

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046133.D
 Acq On : 07 Dec 2021 12:26
 Operator : SY/MD
 Sample : M4938-03 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

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: VU046133.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	74	81	97	rVB	133437	147291	15.39%	1.815%
2	1.919	171	180	196	rVB	91920	118635	12.39%	1.462%
3	2.572	371	383	424	rBV	215531	365484	38.18%	4.504%
4	2.777	443	447	449	rVV	150	134	0.01%	0.002%
5	2.803	449	455	458	rVB	405	460	0.05%	0.006%
6	2.948	497	500	503	rBV2	356	349	0.04%	0.004%
7	3.054	523	533	545	rVB2	3802	6524	0.68%	0.080%
8	3.189	562	575	588	rBV2	2297	4968	0.52%	0.061%
9	3.292	604	607	610	rVB	230	175	0.02%	0.002%
10	3.829	768	774	778	rBV3	545	617	0.06%	0.008%
11	4.079	848	852	854	rBV	249	197	0.02%	0.002%
12	4.176	875	882	884	rBV	176	254	0.03%	0.003%
13	4.279	910	914	920	rBV	192	299	0.03%	0.004%
14	4.401	950	952	958	rVB	167	186	0.02%	0.002%
15	4.449	963	967	973	rBV	185	274	0.03%	0.003%
16	4.571	1001	1005	1010	rBV	166	205	0.02%	0.003%
17	4.636	1010	1025	1066	rVV	81096	240434	25.12%	2.963%
18	4.932	1115	1117	1120	rBV2	276	199	0.02%	0.002%
19	4.951	1120	1123	1125	rVV2	220	135	0.01%	0.002%
20	4.967	1125	1128	1131	rVB	135	118	0.01%	0.001%
21	4.993	1134	1136	1139	rBV	161	129	0.01%	0.002%
22	5.067	1143	1159	1180	rBV	161386	366901	38.33%	4.521%
23	5.234	1209	1211	1216	rVV2	159	142	0.01%	0.002%
24	5.568	1309	1315	1320	rBV	230	317	0.03%	0.004%
25	5.616	1325	1330	1333	rBV	172	189	0.02%	0.002%
26	5.729	1343	1365	1387	rBV2	355613	957274	100.00%	11.796%
27	5.915	1416	1423	1434	rVB4	1725	3110	0.32%	0.038%
28	6.041	1458	1462	1463	rBV	230	164	0.02%	0.002%
29	6.121	1485	1487	1489	rVB	271	150	0.02%	0.002%
30	6.250	1512	1527	1546	rBV	268067	507807	53.05%	6.258%
31	6.533	1604	1615	1625	rBV5	4781	9200	0.96%	0.113%
32	6.613	1638	1640	1643	rBV	140	125	0.01%	0.002%
33	6.694	1650	1665	1681	rBV	214533	412056	43.04%	5.078%
34	6.896	1723	1728	1729	rBV2	229	171	0.02%	0.002%
35	6.928	1729	1738	1748	rVB5	1032	2314	0.24%	0.029%
36	7.041	1760	1773	1789	rBV	113234	198653	20.75%	2.448%

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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

37	7.182	1811	1817	1825	rVB4	942	1311	0.14%	0.016%
38	7.259	1839	1841	1845	rVB	273	197	0.02%	0.002%
39	7.468	1901	1906	1909	rBB	163	190	0.02%	0.002%
40	7.491	1909	1913	1917	rBV	192	251	0.03%	0.003%
41	7.568	1922	1937	1954	rBV	125663	219380	22.92%	2.703%
42	7.687	1970	1974	1978	rVB2	311	190	0.02%	0.002%
43	7.739	1980	1990	2002	rBV	16142	26269	2.74%	0.324%
44	7.793	2003	2007	2016	rVB3	962	1200	0.13%	0.015%
45	7.899	2026	2040	2055	rBV	463440	812124	84.84%	10.008%
46	8.118	2104	2108	2112	rBV	194	246	0.03%	0.003%
47	8.179	2113	2127	2147	rVV	86040	145645	15.21%	1.795%
48	8.465	2208	2216	2226	rVB2	3339	5097	0.53%	0.063%
49	8.571	2234	2249	2257	rBV4	13338	31604	3.30%	0.389%
50	8.632	2257	2268	2287	rVV	267580	482660	50.42%	5.948%
51	8.726	2288	2297	2319	rVV	180174	287250	30.01%	3.540%
52	8.835	2321	2331	2341	rVB	17429	26652	2.78%	0.328%
53	8.915	2349	2356	2371	rVB3	1066	1778	0.19%	0.022%
54	9.166	2428	2434	2437	rVB2	343	285	0.03%	0.004%
55	9.211	2437	2448	2468	rBV	87211	135072	14.11%	1.664%
56	9.365	2490	2496	2497	rBV2	201	192	0.02%	0.002%
57	9.417	2498	2512	2537	rVV	389735	642733	67.14%	7.920%
58	9.574	2555	2561	2565	rVB	552	578	0.06%	0.007%
59	9.642	2579	2582	2585	rBV	291	195	0.02%	0.002%
60	9.687	2590	2596	2598	rBV	694	672	0.07%	0.008%
61	9.957	2677	2680	2684	rBV	171	135	0.01%	0.002%
62	10.073	2709	2716	2724	rBV4	2387	3582	0.37%	0.044%
63	10.105	2724	2726	2730	rVB	355	245	0.03%	0.003%
64	10.478	2841	2842	2847	rVB	160	129	0.01%	0.002%
65	10.671	2894	2902	2910	rVB3	2800	3995	0.42%	0.049%
66	10.758	2916	2929	2947	rVB	302747	483750	50.53%	5.961%
67	10.867	2958	2963	2965	rBV	454	471	0.05%	0.006%
68	10.890	2968	2970	2976	rVB3	486	387	0.04%	0.005%
69	11.089	3027	3032	3035	rBV	239	255	0.03%	0.003%
70	11.118	3039	3041	3043	rVV	185	118	0.01%	0.001%
71	11.150	3049	3051	3061	rVB3	447	382	0.04%	0.005%
72	11.365	3116	3118	3122	rVB	238	123	0.01%	0.002%
73	11.455	3138	3146	3159	rVB2	2027	3497	0.37%	0.043%
74	11.571	3179	3182	3183	rBV2	300	169	0.02%	0.002%
75	11.697	3214	3221	3227	rBV4	1166	1599	0.17%	0.020%
76	11.812	3244	3257	3272	rBV	435850	683296	71.38%	8.420%

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Integrator: RTE
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 Sampling : 1 Min Area: 0 % of largest Peak
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 Stop Thrs : 0 Peak Location: TOP

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 Peak separation: 5

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

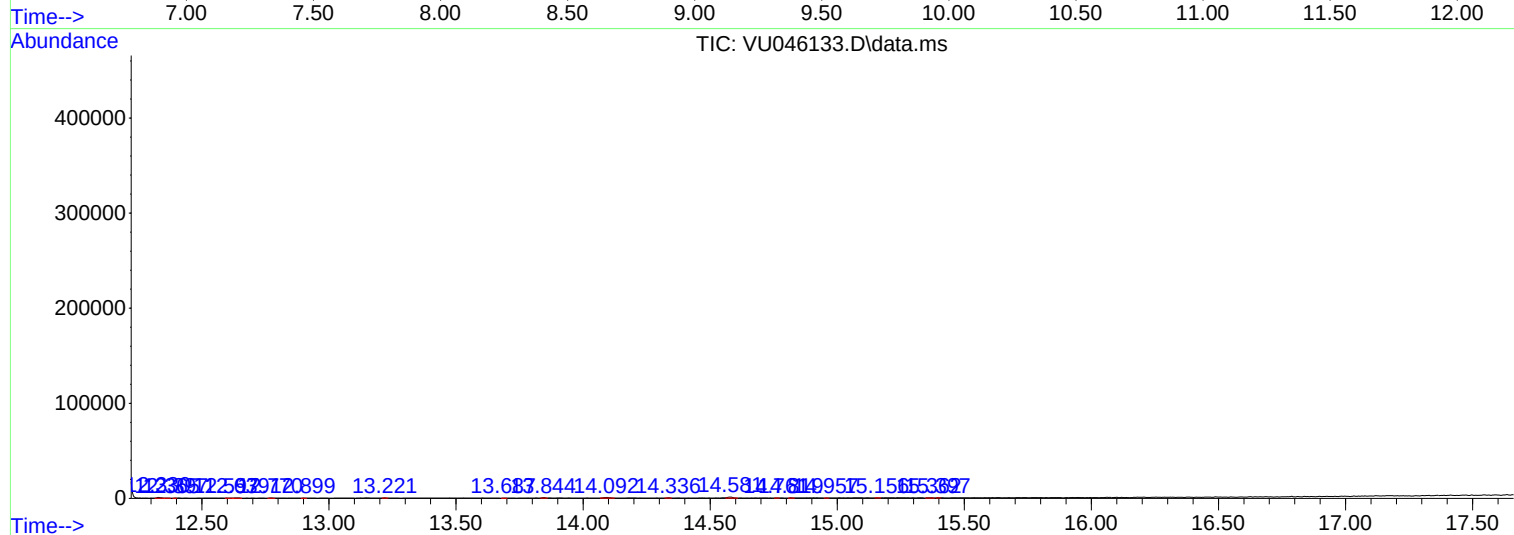
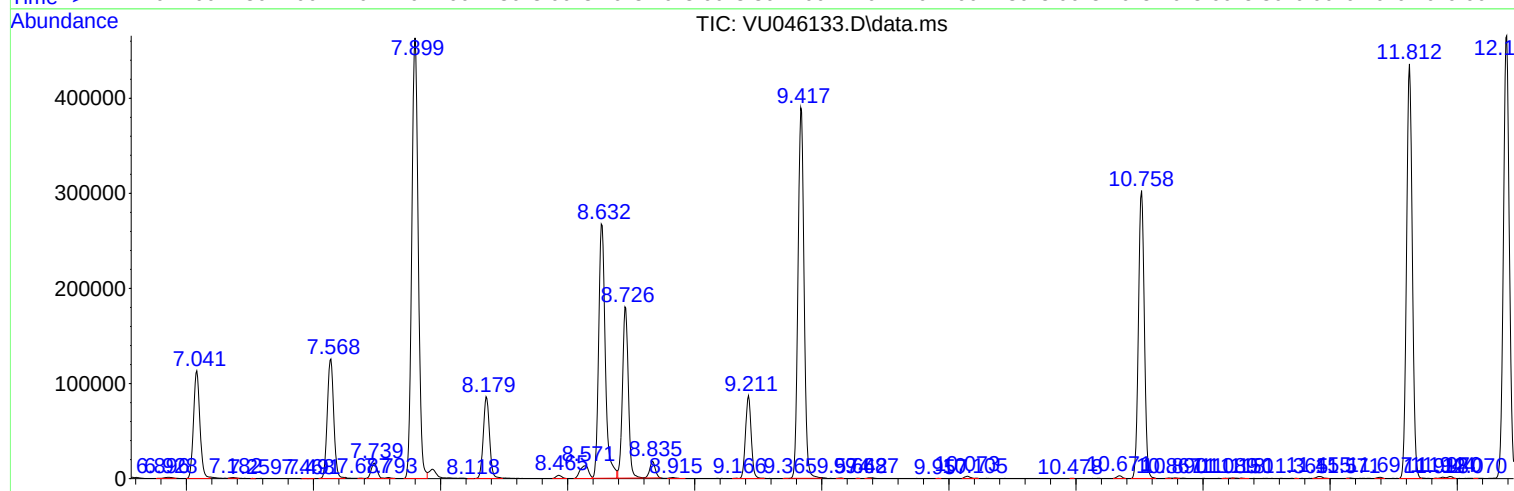
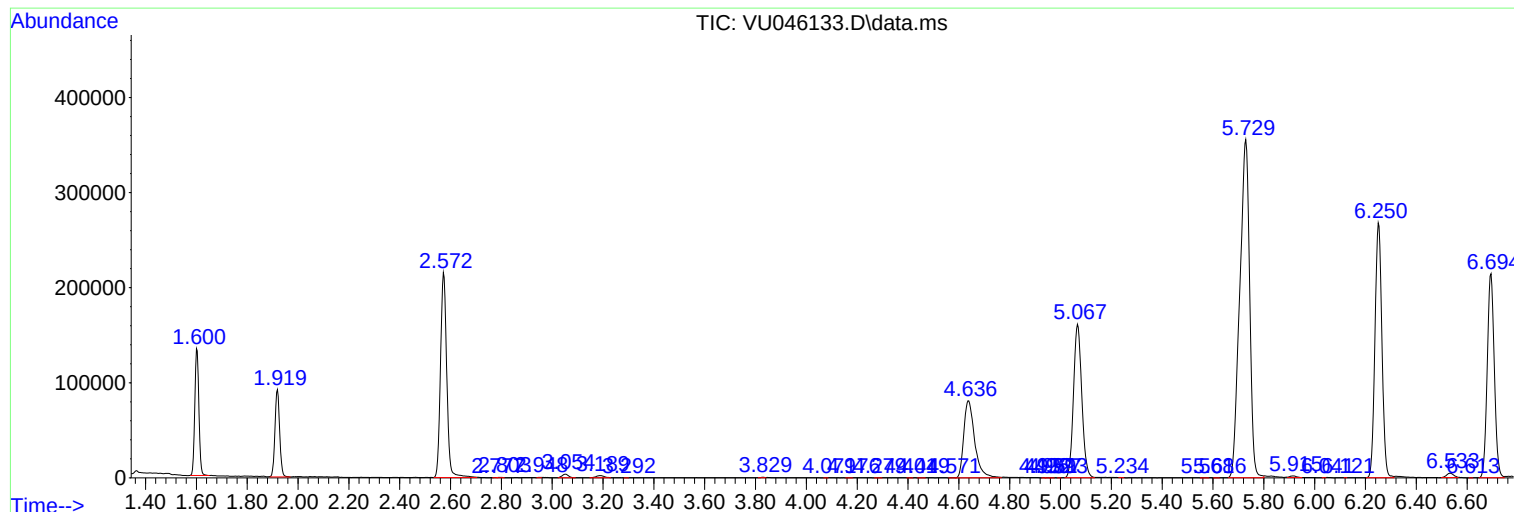
77	11.918	3286	3290	3292	rVV	286	245	0.03%	0.003%
78	11.944	3292	3298	3301	rVV3	1283	1531	0.16%	0.019%
79	11.970	3302	3306	3314	rVV3	2018	2614	0.27%	0.032%
80	12.070	3335	3337	3341	rBV2	123	122	0.01%	0.002%
81	12.195	3358	3376	3394	rBV	465451	753079	78.67%	9.280%
82	12.330	3413	3418	3425	rBV2	900	1010	0.11%	0.012%
83	12.365	3425	3429	3433	rVB2	170	139	0.01%	0.002%
84	12.397	3435	3439	3440	rBV	253	126	0.01%	0.002%
85	12.597	3499	3501	3509	rBV	200	207	0.02%	0.003%
86	12.639	3509	3514	3520	rVB3	389	517	0.05%	0.006%
87	12.770	3551	3555	3560	rBV	267	272	0.03%	0.003%
88	12.899	3592	3595	3599	rBV	240	132	0.01%	0.002%
89	13.221	3691	3695	3699	rVB2	348	244	0.03%	0.003%
90	13.687	3837	3840	3844	rBV	168	154	0.02%	0.002%
91	13.844	3885	3889	3894	rBV2	462	480	0.05%	0.006%
92	14.092	3958	3966	3976	rBV2	672	1167	0.12%	0.014%
93	14.336	4037	4042	4046	rBV2	353	356	0.04%	0.004%
94	14.581	4112	4118	4127	rVB3	1050	1572	0.16%	0.019%
95	14.761	4171	4174	4178	rBV2	240	182	0.02%	0.002%
96	14.819	4188	4192	4196	rBV2	266	310	0.03%	0.004%
97	14.957	4232	4235	4238	rBV2	151	122	0.01%	0.002%
98	15.156	4294	4297	4302	rBV	253	236	0.02%	0.003%
99	15.362	4356	4361	4367	rBV3	341	546	0.06%	0.007%
100	15.397	4369	4372	4375	rVV	301	171	0.02%	0.002%

Sum of corrected areas: 8115078

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ALS Vial : 7 Sample Multiplier: 1

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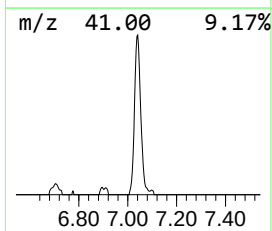
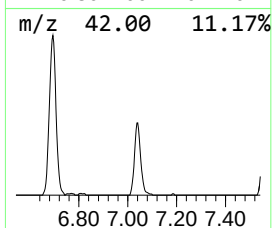
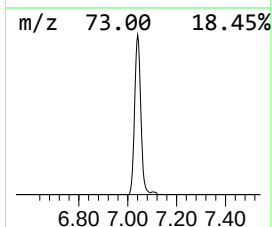
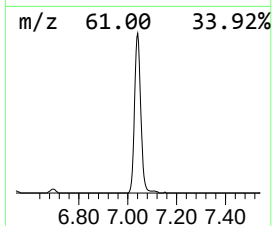
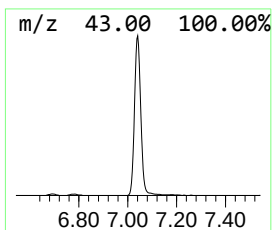
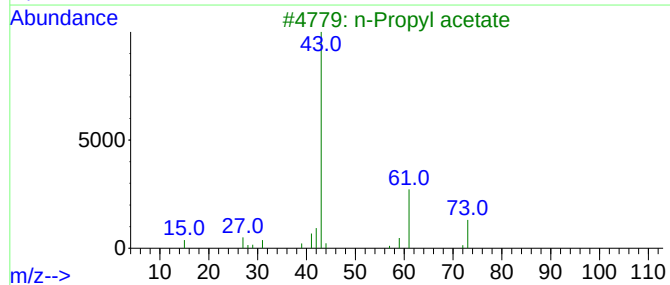
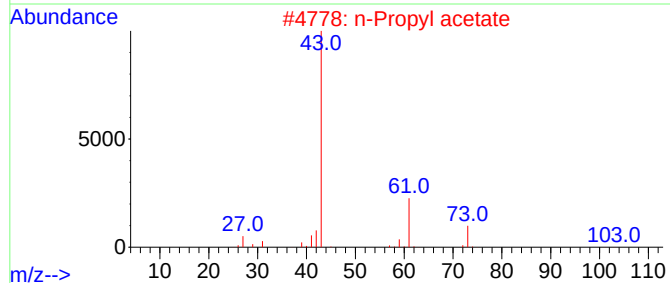
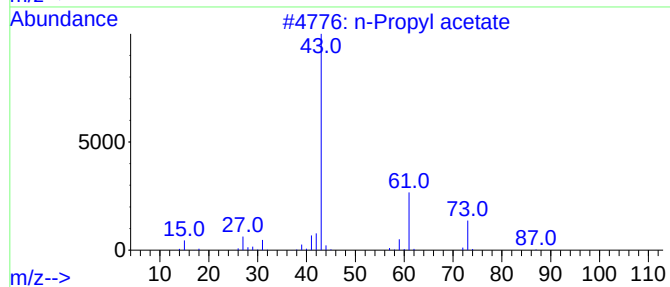
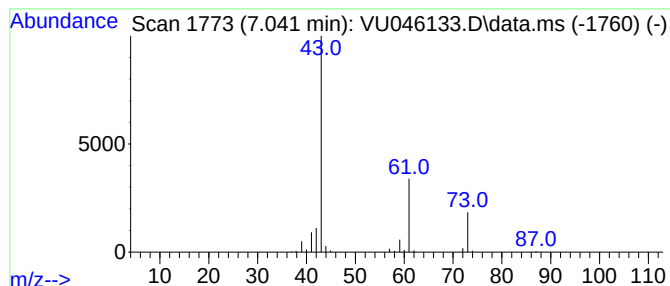
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	19.56 ug/L	198653	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	64
5	Isopropyl acetate			102	C5H10O2	000108-21-4	36



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

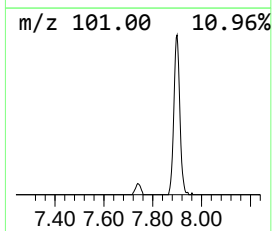
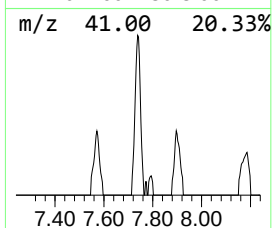
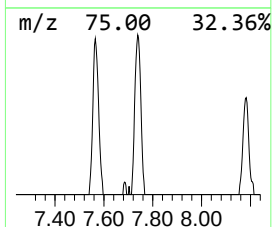
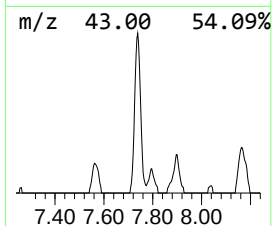
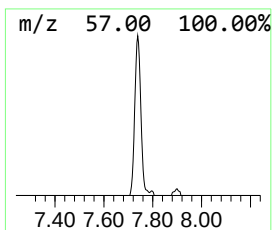
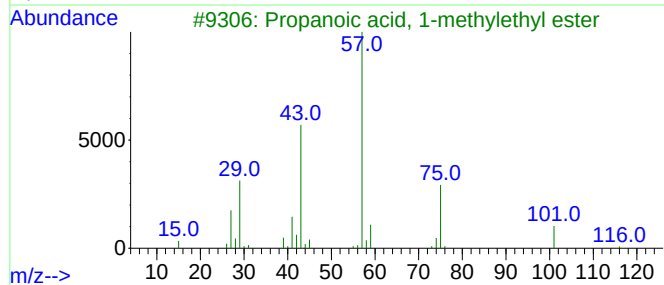
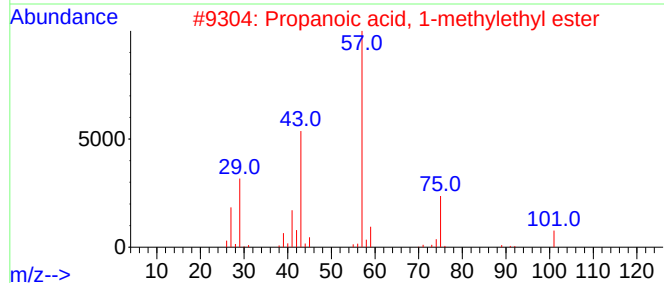
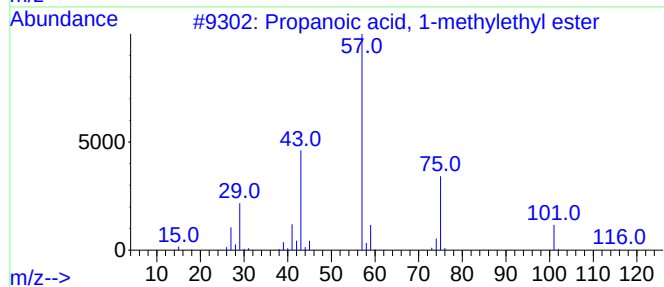
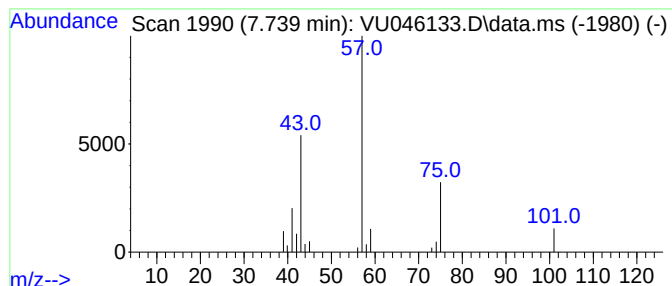
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	2.59 ug/L	26269	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59



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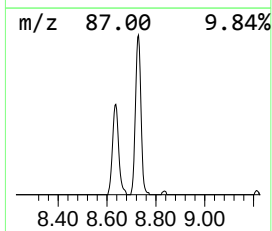
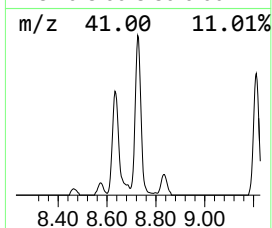
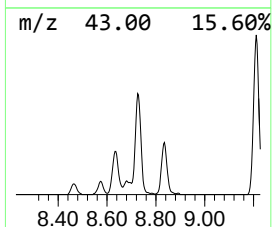
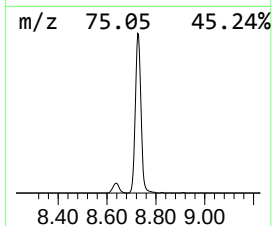
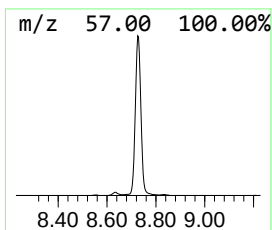
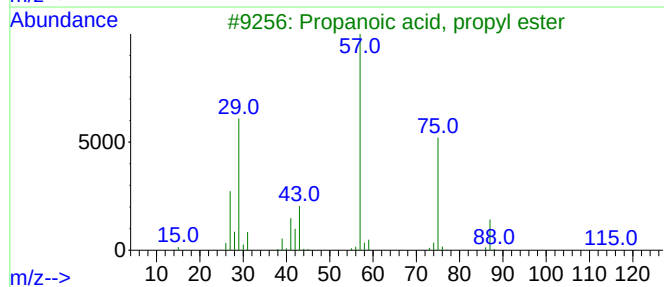
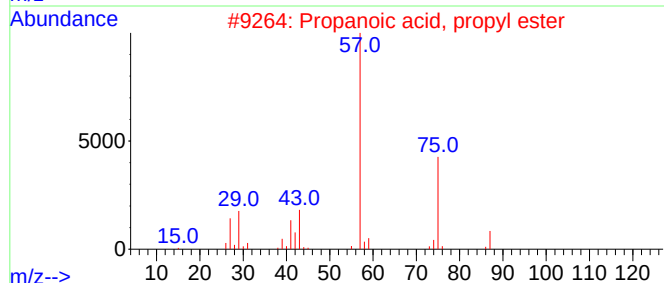
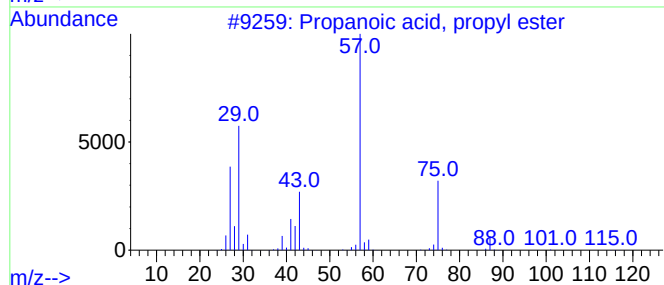
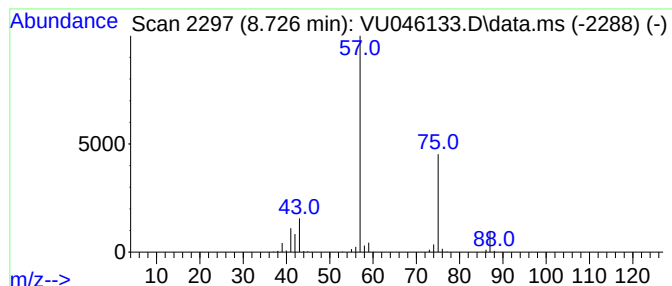
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	22.35 ug/L	287250	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	47



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Acq On : 07 Dec 2021 12:26
Operator : SY/MD
Sample : M4938-03 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

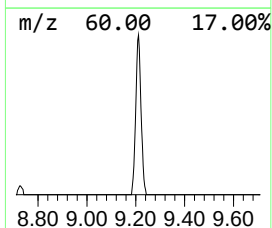
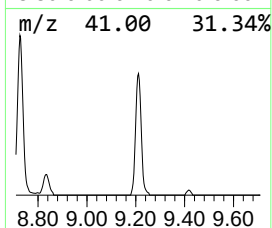
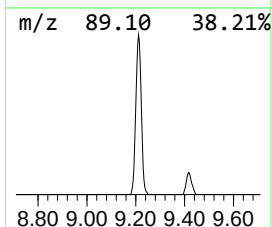
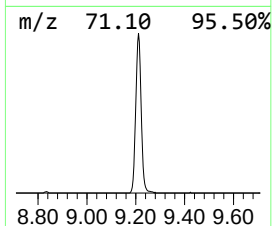
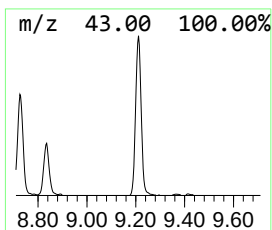
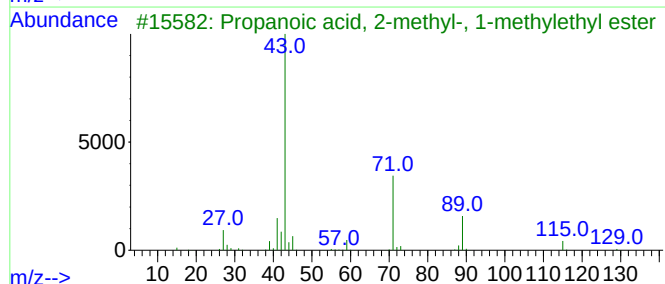
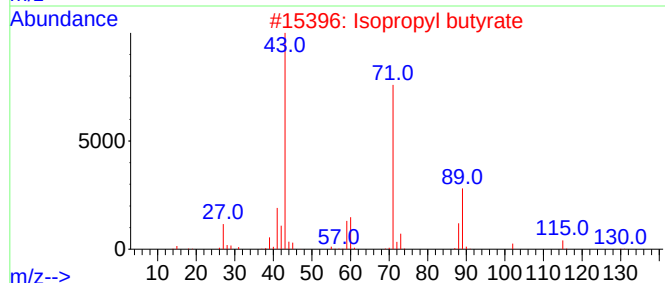
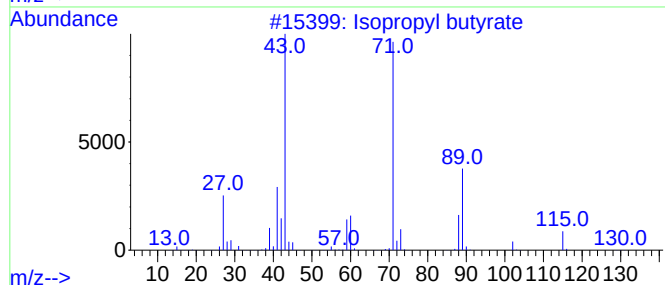
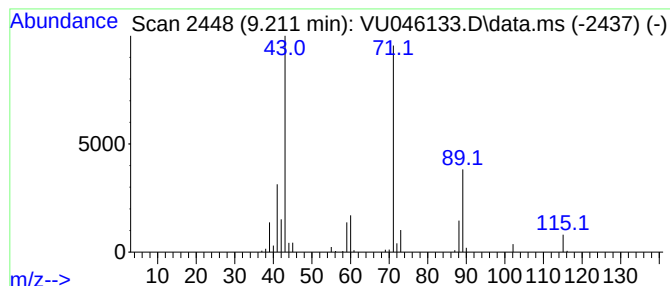
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Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	10.51 ug/L	135072	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	72
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046133.D
Acq On : 07 Dec 2021 12:26
Operator : SY/MD
Sample : M4938-03 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

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	19.6	ug/L	198653	1	6.250	507807	50.0
Propanoic acid,...	7.739	2.6	ug/L	26269	1	6.250	507807	50.0
Propanoic acid,...	8.726	22.4	ug/L	287250	2	9.420	642733	50.0
Isopropyl butyrate	9.211	10.5	ug/L	135072	2	9.420	642733	50.0