

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
 Data File : VU047233.D
 Acq On : 22 Feb 2022 15:51
 Operator : SY/MD
 Sample : PB142831TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB831

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\SFAMULM021022WMA.M
 Title : VOC Analysis

Signal : TIC: VU047233.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	105	rVB	194084	232342	15.79%	1.755%
2	1.919	171	180	197	rBV	159186	216973	14.74%	1.639%
3	2.575	371	384	417	rBV	329827	557906	37.91%	4.215%
4	2.794	449	452	454	rBV2	287	203	0.01%	0.002%
5	2.861	471	473	477	rVB3	279	173	0.01%	0.001%
6	2.890	477	482	484	rBV2	215	193	0.01%	0.001%
7	2.912	486	489	490	rBV3	286	133	0.01%	0.001%
8	2.951	498	501	502	rBV3	351	219	0.01%	0.002%
9	3.051	523	532	550	rVB2	4835	8521	0.58%	0.064%
10	3.189	566	575	582	rBV4	769	1297	0.09%	0.010%
11	3.263	593	598	603	rVB2	137	152	0.01%	0.001%
12	3.401	633	641	644	rBV3	369	451	0.03%	0.003%
13	3.437	649	652	658	rVB2	348	240	0.02%	0.002%
14	3.523	676	679	683	rBV2	191	170	0.01%	0.001%
15	3.572	691	694	696	rVB2	264	138	0.01%	0.001%
16	3.839	773	777	781	rVB2	580	477	0.03%	0.004%
17	3.880	786	790	793	rVB4	257	191	0.01%	0.001%
18	3.967	814	817	819	rVV2	253	135	0.01%	0.001%
19	4.035	836	838	843	rVB2	348	197	0.01%	0.001%
20	4.064	843	847	851	rVB2	165	157	0.01%	0.001%
21	4.089	851	855	860	rBV2	146	174	0.01%	0.001%
22	4.112	860	862	865	rBV3	246	162	0.01%	0.001%
23	4.150	872	874	880	rBV3	306	258	0.02%	0.002%
24	4.228	893	898	904	rVB3	204	278	0.02%	0.002%
25	4.256	904	907	910	rBV2	208	141	0.01%	0.001%
26	4.330	928	930	935	rVB2	233	180	0.01%	0.001%
27	4.372	941	943	947	rVB2	275	139	0.01%	0.001%
28	4.414	953	956	961	rVB3	263	217	0.01%	0.002%
29	4.485	972	978	982	rBV3	230	219	0.01%	0.002%
30	4.629	1007	1023	1055	rBV	153491	403069	27.39%	3.045%
31	4.874	1096	1099	1104	rVB2	342	252	0.02%	0.002%
32	5.002	1135	1139	1141	rBV2	194	171	0.01%	0.001%
33	5.067	1141	1159	1185	rBV	261477	572407	38.90%	4.325%
34	5.224	1206	1208	1211	rBV3	689	338	0.02%	0.003%
35	5.289	1224	1228	1235	rVB4	686	882	0.06%	0.007%
36	5.363	1249	1251	1257	rVB3	285	173	0.01%	0.001%

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 Title : VOC Analysis

37	5.472	1282	1285	1287	rVB3	465	263	0.02%	0.002%
38	5.504	1290	1295	1300	rVB3	156	187	0.01%	0.001%
39	5.536	1303	1305	1308	rVB2	293	189	0.01%	0.001%
40	5.626	1330	1333	1337	rVB2	219	176	0.01%	0.001%
41	5.729	1343	1365	1390	rBV2	557658	1471576	100.00%	11.119%
42	5.819	1390	1393	1397	rBV3	318	263	0.02%	0.002%
43	5.890	1411	1415	1416	rBV	392	223	0.02%	0.002%
44	5.916	1416	1423	1434	rVB3	2574	4245	0.29%	0.032%
45	5.961	1434	1437	1438	rBV2	334	169	0.01%	0.001%
46	6.047	1458	1464	1468	rVV3	541	604	0.04%	0.005%
47	6.109	1480	1483	1486	rBV3	327	311	0.02%	0.002%
48	6.128	1487	1489	1492	rVB3	261	128	0.01%	0.001%
49	6.250	1513	1527	1549	rBV	468195	889601	60.45%	6.721%
50	6.523	1610	1612	1616	rBV4	741	607	0.04%	0.005%
51	6.600	1634	1636	1640	rVB4	358	247	0.02%	0.002%
52	6.626	1640	1644	1646	rBV2	325	265	0.02%	0.002%
53	6.694	1649	1665	1683	rBV	341213	654571	44.48%	4.946%
54	6.777	1689	1691	1694	rBV2	619	304	0.02%	0.002%
55	6.809	1698	1701	1706	rVB3	1103	929	0.06%	0.007%
56	6.854	1713	1715	1718	rBV	195	130	0.01%	0.001%
57	7.041	1759	1773	1792	rBV	152811	267561	18.18%	2.022%
58	7.186	1808	1818	1827	rBV8	3019	5022	0.34%	0.038%
59	7.272	1841	1845	1849	rBV4	338	237	0.02%	0.002%
60	7.317	1853	1859	1862	rBV4	385	416	0.03%	0.003%
61	7.350	1867	1869	1873	rVB4	231	188	0.01%	0.001%
62	7.414	1887	1889	1893	rVB2	343	191	0.01%	0.001%
63	7.449	1893	1900	1902	rBV3	281	316	0.02%	0.002%
64	7.568	1923	1937	1955	rBV	213742	368021	25.01%	2.781%
65	7.687	1963	1974	1980	rBV7	1515	2681	0.18%	0.020%
66	7.739	1980	1990	2001	rVB	23126	36687	2.49%	0.277%
67	7.899	2025	2040	2055	rVV	742666	1268789	86.22%	9.586%
68	7.970	2056	2062	2075	rVB	11616	19215	1.31%	0.145%
69	8.063	2089	2091	2092	rBV3	291	146	0.01%	0.001%
70	8.079	2093	2096	2097	rVV2	328	179	0.01%	0.001%
71	8.182	2113	2128	2143	rBV	146737	252737	17.17%	1.910%
72	8.391	2189	2193	2195	rVB3	226	143	0.01%	0.001%
73	8.472	2205	2218	2231	rBV2	20994	38411	2.61%	0.290%
74	8.520	2231	2233	2236	rVV2	496	294	0.02%	0.002%
75	8.575	2236	2250	2257	rVV3	16414	27180	1.85%	0.205%
76	8.636	2257	2269	2286	rVV	549735	907490	61.67%	6.857%

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77	8.729	2287	2298	2315	rVB	249154	390996	26.57%	2.954%
78	8.835	2321	2331	2345	rVB	26255	41940	2.85%	0.317%
79	8.887	2345	2347	2350	rVB3	369	256	0.02%	0.002%
80	8.948	2364	2366	2369	rBV3	415	199	0.01%	0.002%
81	8.989	2374	2379	2381	rBV	275	207	0.01%	0.002%
82	9.044	2393	2396	2398	rVB	251	133	0.01%	0.001%
83	9.160	2429	2432	2437	rBV3	301	245	0.02%	0.002%
84	9.211	2437	2448	2462	rBV	147358	228139	15.50%	1.724%
85	9.417	2500	2512	2533	rVB	662221	1101363	74.84%	8.321%
86	10.073	2708	2716	2725	rBV3	6376	9704	0.66%	0.073%
87	10.671	2895	2902	2915	rVB2	7726	12049	0.82%	0.091%
88	10.758	2916	2929	2949	rBV	478934	757825	51.50%	5.726%
89	10.893	2959	2971	2988	rVB	16402	31441	2.14%	0.238%
90	11.115	3038	3040	3049	rVB5	1268	1167	0.08%	0.009%
91	11.198	3062	3066	3069	rBV4	800	877	0.06%	0.007%
92	11.462	3140	3148	3159	rVB5	6480	11284	0.77%	0.085%
93	11.700	3214	3222	3230	rVB6	3431	5146	0.35%	0.039%
94	11.812	3244	3257	3272	rBV	801753	1256019	85.35%	9.490%
95	12.195	3362	3376	3395	rVB	712591	1142946	77.67%	8.636%
96	12.327	3412	3417	3428	rVB5	2559	3517	0.24%	0.027%
97	12.636	3508	3513	3521	rVB5	1283	1857	0.13%	0.014%
98	12.774	3547	3556	3571	rVB2	9513	15554	1.06%	0.118%
99	13.144	3669	3671	3680	rVB3	1563	1891	0.13%	0.014%
100	13.468	3769	3772	3774	rBV2	438	298	0.02%	0.002%

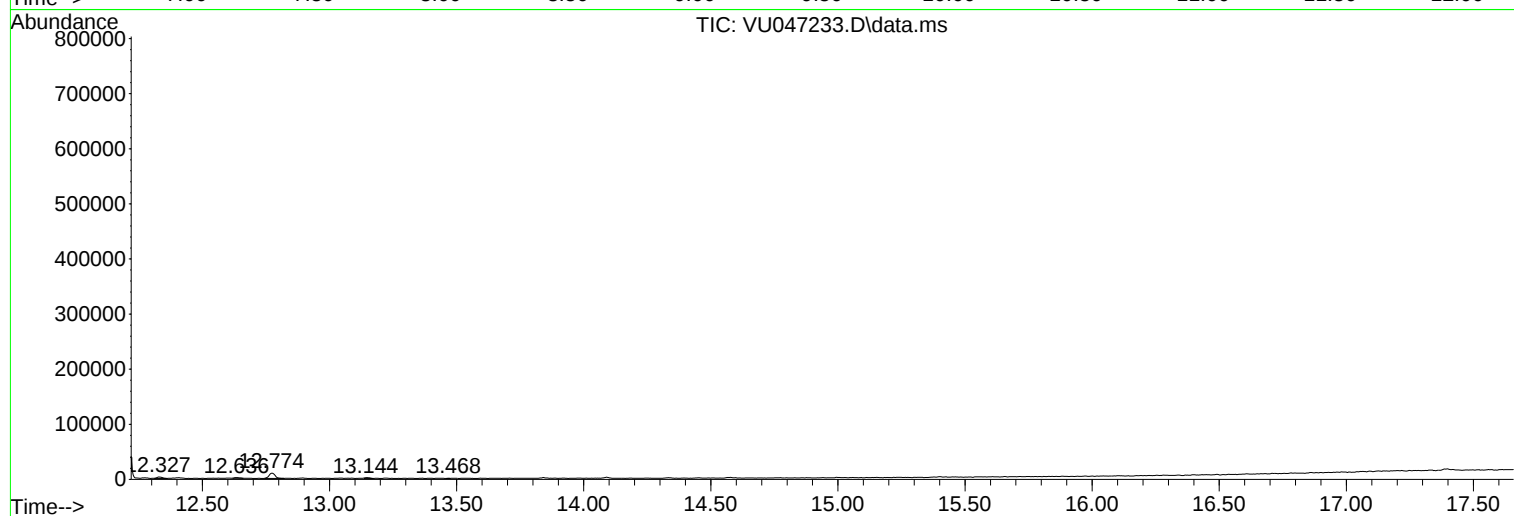
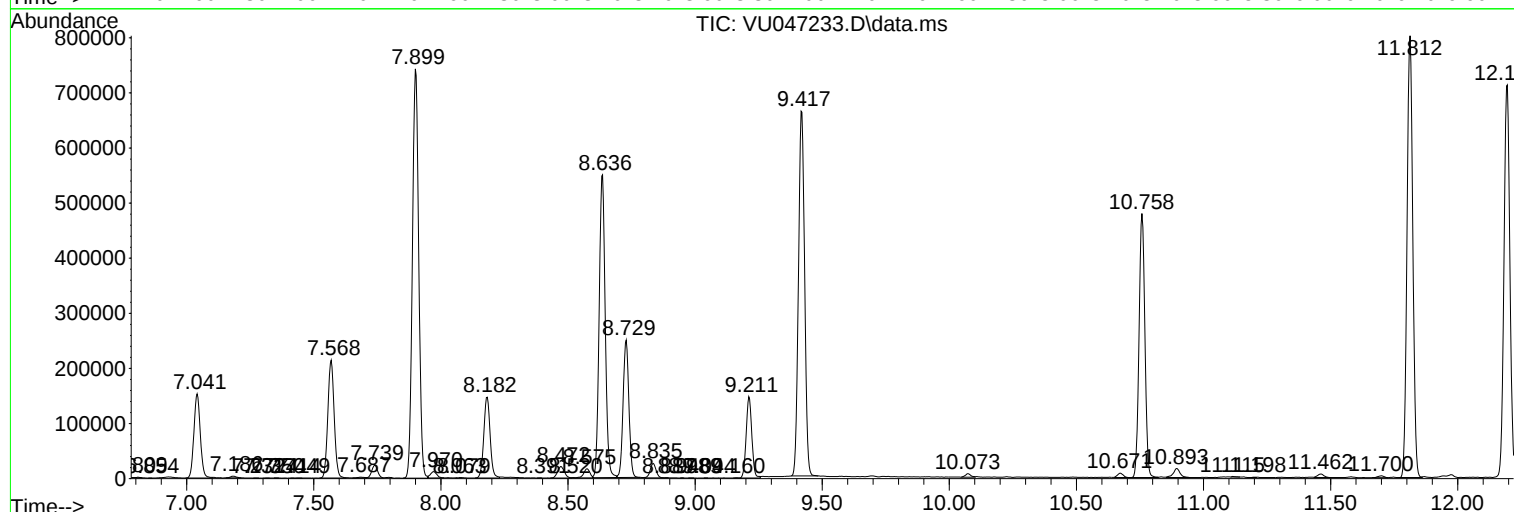
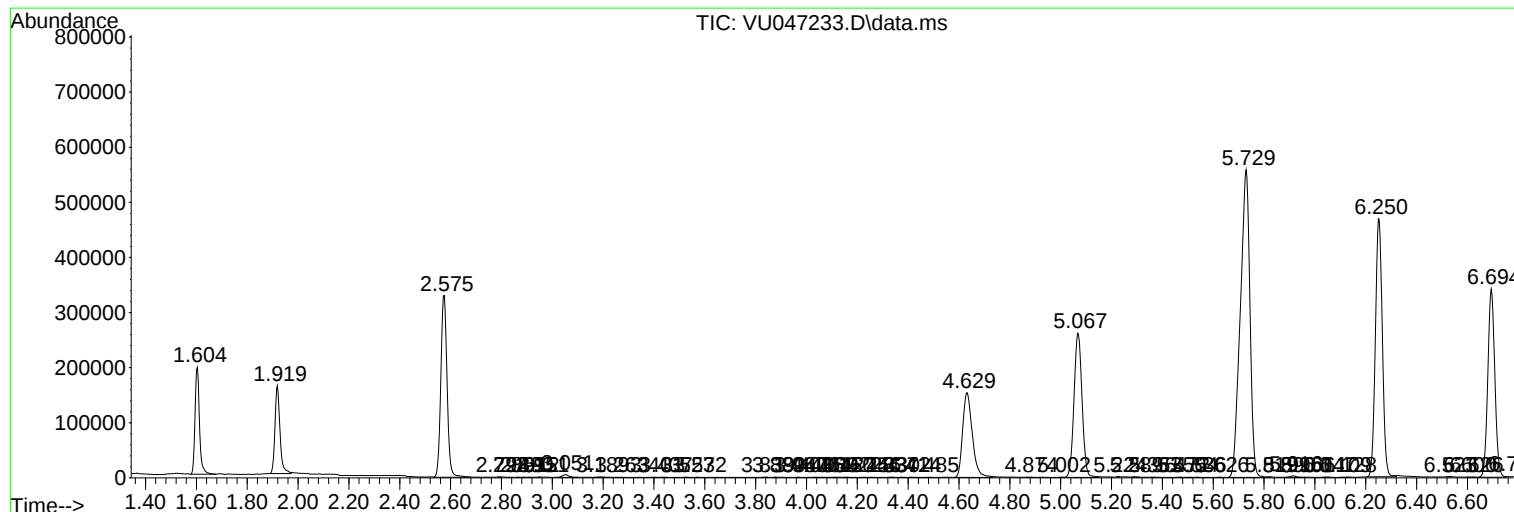
Sum of corrected areas: 13235273

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P



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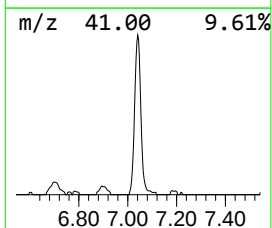
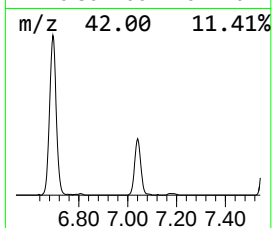
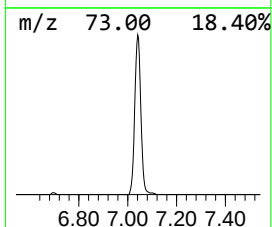
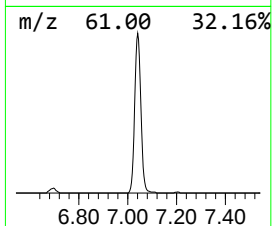
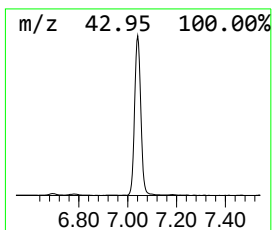
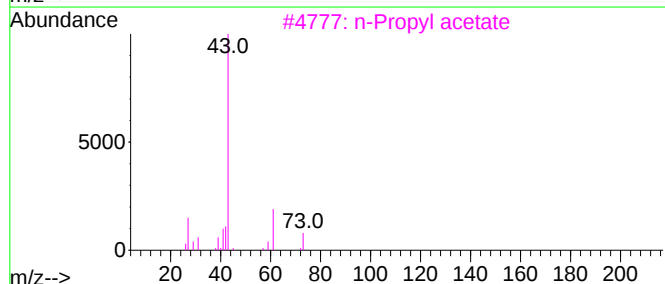
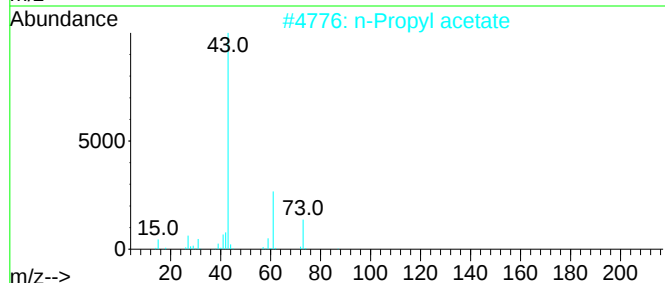
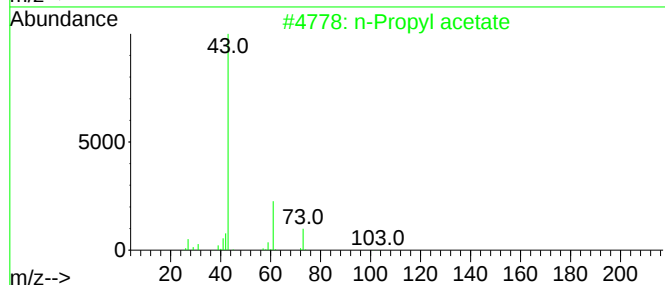
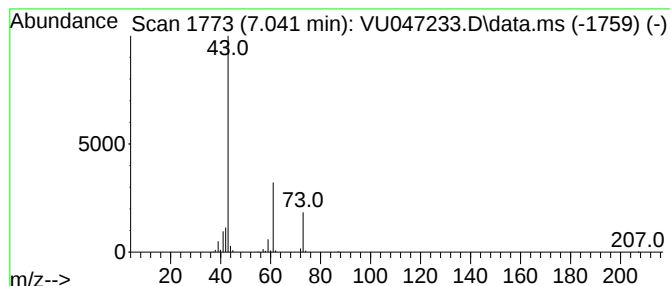
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

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	15.04 ug/L	267561	1,4-Difluorobenzene	6.253

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	50



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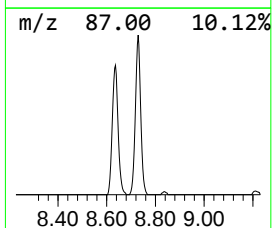
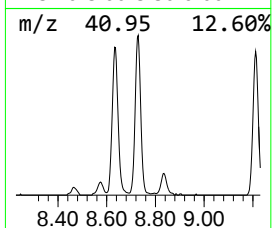
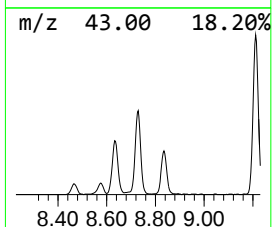
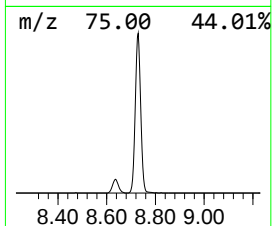
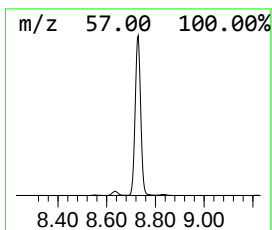
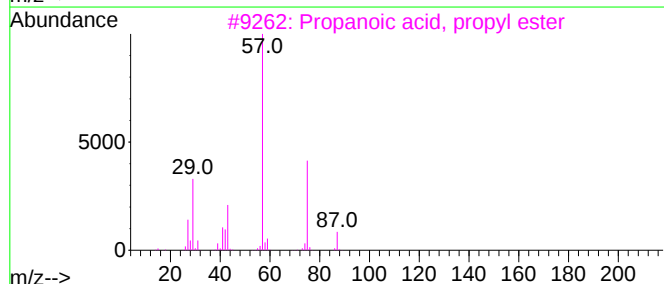
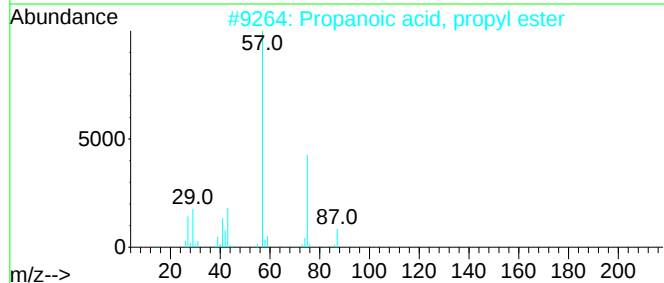
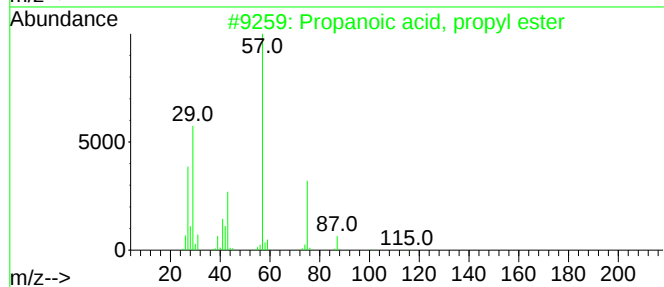
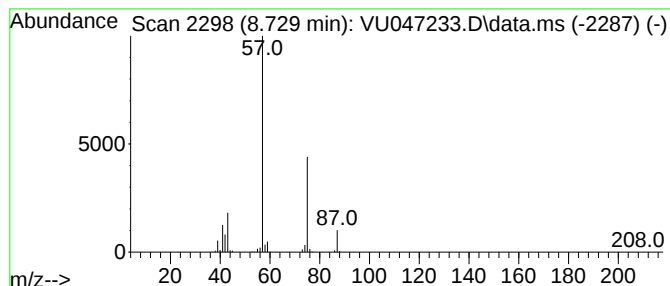
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

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.
8.729	17.75 ug/L	390996	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	72



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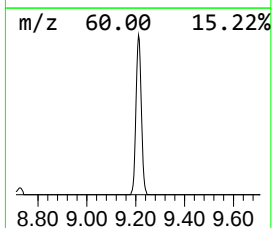
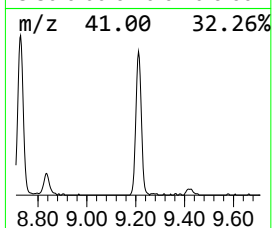
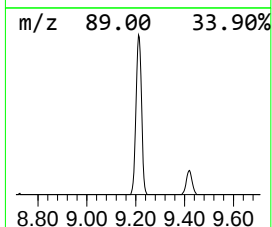
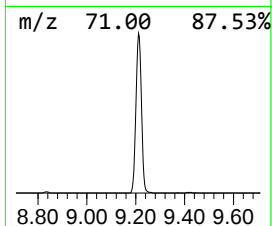
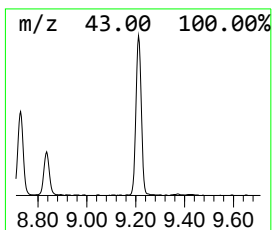
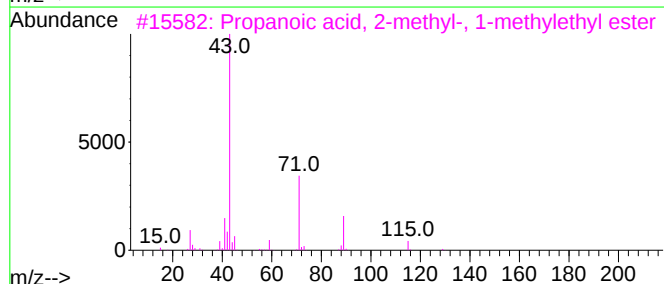
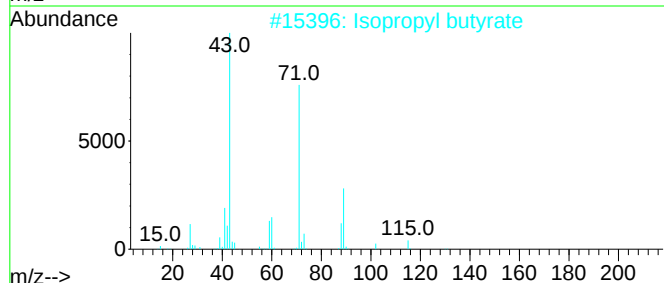
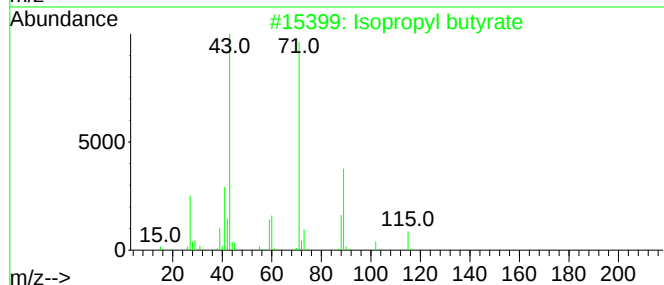
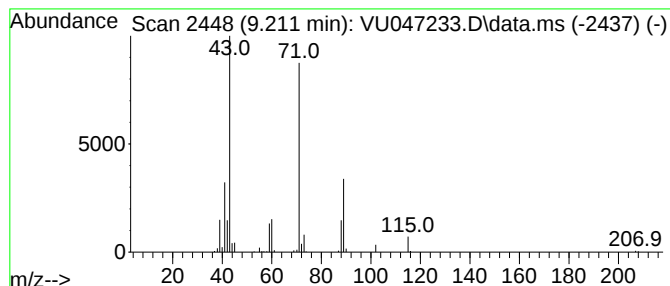
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

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	10.36 ug/L	228139	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			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
Data File : VU047233.D
Acq On : 22 Feb 2022 15:51
Operator : SY/MD
Sample : PB142831TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB831

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.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	15.0	ug/L	267561	1	6.253	889601	50.0
Propanoic acid,...	8.729	17.8	ug/L	390996	2	9.420	1101360	50.0
Isopropyl butyrate	9.211	10.4	ug/L	228139	2	9.420	1101360	50.0