

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU122420\
 Data File : VU041799.D
 Acq On : 24 Dec 2020 10:06
 Operator : SY/MD
 Sample : PB133786TB 10X
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB001

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SFAMULM121620WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	75	82	93	rVB	194459	204513	17.02%	2.063%
2	1.919	172	180	194	rVB	170499	211844	17.63%	2.137%
3	2.578	373	385	402	rBV	321973	529587	44.08%	5.343%
4	2.841	464	467	468	rBV	281	176	0.01%	0.002%
5	2.886	479	481	486	rBV	222	117	0.01%	0.001%
6	3.022	518	523	527	rBV2	296	437	0.04%	0.004%
7	3.060	527	535	544	rVB	2614	4337	0.36%	0.044%
8	3.124	551	555	560	rBV2	224	272	0.02%	0.003%
9	3.308	610	612	614	rBV	190	107	0.01%	0.001%
10	3.587	694	699	703	rVB2	201	149	0.01%	0.002%
11	3.629	710	712	714	rBV2	200	117	0.01%	0.001%
12	3.642	714	716	719	rVB	245	118	0.01%	0.001%
13	3.671	720	725	728	rBV	311	294	0.02%	0.003%
14	3.732	739	744	749	rBV	305	381	0.03%	0.004%
15	3.845	776	779	781	rBV	193	161	0.01%	0.002%
16	3.919	800	802	805	rBB	168	102	0.01%	0.001%
17	3.970	816	818	819	rBV	243	98	0.01%	0.001%
18	4.009	824	830	834	rBB	192	254	0.02%	0.003%
19	4.124	864	866	869	rBB	204	129	0.01%	0.001%
20	4.147	870	873	876	rBV	136	116	0.01%	0.001%
21	4.192	884	887	889	rBV	206	164	0.01%	0.002%
22	4.227	895	898	900	rBV	139	119	0.01%	0.001%
23	4.343	931	934	936	rBV	190	168	0.01%	0.002%
24	4.433	960	962	966	rVB	340	220	0.02%	0.002%
25	4.456	967	969	971	rBV	149	101	0.01%	0.001%
26	4.472	971	974	977	rVB	192	110	0.01%	0.001%
27	4.542	992	996	999	rVV2	327	258	0.02%	0.003%
28	4.568	1002	1004	1007	rBV	130	117	0.01%	0.001%
29	4.642	1012	1027	1058	rBV	117828	297750	24.78%	3.004%
30	4.793	1072	1074	1076	rBV	294	158	0.01%	0.002%
31	4.874	1096	1099	1101	rBV2	293	232	0.02%	0.002%
32	4.960	1122	1126	1132	rBV	315	469	0.04%	0.005%
33	5.079	1146	1163	1187	rBV	220840	472681	39.34%	4.769%
34	5.205	1199	1202	1204	rBV2	391	274	0.02%	0.003%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU122420\
 Data File : VU041799.D
 Acq On : 24 Dec 2020 10:06
 Operator : SY/MD
 Sample : PB133786TB 10X
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB001

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SFAMULM121620WMA.M
 Title : VOC Analysis

35	5.356	1246	1249	1253	rBB	132	117	0.01%	0.001%
36	5.388	1253	1259	1262	rBV3	561	548	0.05%	0.006%
37	5.452	1277	1279	1283	rBV	184	179	0.01%	0.002%
38	5.484	1287	1289	1291	rBV	232	147	0.01%	0.001%
39	5.536	1303	1305	1308	rVB	300	169	0.01%	0.002%
40	5.591	1318	1322	1324	rBV	154	161	0.01%	0.002%
41	5.645	1336	1339	1342	rBB	169	133	0.01%	0.001%
42	5.738	1345	1368	1394	rBV2	456552	1201460	100.00%	12.121%
43	5.919	1417	1424	1427	rBV5	1797	1901	0.16%	0.019%
44	5.992	1442	1447	1454	rBV3	561	579	0.05%	0.006%
45	6.028	1454	1458	1462	rBV2	415	420	0.03%	0.004%
46	6.089	1475	1477	1480	rBV	240	101	0.01%	0.001%
47	6.147	1490	1495	1496	rBV3	823	710	0.06%	0.007%
48	6.259	1517	1530	1552	rBV	373070	706281	58.79%	7.126%
49	6.536	1607	1616	1626	rBV5	4713	8043	0.67%	0.081%
50	6.610	1634	1639	1643	rBV2	684	527	0.04%	0.005%
51	6.700	1653	1667	1685	rBV	271978	523008	43.53%	5.277%
52	6.873	1718	1721	1723	rBV	290	129	0.01%	0.001%
53	6.899	1726	1729	1730	rBV	321	202	0.02%	0.002%
54	7.047	1763	1775	1795	rBV	98227	172901	14.39%	1.744%
55	7.185	1815	1818	1828	rVB6	1300	1778	0.15%	0.018%
56	7.275	1843	1846	1851	rBV	323	223	0.02%	0.002%
57	7.346	1865	1868	1873	rVB	213	224	0.02%	0.002%
58	7.385	1877	1880	1882	rBV	264	200	0.02%	0.002%
59	7.500	1913	1916	1921	rBB	192	200	0.02%	0.002%
60	7.571	1923	1938	1961	rVV	156751	275666	22.94%	2.781%
61	7.745	1982	1992	2003	rBV2	16205	25260	2.10%	0.255%
62	7.832	2017	2019	2021	rBV	198	103	0.01%	0.001%
63	7.902	2027	2041	2069	rBV	564815	978963	81.48%	9.877%
64	8.182	2115	2128	2146	rBV	109207	189610	15.78%	1.913%
65	8.343	2173	2178	2183	rVB2	422	487	0.04%	0.005%
66	8.465	2209	2216	2217	rBV	3818	3196	0.27%	0.032%
67	8.578	2236	2251	2258	rBV3	11303	17667	1.47%	0.178%
68	8.635	2258	2269	2288	rVV	390435	660877	55.01%	6.667%
69	8.729	2289	2298	2312	rVB	179671	278556	23.18%	2.810%
70	8.835	2324	2331	2344	rVB	17805	27267	2.27%	0.275%
71	9.121	2418	2420	2422	rBV2	178	109	0.01%	0.001%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU122420\
 Data File : VU041799.D
 Acq On : 24 Dec 2020 10:06
 Operator : SY/MD
 Sample : PB133786TB 10X
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB001

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SFAMULM121620WMA.M
 Title : VOC Analysis

72	9.172	2431	2436	2437	rBV2	300	241	0.02%	0.002%
73	9.211	2438	2448	2469	rVB	97060	151745	12.63%	1.531%
74	9.340	2485	2488	2490	rBV2	224	136	0.01%	0.001%
75	9.417	2499	2512	2535	rBV	517932	846393	70.45%	8.539%
76	9.603	2567	2570	2575	rVB2	243	203	0.02%	0.002%
77	9.693	2593	2598	2601	rBV3	488	458	0.04%	0.005%
78	9.828	2638	2640	2643	rBV	145	111	0.01%	0.001%
79	10.073	2709	2716	2724	rBV5	3529	4900	0.41%	0.049%
80	10.172	2744	2747	2749	rBV	170	111	0.01%	0.001%
81	10.613	2882	2884	2887	rBV	321	156	0.01%	0.002%
82	10.754	2916	2928	2946	rVB	386002	619553	51.57%	6.251%
83	11.375	3118	3121	3125	rVB	202	133	0.01%	0.001%
84	11.462	3144	3148	3149	rBV2	241	167	0.01%	0.002%
85	11.532	3167	3170	3174	rBV2	228	223	0.02%	0.002%
86	11.713	3223	3226	3229	rBV2	281	189	0.02%	0.002%
87	11.738	3232	3234	3240	rVB2	510	491	0.04%	0.005%
88	11.809	3243	3256	3271	rBV	431977	682321	56.79%	6.884%
89	11.918	3287	3290	3292	rBV	332	149	0.01%	0.002%
90	12.060	3329	3334	3337	rBV	424	336	0.03%	0.003%
91	12.076	3337	3339	3342	rVB	297	139	0.01%	0.001%
92	12.188	3361	3374	3389	rBV	489430	793343	66.03%	8.004%
93	12.378	3430	3433	3436	rVB	281	179	0.01%	0.002%
94	13.208	3686	3691	3700	rBV3	705	934	0.08%	0.009%
95	13.828	3881	3884	3891	rVB3	964	972	0.08%	0.010%
96	14.044	3948	3951	3953	rBV	265	125	0.01%	0.001%
97	14.079	3953	3962	3969	rBV3	1404	2367	0.20%	0.024%
98	14.249	4013	4015	4017	rBV	329	118	0.01%	0.001%
99	14.317	4033	4036	4045	rVB5	1301	1311	0.11%	0.013%
100	14.426	4068	4070	4073	rBV2	466	268	0.02%	0.003%

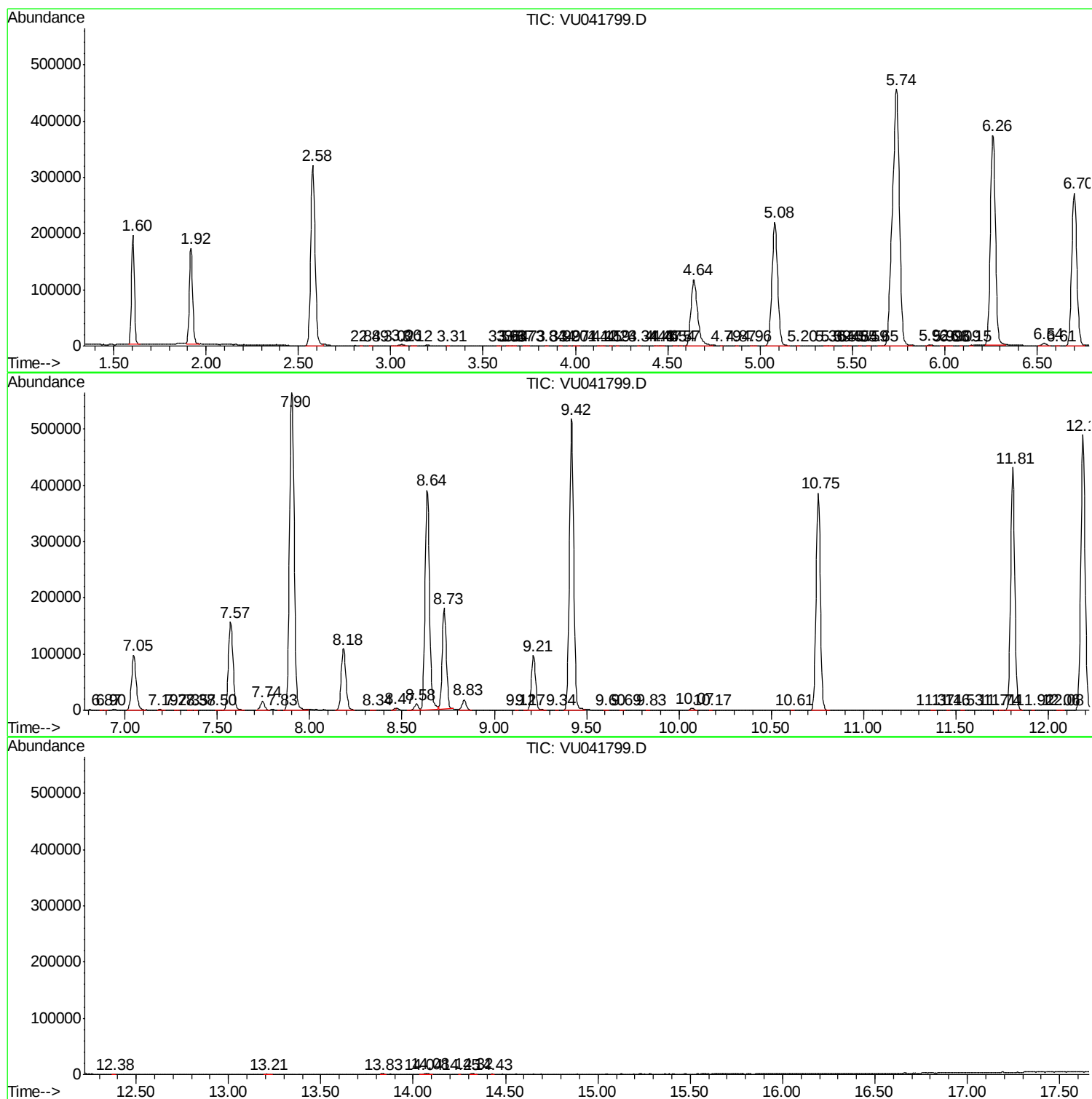
Sum of corrected areas: 9912004

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU122420\
Data File : VU041799.D
Acq On : 24 Dec 2020 10:06
Operator : SY/MD
Sample : PB133786TB 10X
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB001

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SFAMULM121620WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU122420\
Data File : VU041799.D
Acq On : 24 Dec 2020 10:06
Operator : SY/MD
Sample : PB133786TB 10X
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB001

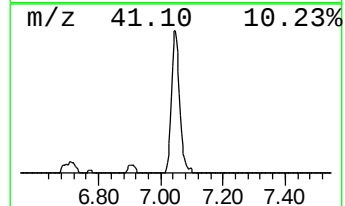
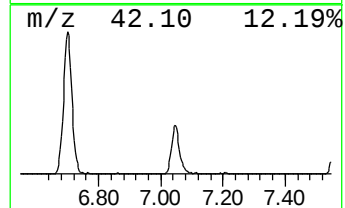
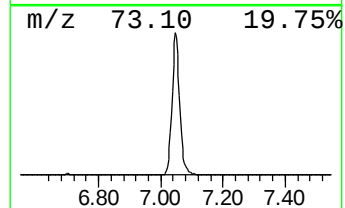
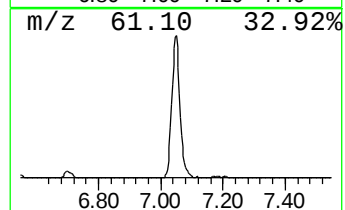
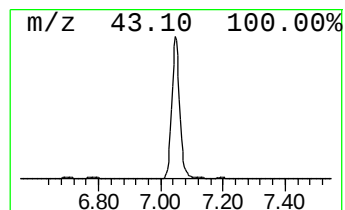
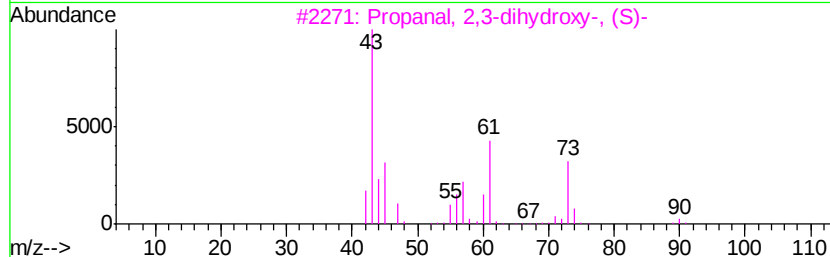
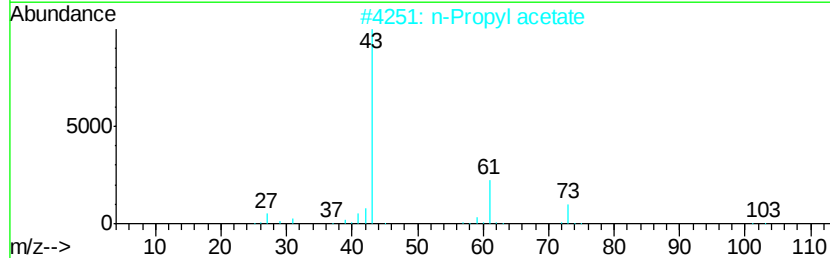
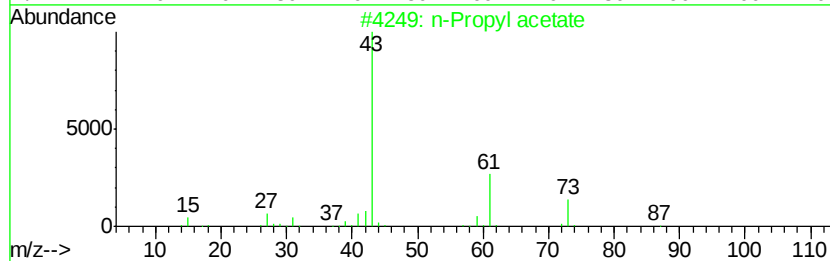
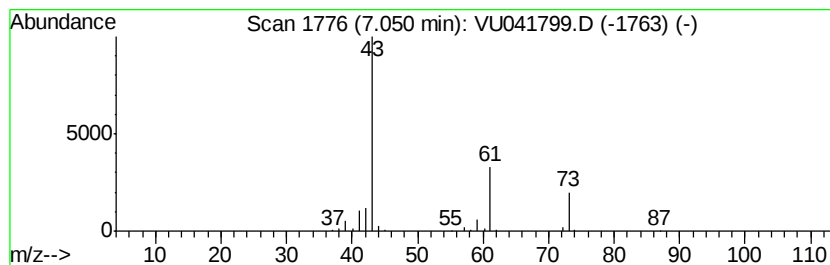
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SFAMULM121620WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	12.24 ug/L	172901	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		n-Propyl acetate	102	C5H10O2	000109-60-4	83
3		Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	38
4		Isopropyl acetate	102	C5H10O2	000108-21-4	28
5		Cyclobutylamine	71	C4H9N	002516-34-9	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU122420\
Data File : VU041799.D
Acq On : 24 Dec 2020 10:06
Operator : SY/MD
Sample : PB133786TB 10X
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB001

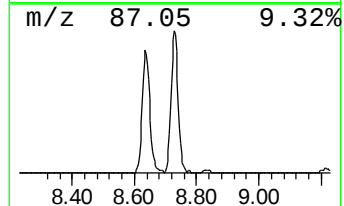
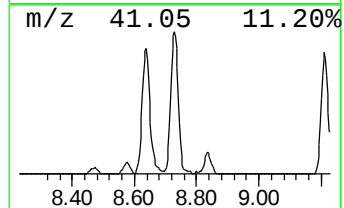
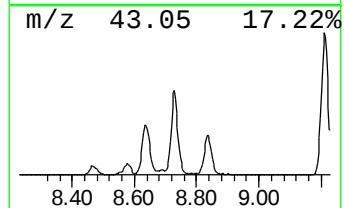
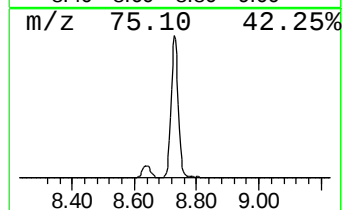
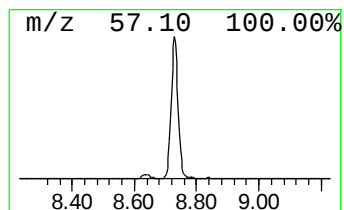
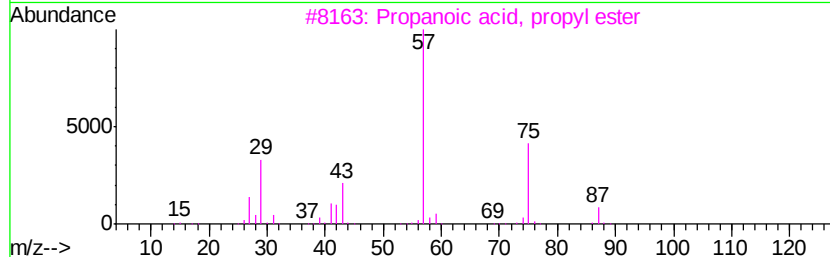
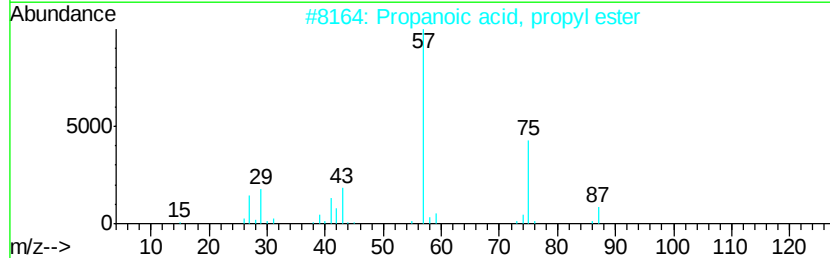
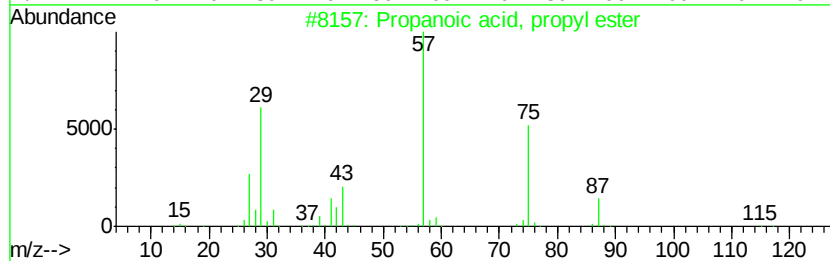
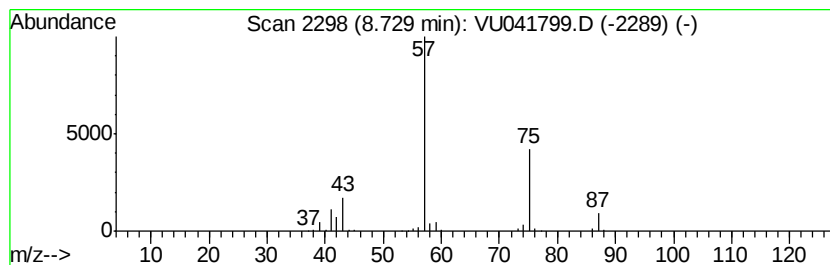
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SFAMULM121620WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.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.
8.73	16.46 ug/L	278556	Chlorobenzene-d5	9.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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, butyl ester	130	C7H14O2	000590-01-2	33



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU122420\
Data File : VU041799.D
Acq On : 24 Dec 2020 10:06
Operator : SY/MD
Sample : PB133786TB 10X
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB001

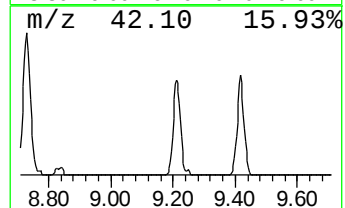
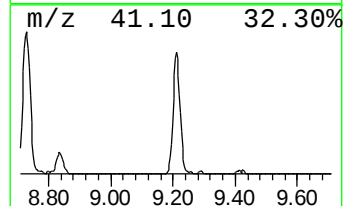
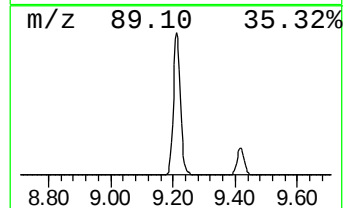
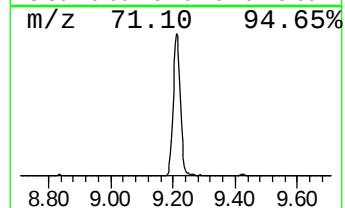
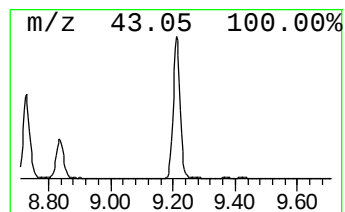
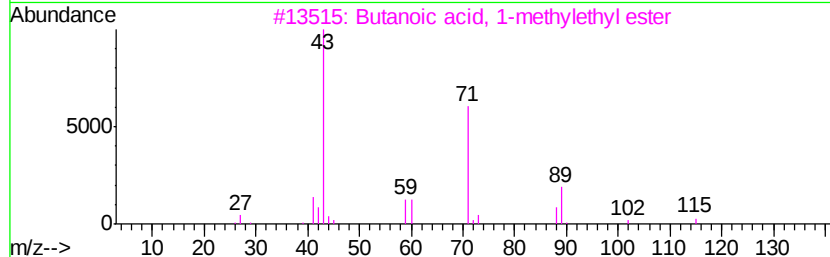
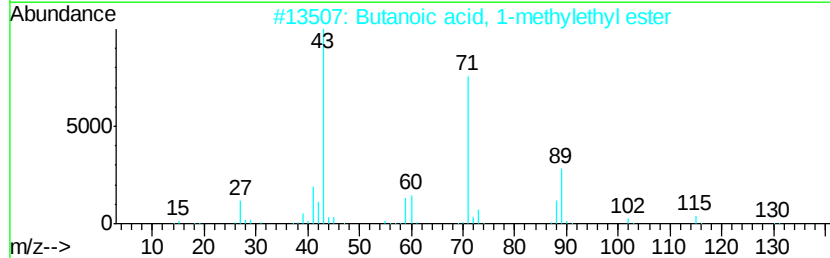
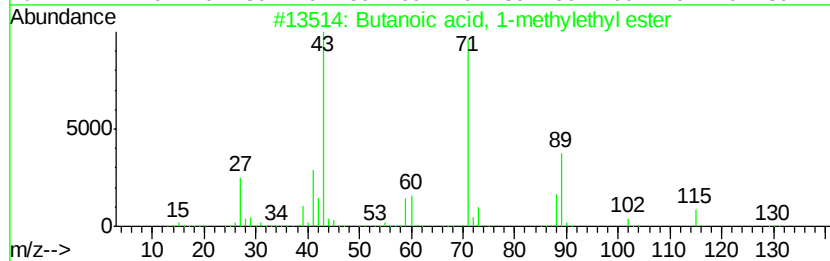
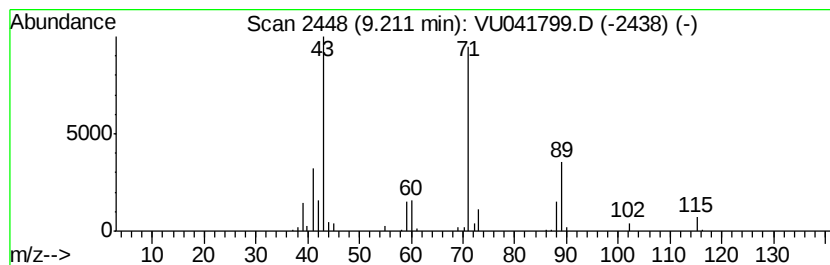
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SFAMULM121620WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.21	8.96 ug/L	151745	Chlorobenzene-d5	9.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91		
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90		
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83		
4	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72		
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72		



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU122420\
Data File : VU041799.D
Acq On : 24 Dec 2020 10:06
Operator : SY/MD
Sample : PB133786TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB001

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SFAMULM121620WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.05	12.2	ug/L	172901	1	6.26	706281	50.0
Propanoic acid, p...	8.73	16.5	ug/L	278556	2	9.42	846393	50.0
Butanoic acid, 1-...	9.21	9.0	ug/L	151745	2	9.42	846393	50.0