

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
 Data File : VU046118.D
 Acq On : 06 Dec 2021 17:57
 Operator : SY/MD
 Sample : M4938-08 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8E4

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: VU046118.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	73	81	92	rVB	93527	102390	13.11%	1.523%
2	1.916	171	179	191	rVB	68045	84786	10.85%	1.261%
3	2.141	247	249	252	rVB	424	217	0.03%	0.003%
4	2.379	319	323	327	rVB2	368	281	0.04%	0.004%
5	2.430	336	339	344	rVB	257	202	0.03%	0.003%
6	2.510	359	364	368	rBV3	287	368	0.05%	0.005%
7	2.571	371	383	400	rBV	165541	273609	35.02%	4.068%
8	2.797	446	453	461	rVV	734	1157	0.15%	0.017%
9	2.919	489	491	496	rVB2	286	208	0.03%	0.003%
10	3.051	523	532	541	rBV3	2617	4423	0.57%	0.066%
11	3.186	566	574	585	rVB2	959	2057	0.26%	0.031%
12	3.359	623	628	633	rBV2	450	335	0.04%	0.005%
13	3.838	773	777	783	rVB3	313	269	0.03%	0.004%
14	4.211	890	893	896	rBV	190	182	0.02%	0.003%
15	4.285	912	916	922	rBV	181	291	0.04%	0.004%
16	4.311	922	924	930	rVB	265	194	0.02%	0.003%
17	4.633	1008	1024	1050	rBV	73701	193518	24.77%	2.878%
18	4.883	1099	1102	1107	rVB3	312	258	0.03%	0.004%
19	4.977	1127	1131	1140	rVB	236	381	0.05%	0.006%
20	5.067	1140	1159	1180	rBV	133604	308777	39.52%	4.591%
21	5.288	1224	1228	1237	rVV2	384	623	0.08%	0.009%
22	5.427	1268	1271	1275	rVB2	234	186	0.02%	0.003%
23	5.581	1315	1319	1321	rBV	294	226	0.03%	0.003%
24	5.729	1339	1365	1386	rBV2	288894	781267	100.00%	11.617%
25	5.854	1402	1404	1410	rVB2	476	259	0.03%	0.004%
26	5.915	1414	1423	1433	rVB3	1462	2138	0.27%	0.032%
27	6.031	1453	1459	1461	rBV	398	338	0.04%	0.005%
28	6.092	1473	1478	1480	rBV	159	196	0.03%	0.003%
29	6.250	1513	1527	1559	rBV	242498	460356	58.92%	6.845%
30	6.436	1581	1585	1589	rBV3	220	226	0.03%	0.003%
31	6.533	1606	1615	1616	rBV2	3154	3700	0.47%	0.055%
32	6.694	1651	1665	1683	rBV	181981	348269	44.58%	5.179%
33	6.761	1683	1686	1687	rBV3	599	353	0.05%	0.005%
34	6.864	1709	1718	1720	rBV2	211	302	0.04%	0.004%
35	6.883	1720	1724	1726	rVV	256	217	0.03%	0.003%
36	6.938	1732	1741	1748	rVB3	842	1599	0.20%	0.024%

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 Title : VOC Analysis

37	7.041	1761	1773	1798	rBV	81423	140323	17.96%	2.087%
38	7.189	1812	1819	1824	rBV4	715	590	0.08%	0.009%
39	7.346	1864	1868	1875	rVB2	192	181	0.02%	0.003%
40	7.568	1920	1937	1960	rBV	104495	181491	23.23%	2.699%
41	7.697	1974	1977	1980	rBV2	308	219	0.03%	0.003%
42	7.742	1980	1991	2000	rBV2	13684	22805	2.92%	0.339%
43	7.899	2026	2040	2057	rBV	380160	652529	83.52%	9.703%
44	8.028	2076	2080	2087	rVB3	555	611	0.08%	0.009%
45	8.179	2114	2127	2142	rBV	70267	116941	14.97%	1.739%
46	8.288	2159	2161	2166	rVB3	305	235	0.03%	0.003%
47	8.320	2168	2171	2174	rBV	286	186	0.02%	0.003%
48	8.468	2208	2217	2225	rVB3	3179	4867	0.62%	0.072%
49	8.574	2236	2250	2257	rBV2	9038	13654	1.75%	0.203%
50	8.632	2257	2268	2288	rVV	234456	410232	52.51%	6.100%
51	8.729	2288	2298	2319	rVV	142125	227054	29.06%	3.376%
52	8.835	2323	2331	2340	rVB	9256	14211	1.82%	0.211%
53	8.915	2348	2356	2368	rVB3	1533	2638	0.34%	0.039%
54	9.041	2389	2395	2399	rBV2	216	229	0.03%	0.003%
55	9.211	2438	2448	2468	rVB	73340	111639	14.29%	1.660%
56	9.356	2490	2493	2496	rBV	297	216	0.03%	0.003%
57	9.420	2499	2513	2534	rBV	344986	574469	73.53%	8.542%
58	9.571	2553	2560	2567	rVB	902	1313	0.17%	0.020%
59	9.697	2590	2599	2607	rVB3	1727	2772	0.35%	0.041%
60	10.073	2709	2716	2722	rVV2	1558	2351	0.30%	0.035%
61	10.111	2724	2728	2736	rVB4	1035	1359	0.17%	0.020%
62	10.484	2840	2844	2850	rVV2	663	731	0.09%	0.011%
63	10.671	2894	2902	2909	rBV3	1916	2481	0.32%	0.037%
64	10.758	2917	2929	2946	rBV	256408	411394	52.66%	6.117%
65	10.925	2976	2981	2985	rVV2	299	289	0.04%	0.004%
66	11.092	3025	3033	3038	rBV	902	996	0.13%	0.015%
67	11.115	3038	3040	3048	rBV3	271	357	0.05%	0.005%
68	11.468	3138	3150	3161	rBV5	1875	3665	0.47%	0.054%
69	11.652	3202	3207	3211	rVV2	245	280	0.04%	0.004%
70	11.697	3214	3221	3228	rVB4	748	978	0.13%	0.015%
71	11.745	3231	3236	3243	rVB3	792	1010	0.13%	0.015%
72	11.812	3244	3257	3272	rBV	385313	604593	77.39%	8.990%
73	11.893	3278	3282	3284	rBV	399	216	0.03%	0.003%
74	11.944	3295	3298	3299	rBV2	349	191	0.02%	0.003%
75	11.973	3299	3307	3317	rVB6	1558	2303	0.29%	0.034%
76	12.098	3340	3346	3350	rBV2	463	470	0.06%	0.007%

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77	12.195	3361	3376	3391	rVV	388984	620676	79.44%	9.229%
78	12.333	3413	3419	3422	rVB2	692	688	0.09%	0.010%
79	12.372	3428	3431	3435	rBV2	274	195	0.02%	0.003%
80	12.404	3438	3441	3445	rBV	347	256	0.03%	0.004%
81	12.471	3459	3462	3468	rVB2	248	262	0.03%	0.004%
82	12.561	3486	3490	3498	rVB2	239	356	0.05%	0.005%
83	12.600	3498	3502	3507	rBV2	332	279	0.04%	0.004%
84	12.767	3551	3554	3561	rVB2	226	217	0.03%	0.003%
85	12.967	3612	3616	3618	rBV2	223	197	0.03%	0.003%
86	13.143	3666	3671	3676	rBV2	315	333	0.04%	0.005%
87	13.227	3690	3697	3701	rVB4	943	1079	0.14%	0.016%
88	13.844	3884	3889	3898	rBV4	1209	1392	0.18%	0.021%
89	14.089	3957	3965	3975	rVB	3285	4573	0.59%	0.068%
90	14.134	3975	3979	3985	rVB2	312	294	0.04%	0.004%
91	14.333	4035	4041	4049	rBV3	846	1343	0.17%	0.020%
92	14.577	4109	4117	4125	rVB3	980	1503	0.19%	0.022%
93	14.674	4144	4147	4152	rBV2	213	181	0.02%	0.003%
94	14.716	4157	4160	4165	rVB2	282	241	0.03%	0.004%
95	14.745	4165	4169	4171	rBV	312	233	0.03%	0.003%
96	14.841	4196	4199	4201	rBV	225	174	0.02%	0.003%
97	14.947	4227	4232	4236	rBV	367	415	0.05%	0.006%
98	15.227	4312	4319	4327	rVB4	1279	2073	0.27%	0.031%
99	15.407	4371	4375	4377	rBV2	590	476	0.06%	0.007%
100	16.735	4786	4788	4792	rBV3	685	459	0.06%	0.007%

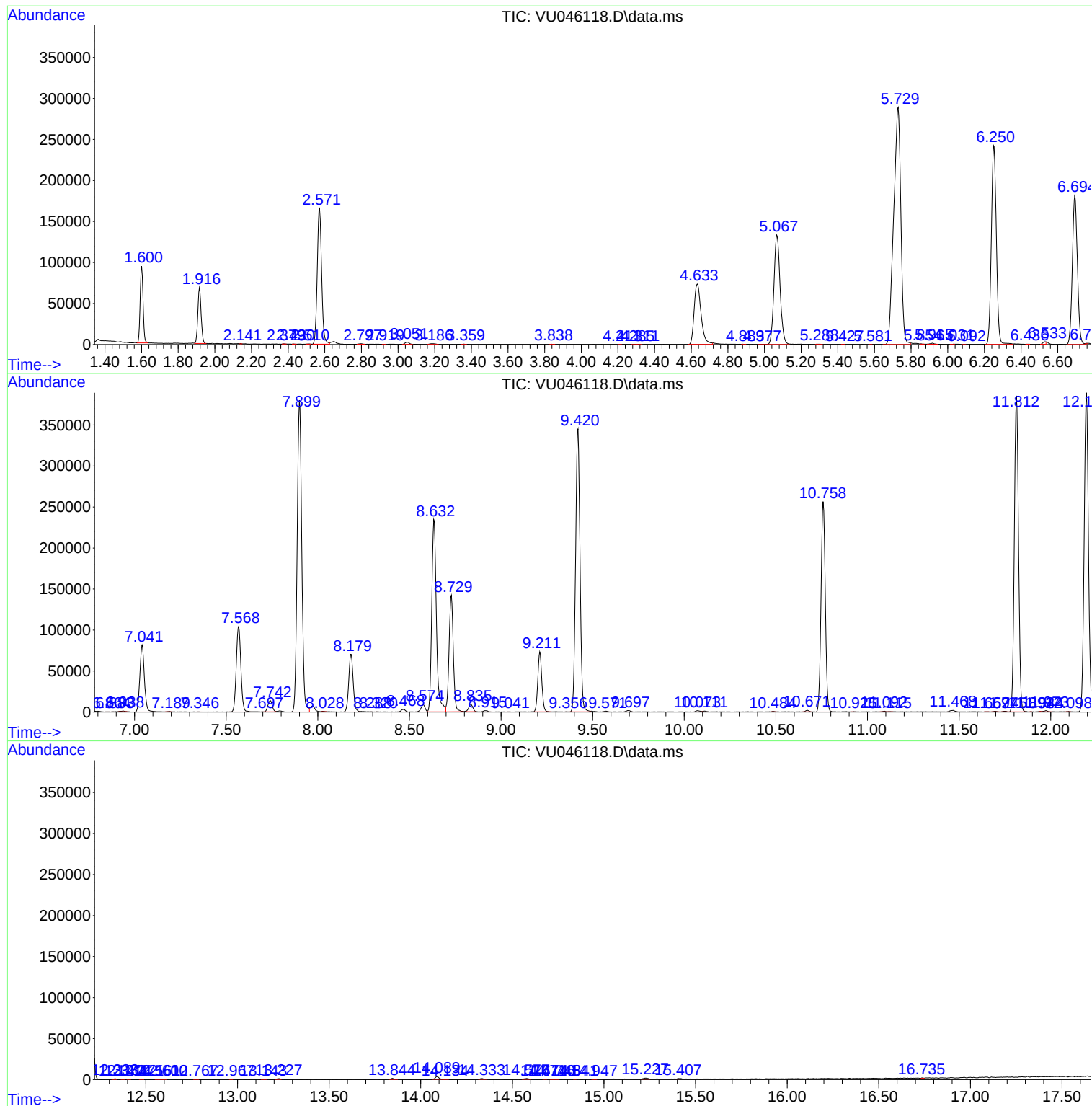
Sum of corrected areas: 6725122

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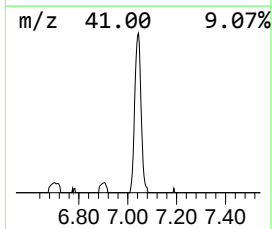
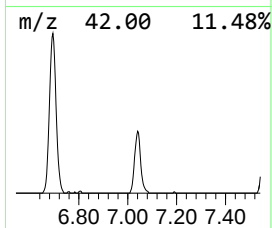
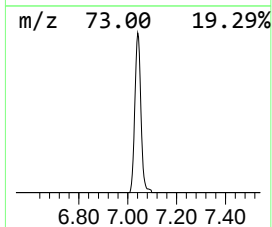
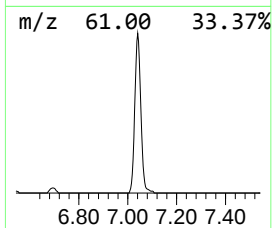
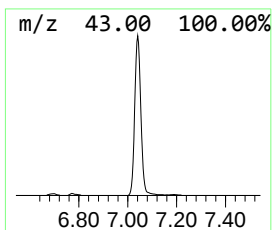
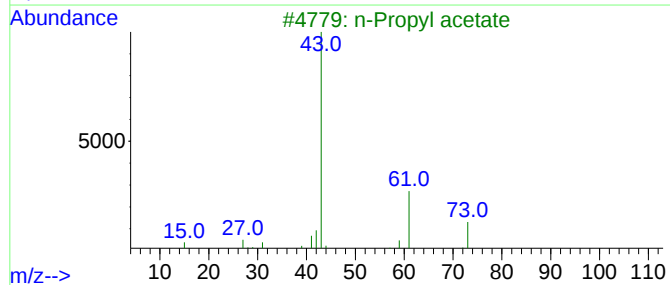
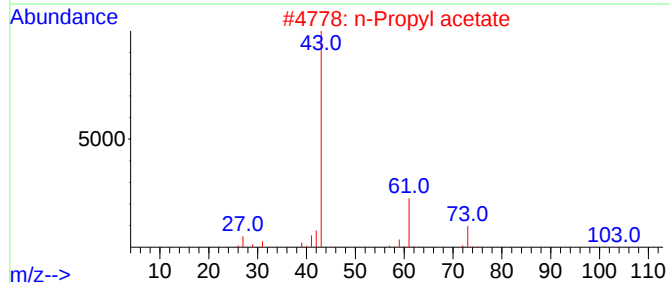
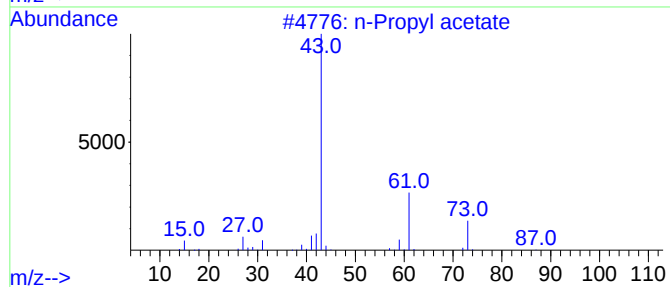
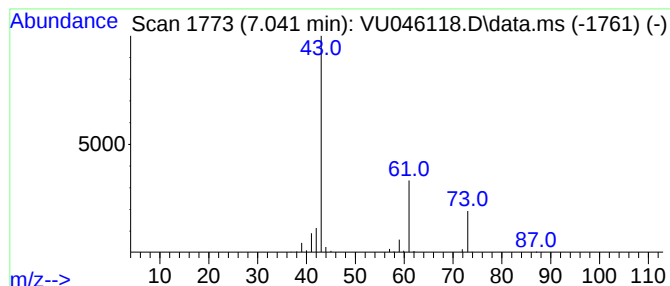
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	15.24 ug/L	140323	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	78
5	n-Propyl acetate			102	C5H10O2	000109-60-4	72



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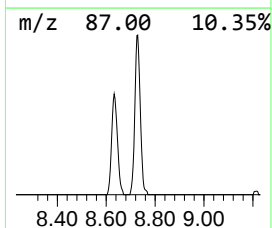
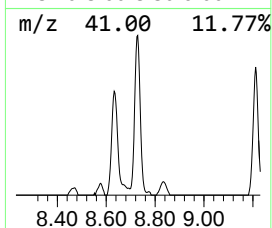
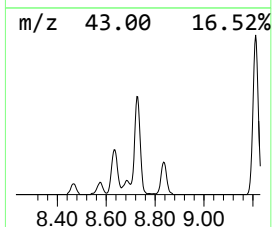
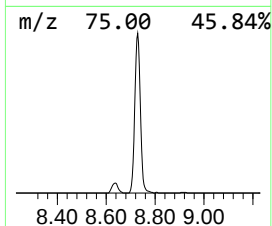
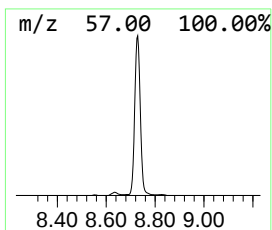
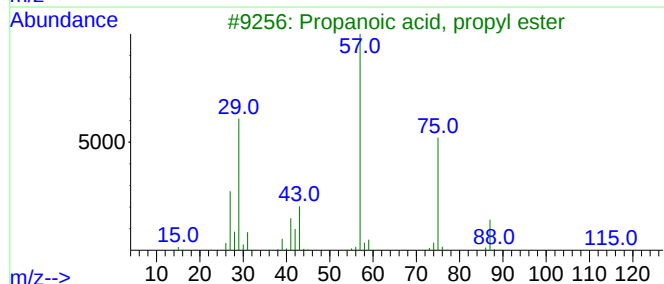
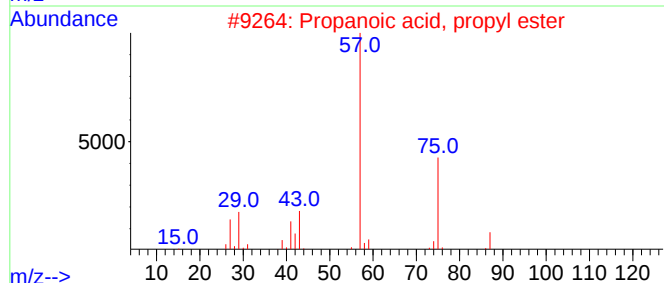
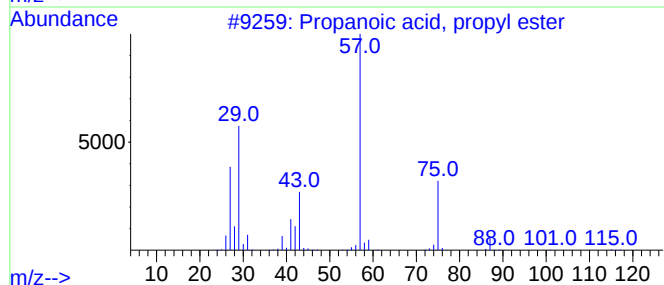
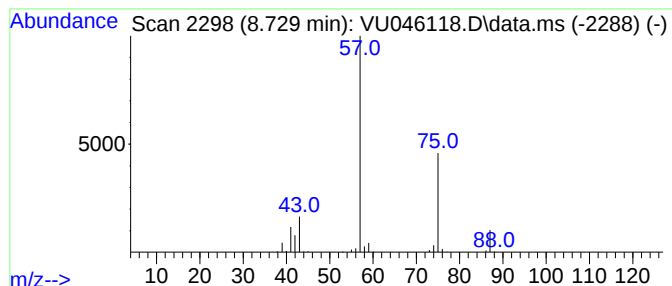
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	19.76 ug/L	227054	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	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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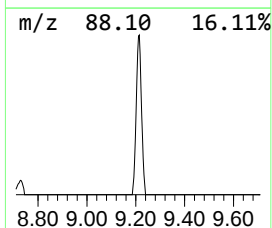
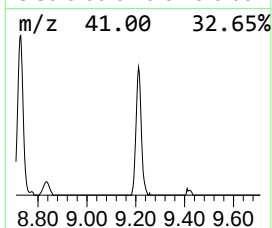
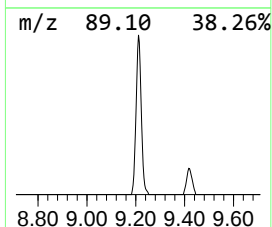
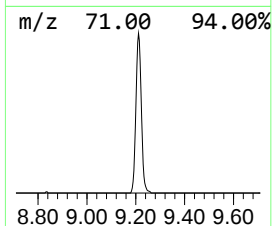
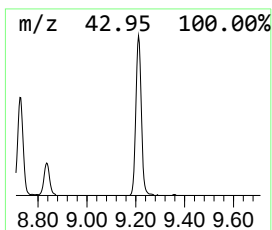
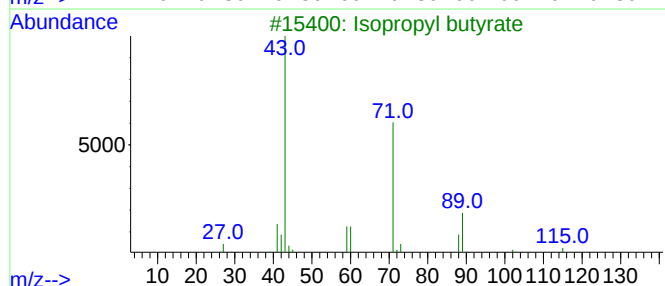
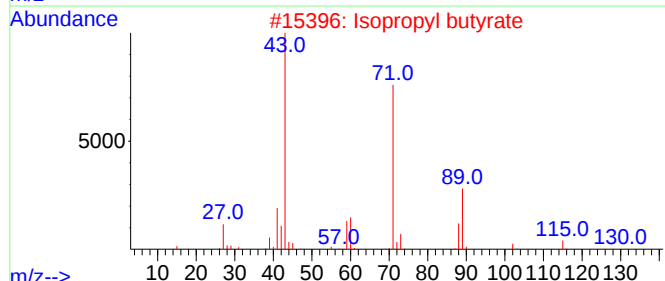
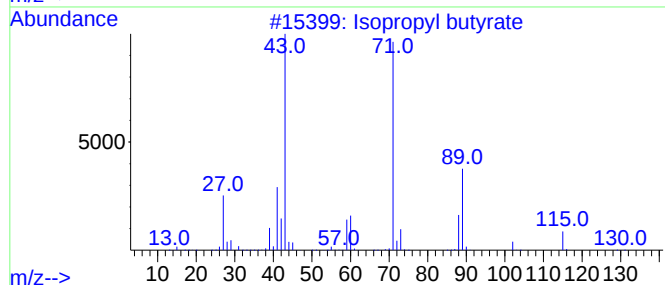
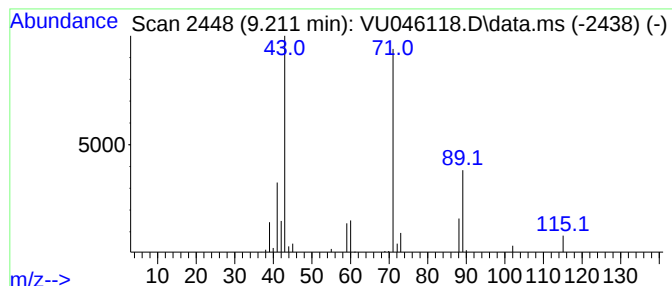
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Quant Title : VOC Analysis

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	9.72 ug/L	111639	Chlorobenzene-d5	9.420

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	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
Data File : VU046118.D
Acq On : 06 Dec 2021 17:57
Operator : SY/MD
Sample : M4938-08 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8E4

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	15.2	ug/L	140323	1	6.250	460356	50.0
Propanoic acid,...	8.729	19.8	ug/L	227054	2	9.420	574469	50.0
Isopropyl butyrate	9.211	9.7	ug/L	111639	2	9.420	574469	50.0