

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
 Data File : VU046110.D
 Acq On : 06 Dec 2021 14:34
 Operator : SY/MD
 Sample : M4938-01 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8D7

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_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046110.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	94	rBV	106671	116142	13.23%	1.638%
2	1.916	170	179	195	rVB	77549	98908	11.27%	1.395%
3	2.112	238	240	242	rBV	361	195	0.02%	0.003%
4	2.517	363	366	370	rVB2	392	198	0.02%	0.003%
5	2.572	370	383	401	rBV	188477	312792	35.63%	4.413%
6	2.778	444	447	448	rBV	304	153	0.02%	0.002%
7	2.790	448	451	459	rVB	430	498	0.06%	0.007%
8	2.900	483	485	490	rVV2	160	141	0.02%	0.002%
9	2.954	498	502	503	rBV2	213	152	0.02%	0.002%
10	3.048	523	531	544	rVB3	4482	8011	0.91%	0.113%
11	3.115	550	552	558	rVB2	183	153	0.02%	0.002%
12	3.189	565	575	586	rBV	1987	4275	0.49%	0.060%
13	3.263	595	598	604	rBV2	246	195	0.02%	0.003%
14	3.347	621	624	627	rVB	235	149	0.02%	0.002%
15	3.610	704	706	711	rVB	190	190	0.02%	0.003%
16	3.852	777	781	784	rBV	153	141	0.02%	0.002%
17	4.115	859	863	867	rBV2	217	172	0.02%	0.002%
18	4.295	916	919	923	rVB2	267	241	0.03%	0.003%
19	4.633	1006	1024	1049	rBV	82684	215000	24.49%	3.033%
20	4.803	1073	1077	1078	rBV3	230	181	0.02%	0.003%
21	4.922	1108	1114	1116	rBV	314	267	0.03%	0.004%
22	5.067	1143	1159	1182	rBV	151361	338997	38.62%	4.782%
23	5.196	1190	1199	1205	rVV3	393	683	0.08%	0.010%
24	5.295	1224	1230	1237	rVB2	514	652	0.07%	0.009%
25	5.385	1255	1258	1260	rVV	375	215	0.02%	0.003%
26	5.456	1273	1280	1282	rBV	160	227	0.03%	0.003%
27	5.729	1342	1365	1386	rBV2	328780	877771	100.00%	12.383%
28	5.909	1416	1421	1435	rVB5	1251	2190	0.25%	0.031%
29	5.980	1441	1443	1448	rVB	258	198	0.02%	0.003%
30	6.041	1461	1462	1467	rVB2	373	253	0.03%	0.004%
31	6.105	1479	1482	1484	rBV3	246	148	0.02%	0.002%
32	6.250	1513	1527	1544	rBV	251742	474386	54.04%	6.692%
33	6.414	1575	1578	1584	rVB2	277	275	0.03%	0.004%
34	6.472	1594	1596	1599	rVB2	290	157	0.02%	0.002%
35	6.536	1604	1616	1629	rVB6	5233	11357	1.29%	0.160%
36	6.694	1651	1665	1681	rBV	200470	383996	43.75%	5.417%

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Integrator: RTE

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 Title : VOC Analysis

37	6.765	1684	1687	1690	rBV2	541	468	0.05%	0.007%
38	6.890	1723	1726	1730	rBV	350	302	0.03%	0.004%
39	6.922	1730	1736	1737	rBV	530	441	0.05%	0.006%
40	7.041	1760	1773	1797	rBV	74826	130813	14.90%	1.845%
41	7.179	1814	1816	1821	rVB3	569	428	0.05%	0.006%
42	7.215	1825	1827	1833	rVB2	328	258	0.03%	0.004%
43	7.568	1923	1937	1955	rBV	117505	203141	23.14%	2.866%
44	7.687	1970	1974	1981	rVB3	416	507	0.06%	0.007%
45	7.739	1981	1990	2000	rBV2	11032	16973	1.93%	0.239%
46	7.790	2000	2006	2007	rBV2	338	306	0.03%	0.004%
47	7.900	2025	2040	2056	rBV	420529	732884	83.49%	10.339%
48	8.179	2112	2127	2143	rBV	78194	131905	15.03%	1.861%
49	8.273	2152	2156	2165	rBV4	455	632	0.07%	0.009%
50	8.314	2165	2169	2170	rBV2	236	158	0.02%	0.002%
51	8.343	2175	2178	2183	rBV2	139	137	0.02%	0.002%
52	8.466	2208	2216	2227	rVB3	1805	2744	0.31%	0.039%
53	8.572	2237	2249	2256	rBV7	5387	10942	1.25%	0.154%
54	8.633	2257	2268	2289	rVV	252599	436188	49.69%	6.153%
55	8.726	2289	2297	2313	rVB	84931	132607	15.11%	1.871%
56	8.835	2321	2331	2343	rVB2	7170	11382	1.30%	0.161%
57	8.916	2349	2356	2364	rVV3	931	1457	0.17%	0.021%
58	9.028	2388	2391	2396	rVB2	209	161	0.02%	0.002%
59	9.154	2424	2430	2431	rBV	254	235	0.03%	0.003%
60	9.211	2438	2448	2463	rBV	33387	51776	5.90%	0.730%
61	9.417	2499	2512	2536	rVV	360189	592000	67.44%	8.351%
62	9.652	2581	2585	2589	rVB2	222	180	0.02%	0.003%
63	9.694	2591	2598	2604	rBV3	1071	1366	0.16%	0.019%
64	10.073	2711	2716	2721	rVB4	481	470	0.05%	0.007%
65	10.096	2721	2723	2726	rBV	267	203	0.02%	0.003%
66	10.231	2761	2765	2767	rBV2	199	135	0.02%	0.002%
67	10.600	2876	2880	2884	rVB2	152	180	0.02%	0.003%
68	10.623	2885	2887	2892	rVB2	204	158	0.02%	0.002%
69	10.674	2894	2903	2911	rBV4	1929	2873	0.33%	0.041%
70	10.758	2915	2929	2948	rVB	286269	447463	50.98%	6.312%
71	10.832	2949	2952	2954	rBV	207	148	0.02%	0.002%
72	10.996	3001	3003	3007	rVB2	196	135	0.02%	0.002%
73	11.038	3011	3016	3017	rBV2	190	151	0.02%	0.002%
74	11.118	3039	3041	3043	rBV	296	158	0.02%	0.002%
75	11.459	3138	3147	3156	rBV4	1481	2534	0.29%	0.036%
76	11.571	3179	3182	3189	rVV2	167	237	0.03%	0.003%

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Stop Thrs : 0

Peak Location: TOP

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77	11.697	3215	3221	3226	rVB2	729	756	0.09%	0.011%
78	11.748	3235	3237	3242	rVB	206	136	0.02%	0.002%
79	11.813	3245	3257	3273	rVV	400789	627384	71.47%	8.850%
80	11.887	3277	3280	3282	rVB	353	208	0.02%	0.003%
81	11.925	3289	3292	3293	rBV2	297	192	0.02%	0.003%
82	11.944	3295	3298	3300	rVV2	831	629	0.07%	0.009%
83	11.973	3303	3307	3318	rVB4	1711	2032	0.23%	0.029%
84	12.195	3363	3376	3395	rVB	427661	685564	78.10%	9.671%
85	12.334	3413	3419	3423	rBV4	582	570	0.06%	0.008%
86	12.404	3437	3441	3443	rBV2	271	155	0.02%	0.002%
87	12.616	3503	3507	3509	rBV	264	170	0.02%	0.002%
88	13.305	3719	3721	3726	rBV	142	140	0.02%	0.002%
89	13.780	3866	3869	3872	rVB2	244	165	0.02%	0.002%
90	13.841	3886	3888	3892	rVB2	331	243	0.03%	0.003%
91	14.092	3960	3966	3975	rVB2	772	1190	0.14%	0.017%
92	14.382	4053	4056	4059	rBV	237	138	0.02%	0.002%
93	14.411	4061	4065	4066	rBV	287	161	0.02%	0.002%
94	14.491	4087	4090	4093	rBV3	274	169	0.02%	0.002%
95	14.575	4109	4116	4117	rBV	597	576	0.07%	0.008%
96	14.809	4187	4189	4191	rBV	237	152	0.02%	0.002%
97	14.999	4246	4248	4251	rBV2	281	176	0.02%	0.002%
98	15.153	4293	4296	4298	rBV	274	183	0.02%	0.003%
99	15.231	4311	4320	4328	rVB4	1316	2356	0.27%	0.033%
100	15.716	4469	4471	4476	rBV2	369	378	0.04%	0.005%

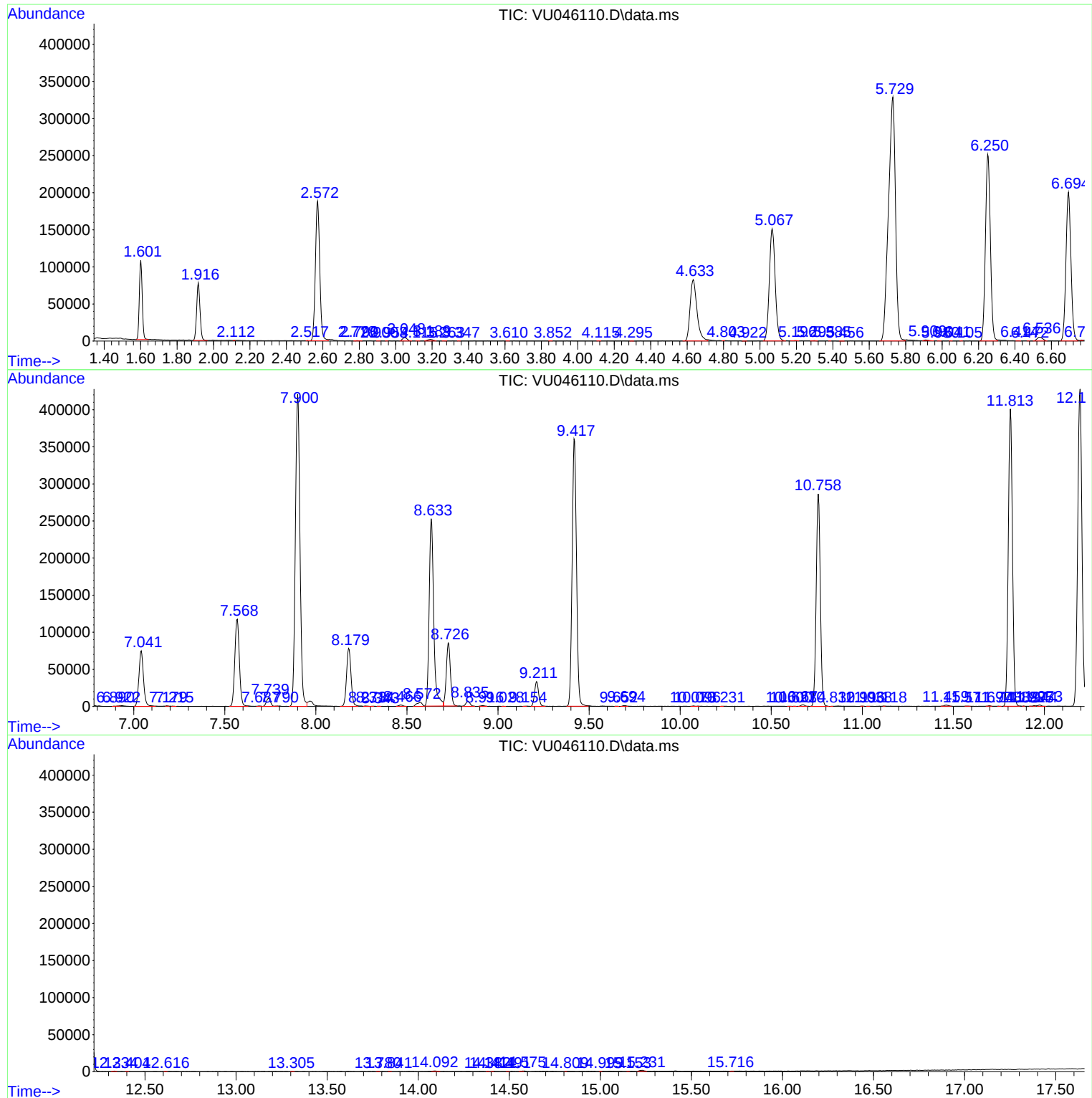
Sum of corrected areas: 7088718

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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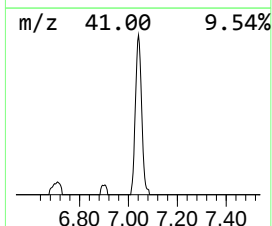
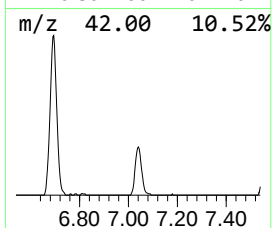
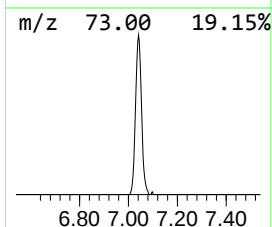
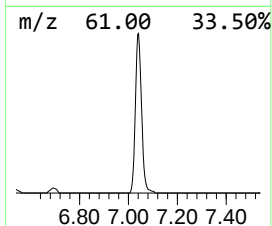
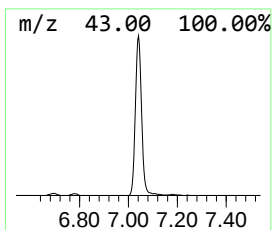
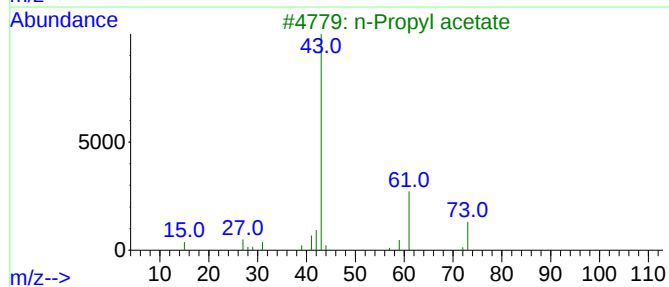
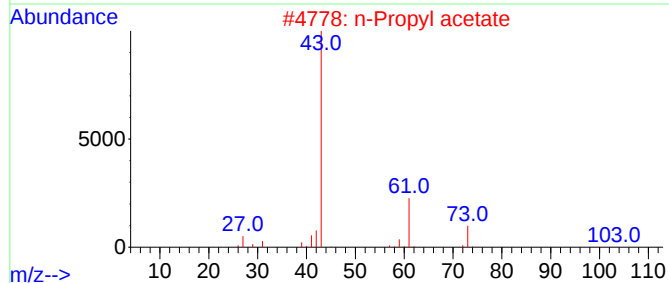
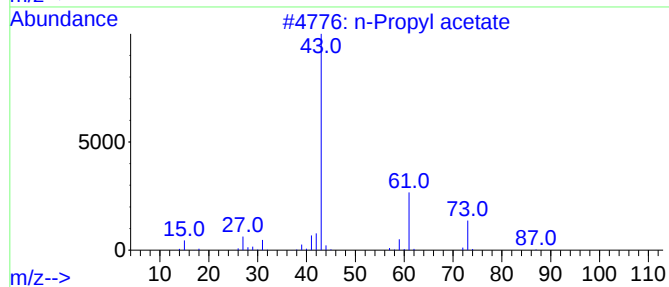
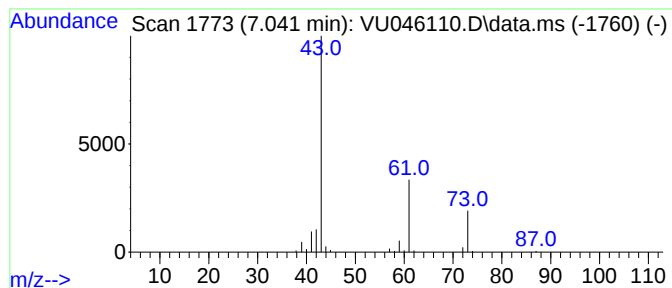
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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.
7.041	13.79 ug/L	130813	1,4-Difluorobenzene	6.250

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	72
5	Isopropyl acetate			102	C5H10O2	000108-21-4	28



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Instrument :
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ClientSampleId :
EX8D7

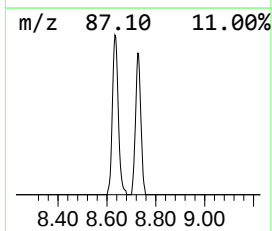
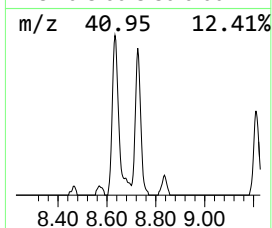
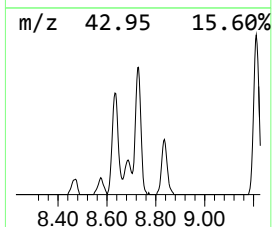
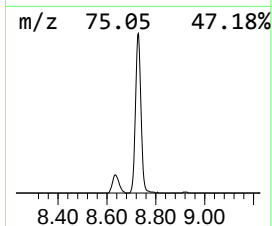
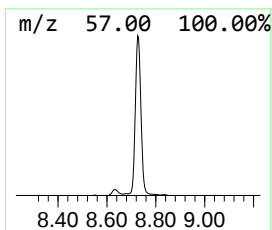
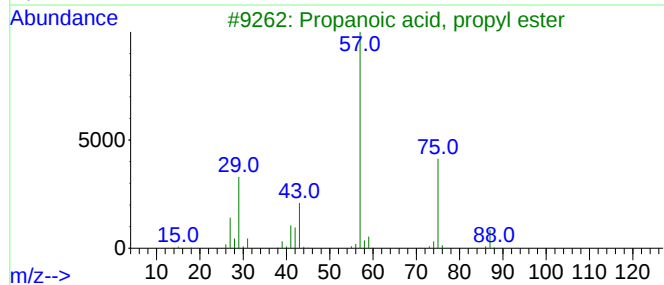
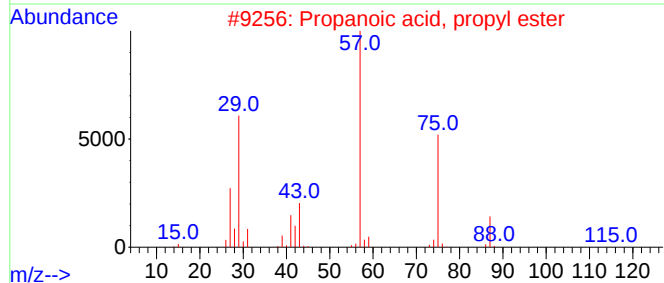
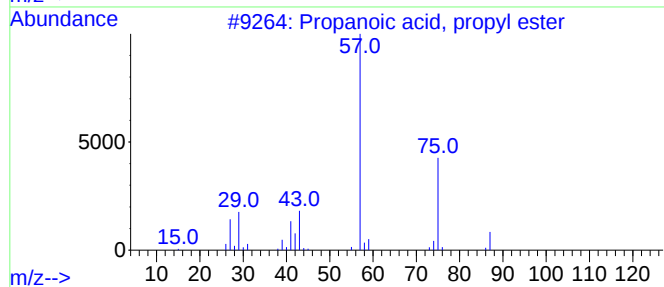
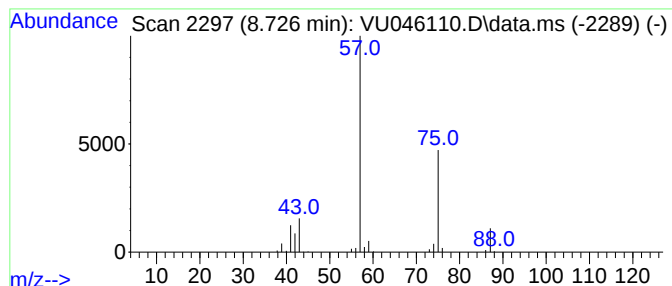
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	11.20 ug/L	132607	Chlorobenzene-d5	9.420

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	50
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	47
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	43



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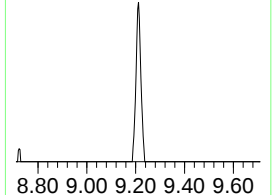
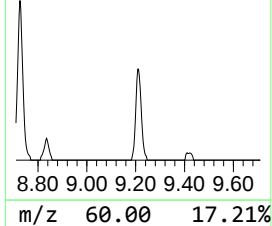
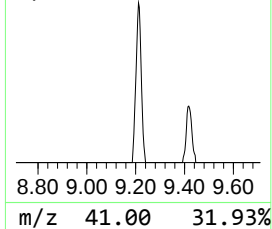
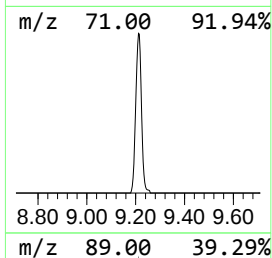
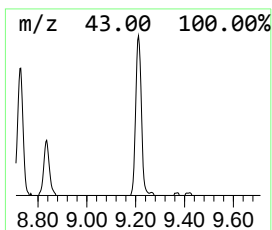
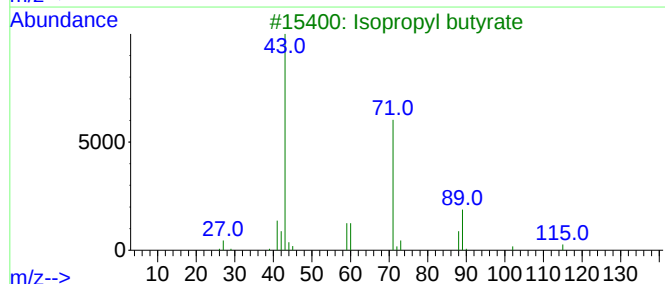
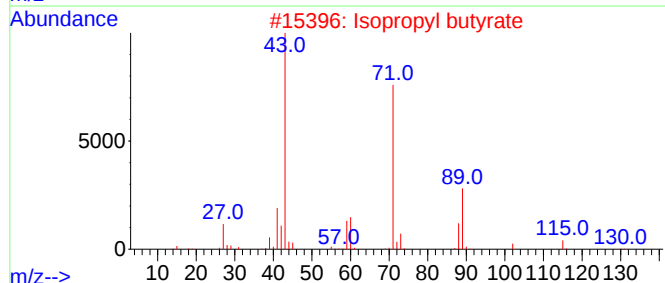
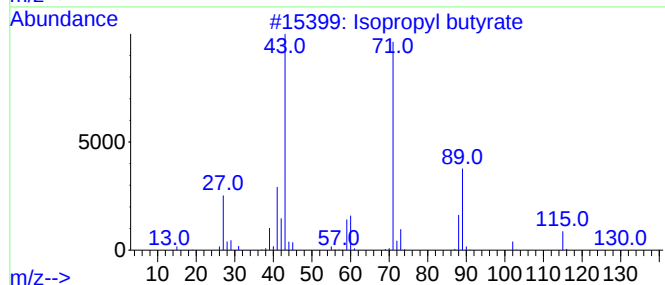
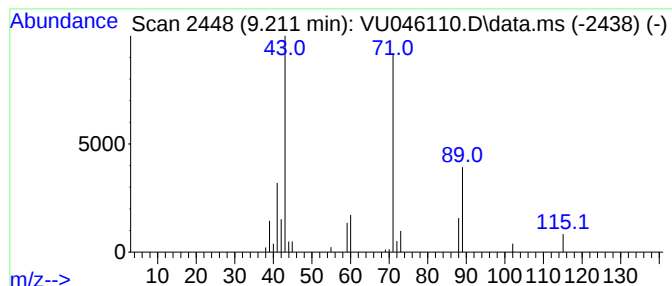
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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.
9.211	4.37 ug/L	51776	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
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_U\Data\VU120621\
Data File : VU046110.D
Acq On : 06 Dec 2021 14:34
Operator : SY/MD
Sample : M4938-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8D7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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	7.041	13.8	ug/L	130813	1	6.250	474386	50.0
Propanoic acid,...	8.726	11.2	ug/L	132607	2	9.420	592000	50.0
Isopropyl butyrate	9.211	4.4	ug/L	51776	2	9.420	592000	50.0