1343	1791	0.14%	0.016%
7	2.819	550	553	555	rBV3	217	164	0.01%	0.002%
8	2.957	594	596	598	rBV	281	177	0.01%	0.002%
9	3.002	605	610	612	rBV2	344	316	0.02%	0.003%
10	3.040	617	622	627	rVB2	602	622	0.05%	0.006%
11	3.069	627	631	632	rBV	309	152	0.01%	0.001%
12	3.089	635	637	640	rBV2	334	242	0.02%	0.002%
13	3.172	660	663	665	rBV2	482	335	0.03%	0.003%
14	3.269	688	693	697	rBV	532	511	0.04%	0.005%
15	3.330	708	712	713	rBV2	251	158	0.01%	0.001%
16	3.391	729	731	735	rBV	433	235	0.02%	0.002%
17	3.433	740	744	749	rBV2	229	170	0.01%	0.002%
18	3.561	780	784	786	rVV2	286	207	0.02%	0.002%
19	3.828	863	867	869	rBV	342	189	0.01%	0.002%
20	3.876	872	882	917	rBV	110774	294264	22.68%	2.694%
21	4.349	1013	1029	1060	rBV	196097	505624	38.98%	4.629%
22	4.671	1124	1129	1134	rBV6	823	968	0.07%	0.009%
23	4.728	1143	1147	1152	rVB3	443	432	0.03%	0.004%
24	4.886	1192	1196	1198	rBV2	359	251	0.02%	0.002%
25	5.047	1229	1246	1277	rBV2	510865	1297230	100.00%	11.876%
26	5.526	1392	1395	1396	rBV	303	154	0.01%	0.001%
27	5.558	1401	1405	1408	rBV3	408	305	0.02%	0.003%
28	5.574	1408	1410	1411	rBV	498	175	0.01%	0.002%
29	5.619	1412	1424	1457	rBV	395252	796819	61.42%	7.295%
30	5.908	1504	1514	1534	rVB3	12773	28889	2.23%	0.264%
31	6.072	1551	1565	1593	rBV	282740	583644	44.99%	5.343%
32	6.336	1643	1647	1649	rBV4	818	634	0.05%	0.006%
33	6.465	1678	1687	1712	rBV	108517	206551	15.92%	1.891%
34	6.989	1836	1850	1872	rBV	157056	289214	22.29%	2.648%
35	7.191	1904	1913	1925	rBV2	18399	31519	2.43%	0.289%
36	7.317	1941	1952	1970	rBV	624132	1089287	83.97%	9.972%

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Integrator: RTE

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

37	7.584	2033	2035	2037	rBV3	430	254	0.02%	0.002%
38	7.625	2039	2048	2068	rVV	105547	186483	14.38%	1.707%
39	7.931	2132	2143	2153	rBV3	4736	8848	0.68%	0.081%
40	8.040	2168	2177	2183	rBV4	13424	20348	1.57%	0.186%
41	8.088	2183	2192	2215	rVV	332925	603583	46.53%	5.526%
42	8.191	2217	2224	2249	rVB	196856	319528	24.63%	2.925%
43	8.590	2345	2348	2349	rBV	357	232	0.02%	0.002%
44	8.619	2355	2357	2362	rBV	382	289	0.02%	0.003%
45	8.683	2366	2377	2398	rBV	108296	175011	13.49%	1.602%
46	8.854	2419	2430	2451	rBV	598102	976677	75.29%	8.941%
47	9.146	2514	2521	2525	rBV4	1803	2313	0.18%	0.021%
48	9.249	2551	2553	2557	rVB3	605	299	0.02%	0.003%
49	9.301	2567	2569	2573	rVB2	453	265	0.02%	0.002%
50	9.336	2578	2580	2583	rBV2	370	194	0.01%	0.002%
51	9.358	2583	2587	2593	rVB4	311	357	0.03%	0.003%
52	9.391	2593	2597	2599	rBV	377	215	0.02%	0.002%
53	9.410	2599	2603	2606	rBV2	361	268	0.02%	0.002%
54	9.445	2612	2614	2615	rBV2	397	177	0.01%	0.002%
55	9.516	2633	2636	2639	rBV2	249	186	0.01%	0.002%
56	9.558	2639	2649	2663	rVV6	3808	7448	0.57%	0.068%
57	9.677	2683	2686	2689	rVB3	432	255	0.02%	0.002%
58	9.786	2719	2720	2725	rVB2	295	233	0.02%	0.002%
59	9.818	2725	2730	2733	rBV2	457	414	0.03%	0.004%
60	9.982	2778	2781	2784	rVB3	284	195	0.02%	0.002%
61	9.998	2784	2786	2788	rBV2	408	167	0.01%	0.002%
62	10.130	2819	2827	2838	rBV6	2733	4305	0.33%	0.039%
63	10.217	2843	2854	2879	rBV	400864	629008	48.49%	5.758%
64	10.510	2942	2945	2948	rBV2	295	165	0.01%	0.002%
65	10.548	2950	2957	2963	rBV4	933	1608	0.12%	0.015%
66	10.609	2973	2976	2981	rVB2	608	527	0.04%	0.005%
67	10.706	3001	3006	3010	rBV3	360	377	0.03%	0.003%
68	10.812	3036	3039	3042	rBV2	341	217	0.02%	0.002%
69	10.834	3042	3046	3047	rBV3	401	246	0.02%	0.002%
70	10.879	3057	3060	3061	rBV	382	203	0.02%	0.002%
71	10.921	3065	3073	3081	rVB6	3598	5375	0.41%	0.049%
72	10.992	3093	3095	3099	rVB	337	164	0.01%	0.002%
73	11.027	3102	3106	3107	rBV	255	151	0.01%	0.001%
74	11.037	3107	3109	3112	rVV2	446	214	0.02%	0.002%
75	11.140	3135	3141	3143	rBV3	970	870	0.07%	0.008%
76	11.185	3152	3155	3156	rBV2	840	508	0.04%	0.005%

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Title : VOC Analysis

77	11.252	3165	3176	3200	rBV	647954	1010381	77.89%	9.250%
78	11.358	3207	3209	3211	rBV2	881	373	0.03%	0.003%
79	11.503	3252	3254	3258	rVB2	482	262	0.02%	0.002%
80	11.545	3262	3267	3273	rBV4	651	798	0.06%	0.007%
81	11.625	3280	3292	3322	rBV	635769	1003877	77.39%	9.190%
82	11.792	3338	3344	3347	rBV4	1199	1304	0.10%	0.012%
83	11.847	3356	3361	3363	rBV2	444	453	0.03%	0.004%
84	11.892	3372	3375	3377	rBV	337	153	0.01%	0.001%
85	11.937	3386	3389	3391	rBV2	401	202	0.02%	0.002%
86	12.037	3419	3420	3424	rVB	430	154	0.01%	0.001%
87	12.162	3455	3459	3461	rBV	411	305	0.02%	0.003%
88	12.175	3461	3463	3466	rVV2	424	201	0.02%	0.002%
89	12.333	3510	3512	3516	rBV2	348	208	0.02%	0.002%
90	12.493	3559	3562	3563	rBV	344	153	0.01%	0.001%
91	12.651	3606	3611	3620	rVB5	2363	3662	0.28%	0.034%
92	12.815	3658	3662	3665	rBV	252	212	0.02%	0.002%
93	12.895	3683	3687	3689	rBV3	530	315	0.02%	0.003%
94	12.998	3718	3719	3723	rVB2	339	157	0.01%	0.001%
95	13.217	3784	3787	3789	rBV	438	249	0.02%	0.002%
96	13.268	3797	3803	3805	rBV2	1943	1907	0.15%	0.017%
97	13.355	3826	3830	3836	rBV2	502	597	0.05%	0.005%
98	13.509	3870	3878	3891	rBV2	3917	6566	0.51%	0.060%
99	13.593	3901	3904	3908	rBV3	566	517	0.04%	0.005%
100	13.754	3948	3954	3959	rBV2	2313	2662	0.21%	0.024%

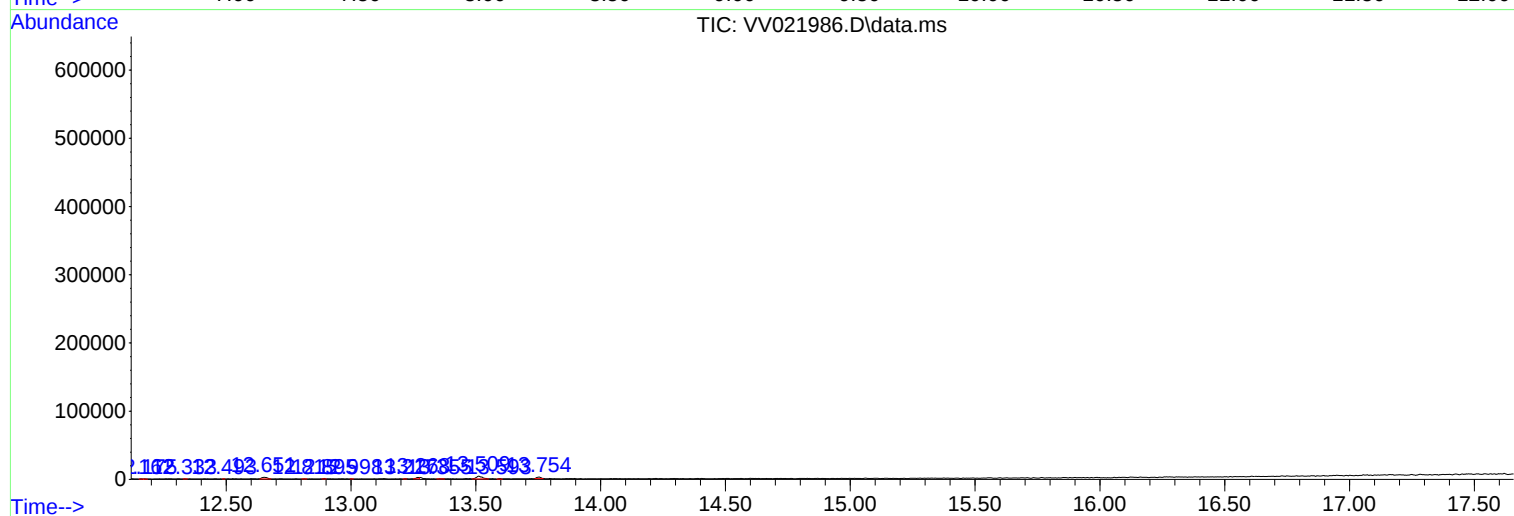
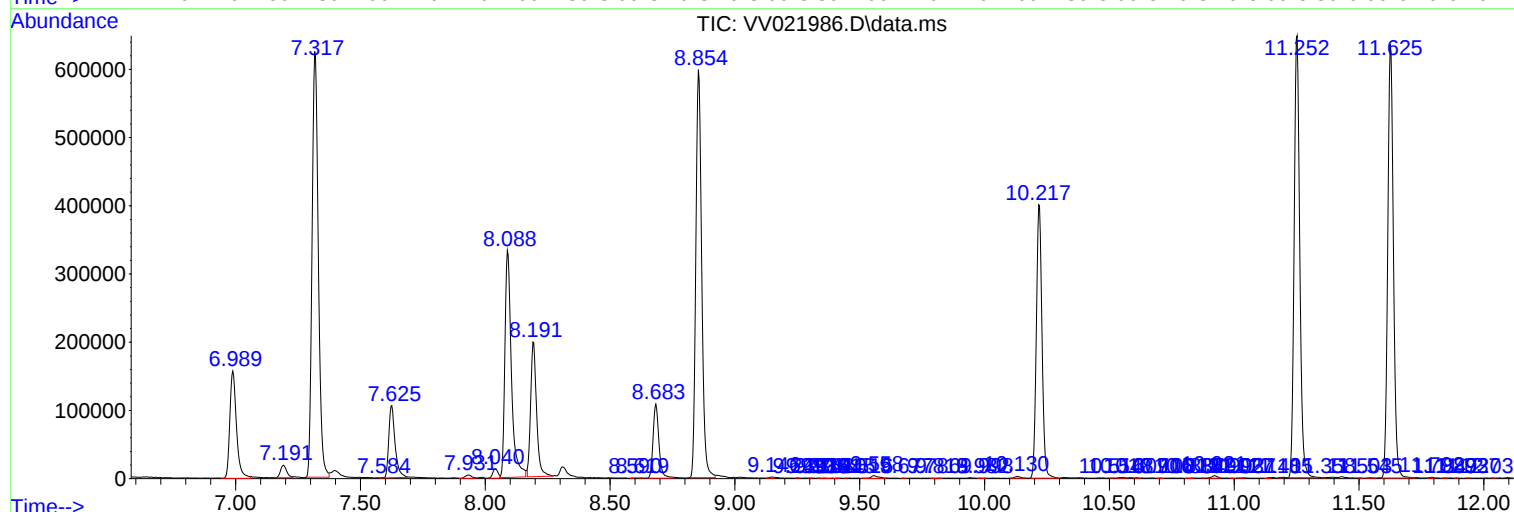
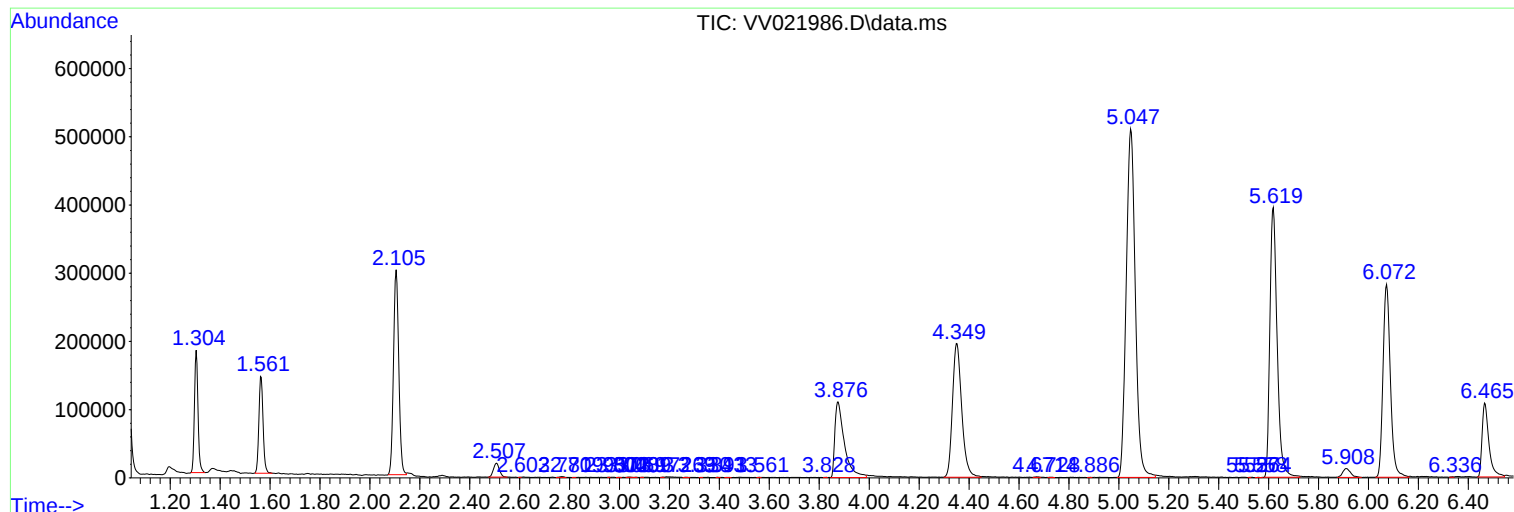
Sum of corrected areas: 10923332

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Instrument :
MSVOA_V
ClientSampleId :
C0AH0

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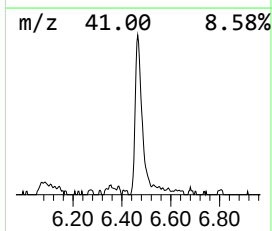
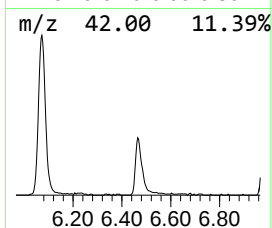
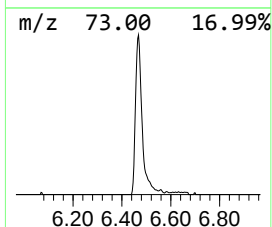
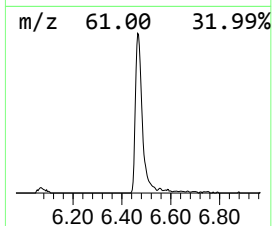
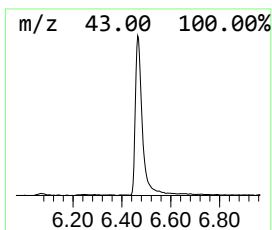
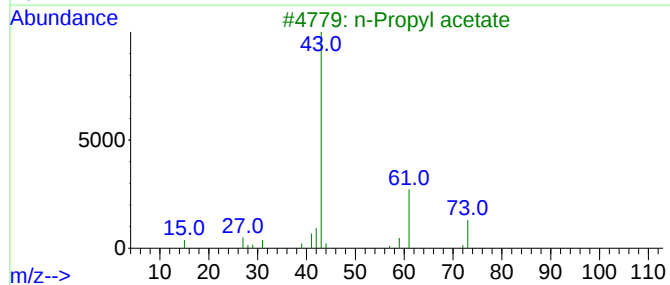
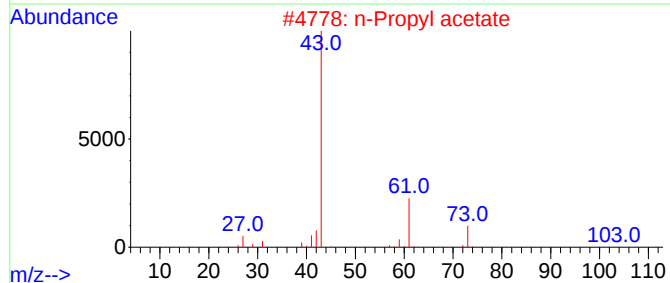
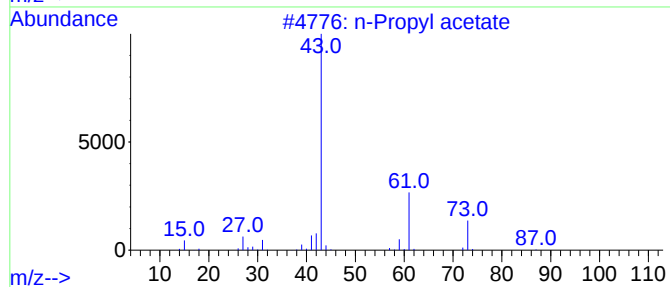
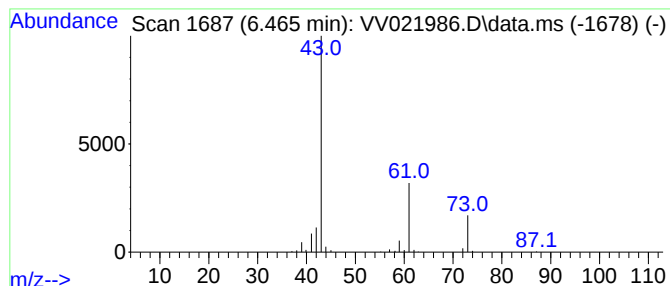
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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	12.96 ug/L	206551	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		Isopropyl acetate	102	C5H10O2	000108-21-4	36



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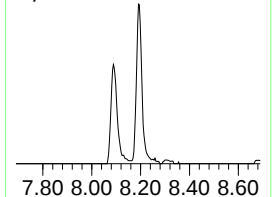
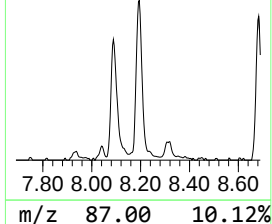
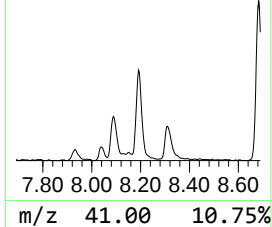
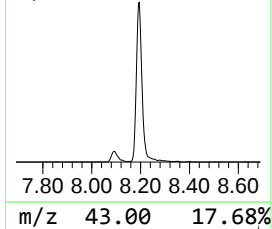
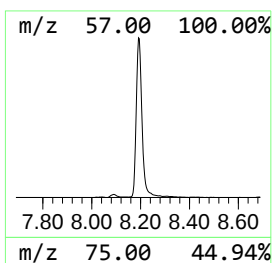
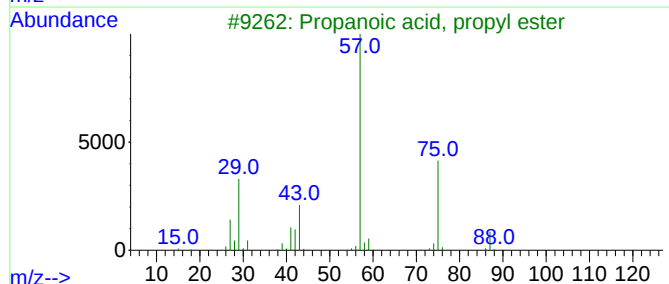
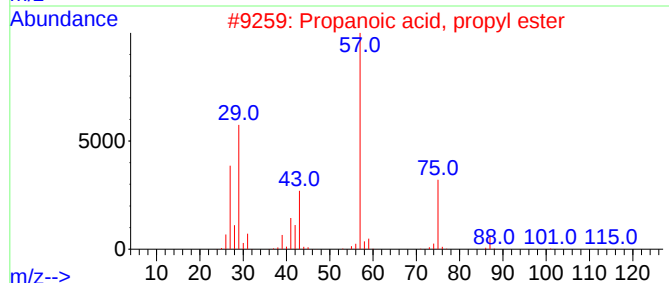
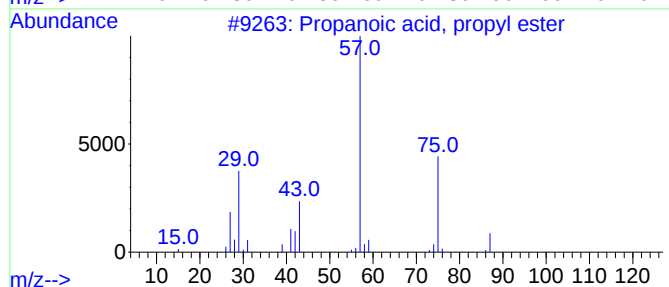
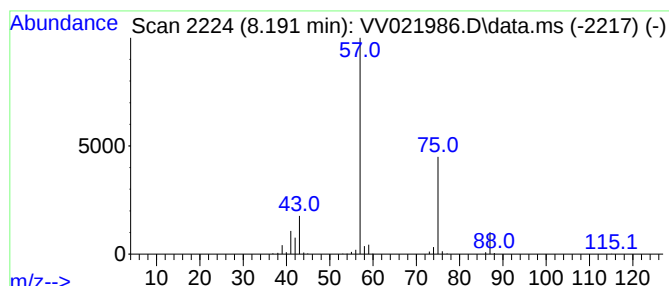
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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	16.36 ug/L	319528	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	59



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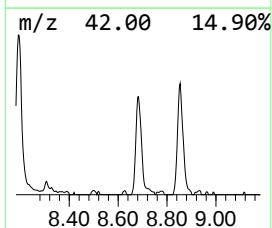
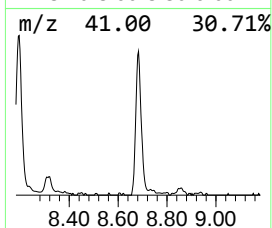
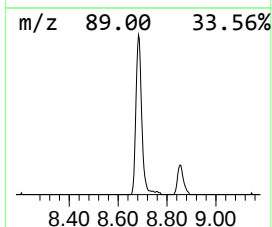
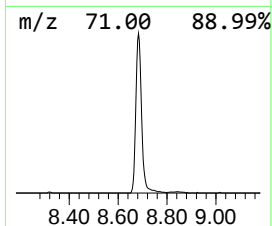
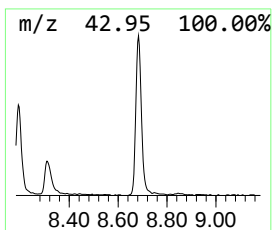
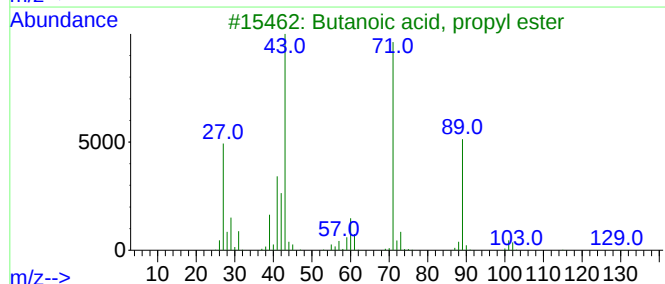
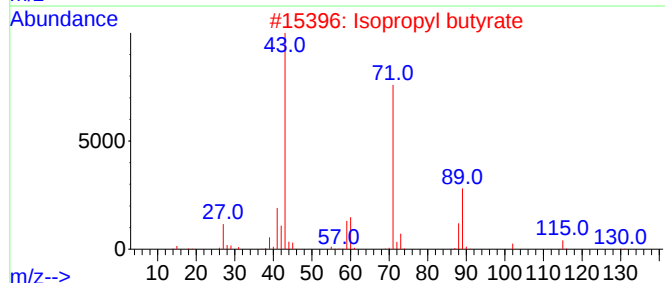
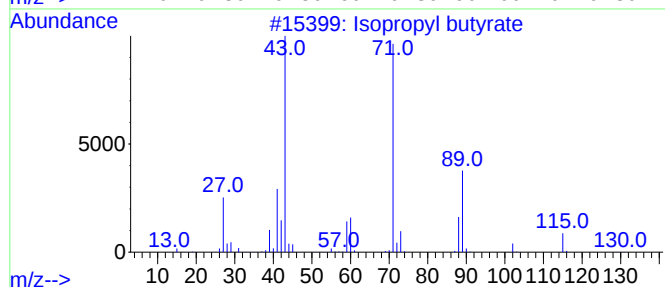
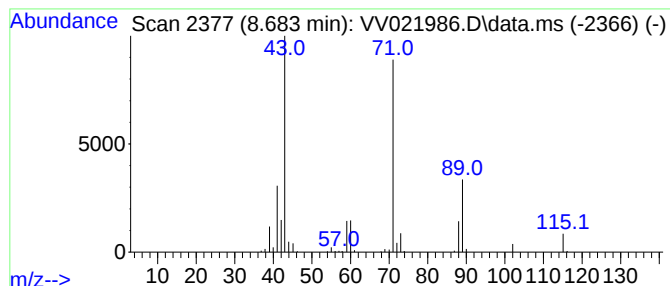
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082721WMA.M
Quant Title : VOC Analysis

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	8.96 ug/L	175011	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			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	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 : VV021986.D
Acq On : 27 Aug 2021 19:18
Operator : SY/MD
Sample : M3552-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AH0

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	13.0	ug/L	206551	1	5.619	796819	50.0
Propanoic acid,...	8.191	16.4	ug/L	319528	2	8.854	976677	50.0
Isopropyl butyrate	8.683	9.0	ug/L	175011	2	8.854	976677	50.0