

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061219\
 Data File : VU032642.D
 Acq On : 12 Jun 2019 11:30
 Operator : JC/SP
 Sample : VLEB01
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB01

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\SOMULM060619WMA.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	1.180	24	28	35	rBV	4406	3930	0.33%	0.047%
2	1.396	88	95	110	rVB	96275	95305	7.97%	1.143%
3	1.675	175	182	199	rVB	71320	88001	7.36%	1.056%
4	2.267	355	366	377	rBV	153516	233562	19.53%	2.802%
5	2.318	377	382	394	rVB3	8256	12640	1.06%	0.152%
6	2.447	413	422	424	rBV3	629	743	0.06%	0.009%
7	2.569	457	460	467	rBV2	285	270	0.02%	0.003%
8	2.617	470	475	481	rBV3	570	773	0.06%	0.009%
9	2.698	491	500	509	rBV2	3948	6401	0.54%	0.077%
10	2.820	536	538	549	rVB3	466	701	0.06%	0.008%
11	2.945	574	577	583	rVB	188	158	0.01%	0.002%
12	3.077	611	618	621	rBV2	217	271	0.02%	0.003%
13	3.415	715	723	727	rBV5	1877	3131	0.26%	0.038%
14	3.624	784	788	792	rBV2	152	162	0.01%	0.002%
15	3.948	886	889	892	rBV	241	166	0.01%	0.002%
16	4.016	906	910	914	rVB2	218	196	0.02%	0.002%
17	4.116	937	941	944	rVB2	238	179	0.01%	0.002%
18	4.170	944	958	987	rBV	58854	154634	12.93%	1.855%
19	4.489	1053	1057	1058	rBV2	285	200	0.02%	0.002%
20	4.572	1077	1083	1088	rBV3	292	417	0.03%	0.005%
21	4.640	1088	1104	1126	rBV	106070	249336	20.85%	2.991%
22	4.894	1179	1183	1187	rVB2	440	360	0.03%	0.004%
23	4.955	1199	1202	1207	rVB2	184	179	0.01%	0.002%
24	5.058	1229	1234	1238	rVB2	198	203	0.02%	0.002%
25	5.083	1238	1242	1248	rBV2	203	246	0.02%	0.003%
26	5.215	1278	1283	1287	rVB2	201	193	0.02%	0.002%
27	5.241	1287	1291	1295	rBV	232	247	0.02%	0.003%
28	5.334	1297	1320	1345	rBV2	217333	632408	52.88%	7.586%
29	5.511	1372	1375	1379	rBV3	184	179	0.01%	0.002%
30	5.553	1380	1388	1400	rVV3	3597	7648	0.64%	0.092%
31	5.691	1429	1431	1439	rVB3	256	262	0.02%	0.003%
32	5.810	1465	1468	1474	rVB2	215	238	0.02%	0.003%
33	5.881	1474	1490	1512	rBV	209732	413960	34.61%	4.966%
34	6.325	1614	1628	1648	rBV	144266	287321	24.02%	3.447%

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 Title : VOC Analysis

35	6.424	1653	1659	1675	rVB	5346	11234	0.94%	0.135%
36	6.537	1687	1694	1698	rBV3	1526	2306	0.19%	0.028%
37	6.579	1702	1707	1714	rVV	3275	4749	0.40%	0.057%
38	6.698	1732	1744	1784	rBV	670421	1195955	100.00%	14.346%
39	7.161	1884	1888	1894	rBV3	238	316	0.03%	0.004%
40	7.222	1896	1907	1929	rBV	83934	149951	12.54%	1.799%
41	7.415	1956	1967	1993	rBV	122080	214681	17.95%	2.575%
42	7.559	1999	2012	2051	rVB	304066	532882	44.56%	6.392%
43	7.788	2079	2083	2086	rBV4	604	518	0.04%	0.006%
44	7.845	2091	2101	2122	rVV2	66992	119590	10.00%	1.435%
45	8.151	2183	2196	2213	rBV	74179	123819	10.35%	1.485%
46	8.257	2214	2229	2235	rVV2	30493	55503	4.64%	0.666%
47	8.305	2235	2244	2266	rVV	209322	380013	31.77%	4.559%
48	8.411	2266	2277	2303	rVV	512413	829106	69.33%	9.946%
49	8.521	2304	2311	2331	rVB	34153	60119	5.03%	0.721%
50	8.694	2363	2365	2371	rVB2	373	289	0.02%	0.003%
51	8.752	2380	2383	2387	rBV3	184	171	0.01%	0.002%
52	8.826	2403	2406	2408	rBV	292	186	0.02%	0.002%
53	8.900	2416	2429	2455	rBV	365184	572740	47.89%	6.870%
54	9.083	2470	2486	2521	rBV	307700	517725	43.29%	6.210%
55	9.228	2529	2531	2534	rVB3	527	297	0.02%	0.004%
56	9.247	2534	2537	2541	rBV2	529	332	0.03%	0.004%
57	9.305	2549	2555	2557	rBV2	196	184	0.02%	0.002%
58	9.392	2579	2582	2585	rVB2	332	191	0.02%	0.002%
59	9.418	2585	2590	2595	rVB2	319	296	0.02%	0.004%
60	9.450	2595	2600	2603	rBV2	253	218	0.02%	0.003%
61	9.511	2616	2619	2628	rVB3	443	533	0.04%	0.006%
62	9.553	2628	2632	2639	rBV2	410	474	0.04%	0.006%
63	9.607	2641	2649	2668	rBV2	3907	7655	0.64%	0.092%
64	9.765	2687	2698	2715	rBV2	20476	34221	2.86%	0.411%
65	9.887	2733	2736	2740	rBV3	202	205	0.02%	0.002%
66	9.919	2744	2746	2751	rVB	379	309	0.03%	0.004%
67	9.958	2751	2758	2761	rBV3	431	457	0.04%	0.005%
68	10.074	2788	2794	2799	rVB	407	435	0.04%	0.005%
69	10.135	2810	2813	2816	rVB2	270	173	0.01%	0.002%
70	10.160	2816	2821	2825	rVB2	259	241	0.02%	0.003%
71	10.257	2846	2851	2854	rBV2	153	160	0.01%	0.002%

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72	10.353	2878	2881	2886	rBV2	240	236	0.02%	0.003%
73	10.427	2891	2904	2925	rBV	198210	325141	27.19%	3.900%
74	10.607	2951	2960	2964	rBV3	1014	1456	0.12%	0.017%
75	10.694	2985	2987	2993	rVB	355	252	0.02%	0.003%
76	10.771	3003	3011	3024	rVB	5266	7383	0.62%	0.089%
77	10.829	3024	3029	3032	rBV	275	297	0.02%	0.004%
78	10.881	3042	3045	3053	rBV2	213	233	0.02%	0.003%
79	10.993	3075	3080	3083	rVB2	200	185	0.02%	0.002%
80	11.032	3089	3092	3095	rVV2	240	196	0.02%	0.002%
81	11.067	3099	3103	3109	rBV2	213	210	0.02%	0.003%
82	11.138	3121	3125	3132	rVB2	258	259	0.02%	0.003%
83	11.479	3217	3231	3263	rBV	312531	503475	42.10%	6.040%
84	11.636	3278	3280	3287	rVB4	320	275	0.02%	0.003%
85	11.781	3321	3325	3330	rBV3	356	372	0.03%	0.004%
86	11.855	3335	3348	3369	rBV	288840	478471	40.01%	5.740%
87	12.003	3392	3394	3402	rVB4	568	411	0.03%	0.005%
88	12.212	3456	3459	3463	rVB2	464	305	0.03%	0.004%
89	12.366	3503	3507	3509	rBV	232	175	0.01%	0.002%
90	12.427	3521	3526	3528	rBV2	180	187	0.02%	0.002%
91	12.475	3537	3541	3551	rVB3	783	1023	0.09%	0.012%
92	13.193	3759	3764	3769	rBV	270	369	0.03%	0.004%
93	13.266	3783	3787	3788	rBV	316	159	0.01%	0.002%
94	13.556	3873	3877	3883	rVV2	257	345	0.03%	0.004%
95	13.585	3883	3886	3890	rVB	320	219	0.02%	0.003%
96	13.749	3934	3937	3940	rBV2	329	264	0.02%	0.003%
97	13.961	3999	4003	4008	rBV3	333	350	0.03%	0.004%
98	14.170	4066	4068	4074	rBV2	302	252	0.02%	0.003%
99	14.408	4139	4142	4147	rVB2	257	208	0.02%	0.002%
100	15.443	4458	4464	4471	rBV3	435	745	0.06%	0.009%

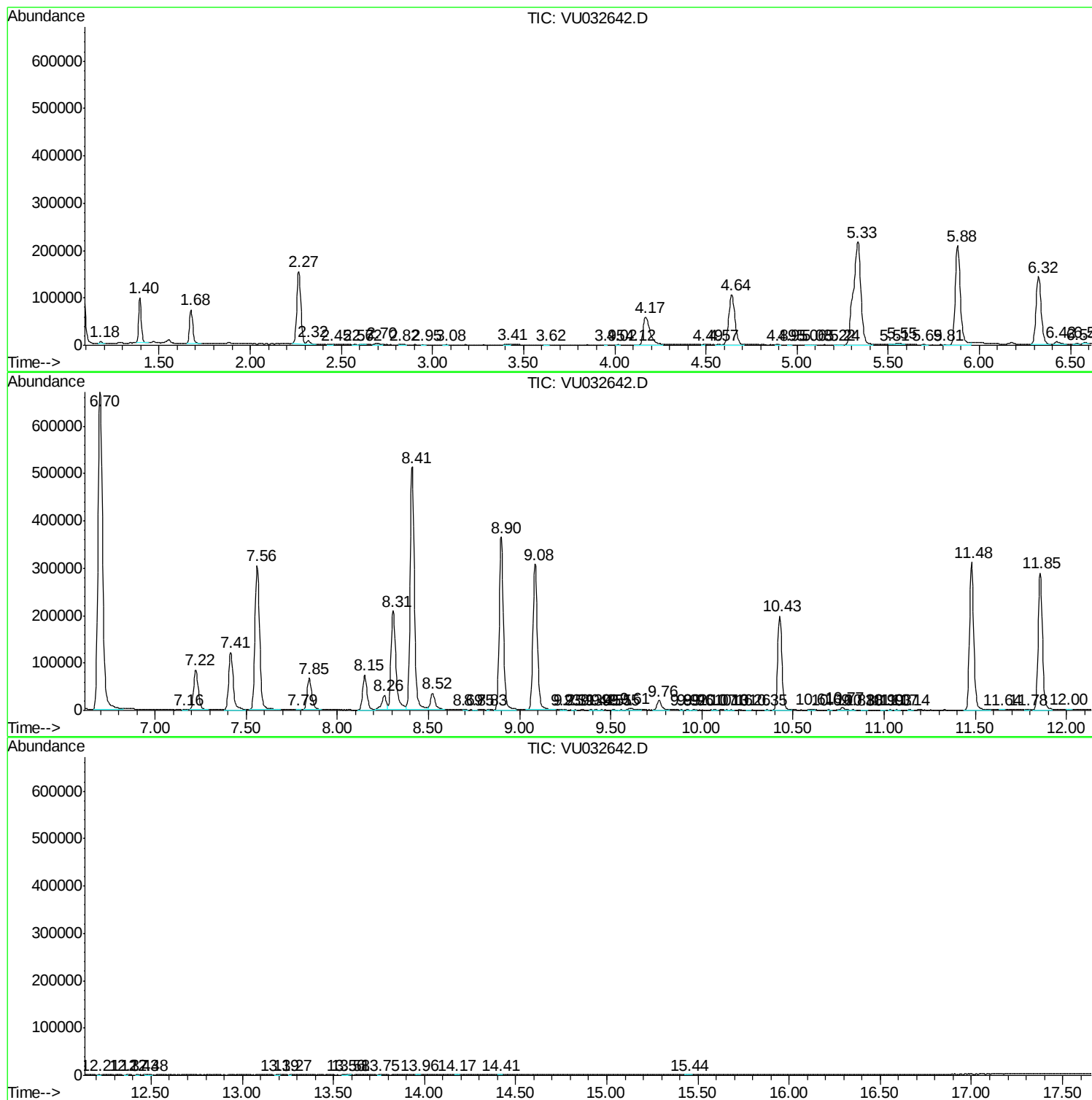
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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



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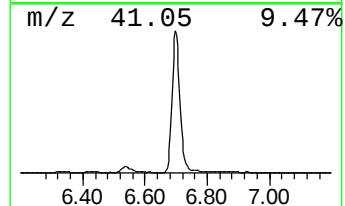
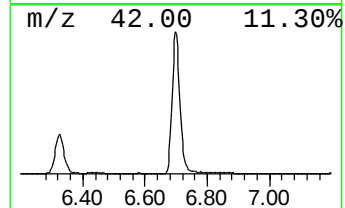
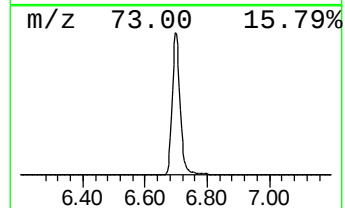
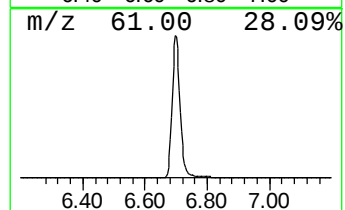
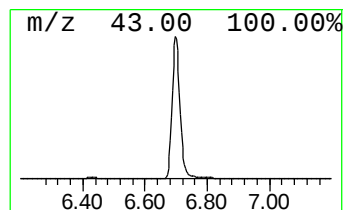
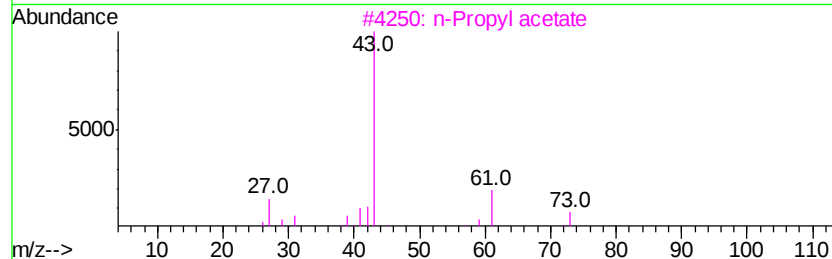
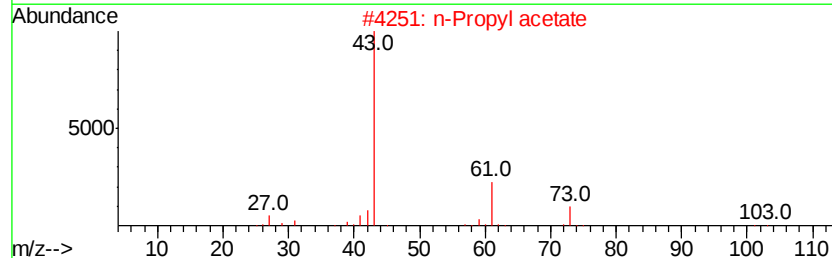
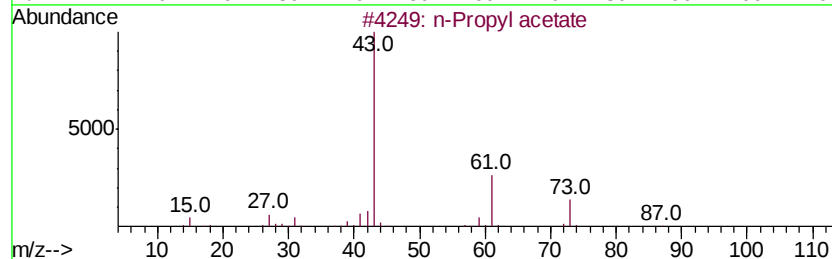
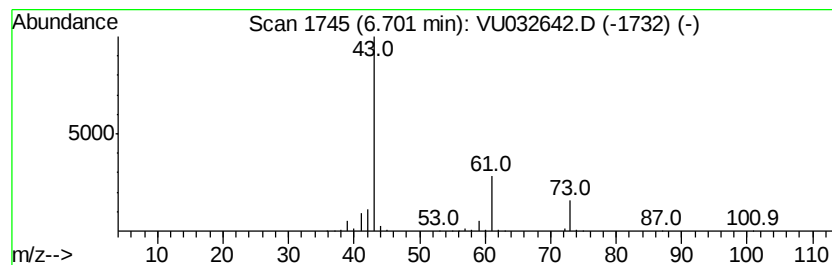
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	144.45 ug/L	1195960	1,4-Difluorobenzene	5.88

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		n-Propyl acetate	102	C5H10O2	000109-60-4	78
4		Isopropyl acetate	102	C5H10O2	000108-21-4	36
5		Isobutyl acetate	116	C6H12O2	000110-19-0	9



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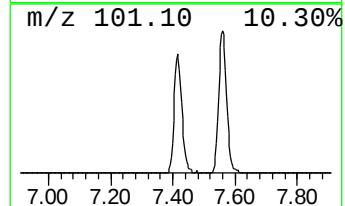
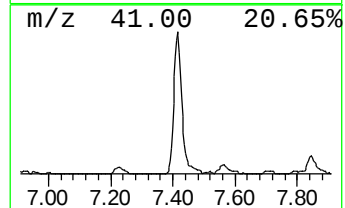
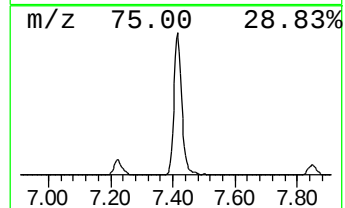
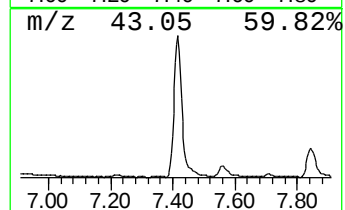
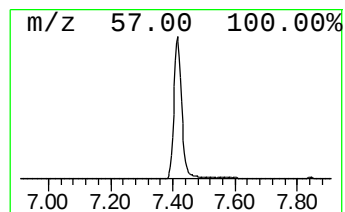
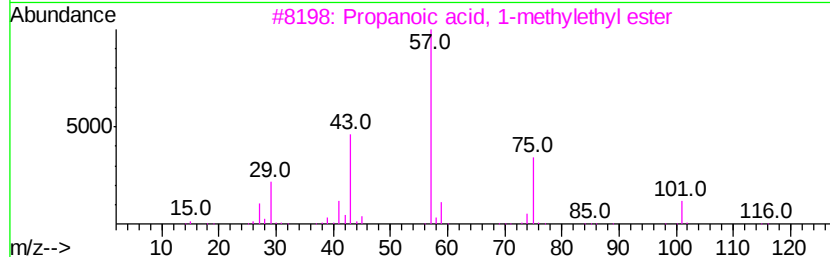
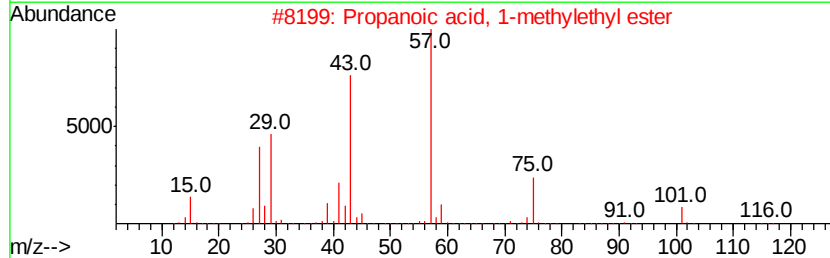
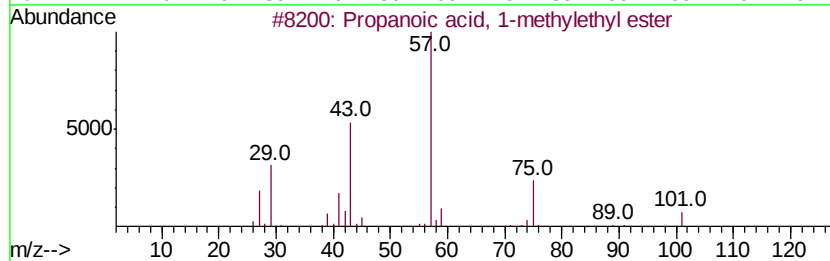
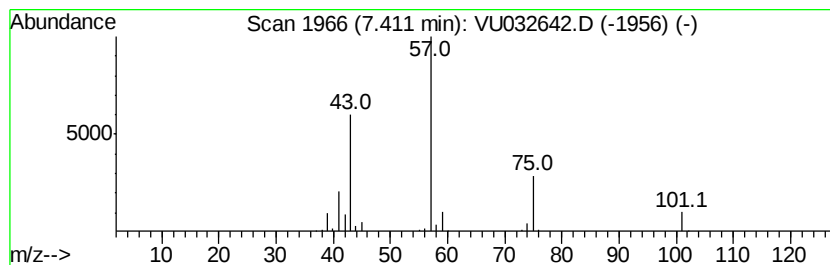
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Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	25.93 ug/L	214681	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
5		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53



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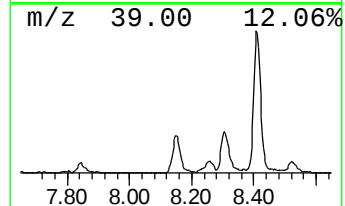
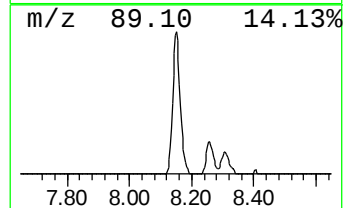
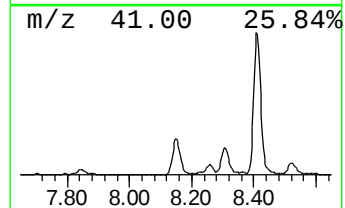
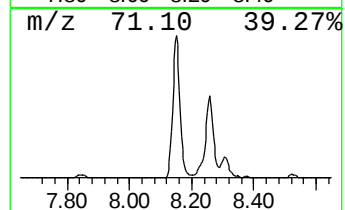
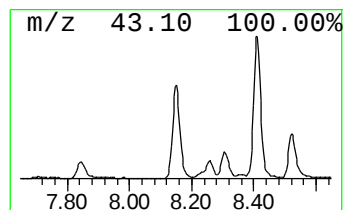
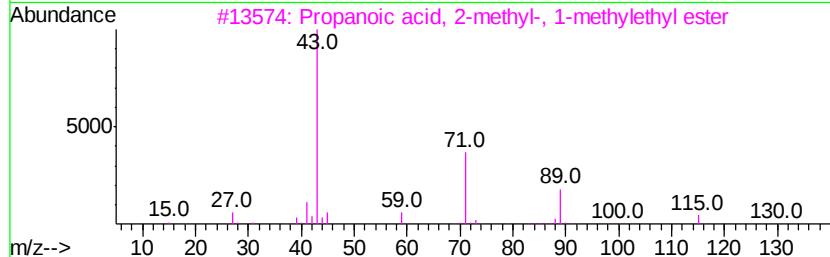
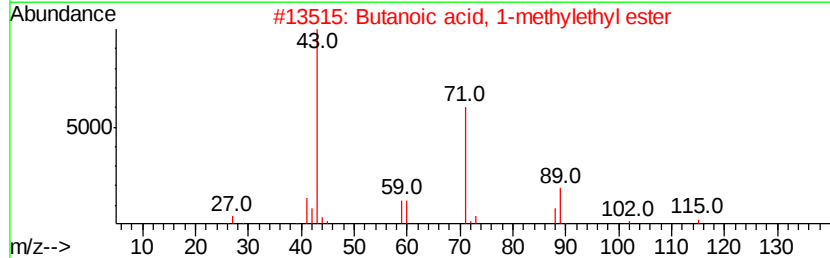
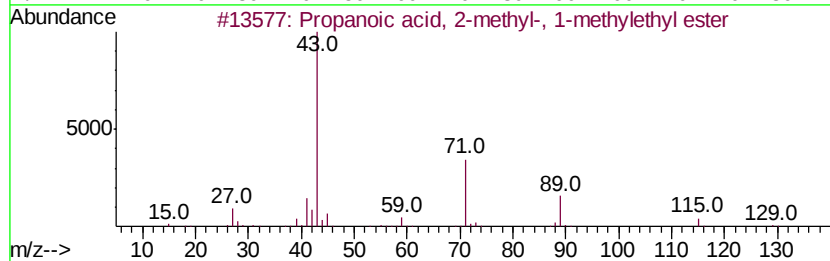
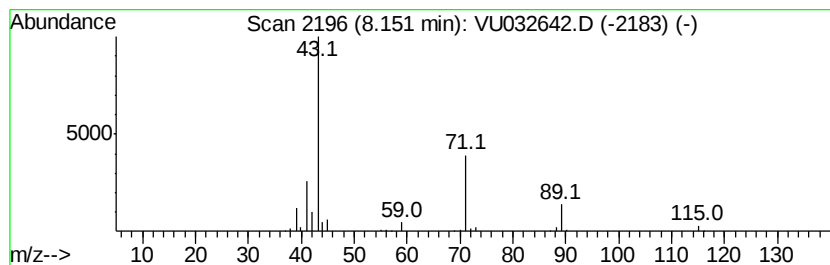
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	11.96 ug/L	123819	Chlorobenzene-d5	9.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83	
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72	
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72	
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64	
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032642.D
Acq On : 12 Jun 2019 11:30
Operator : JC/SP
Sample : VLEB01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

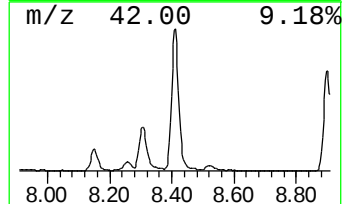
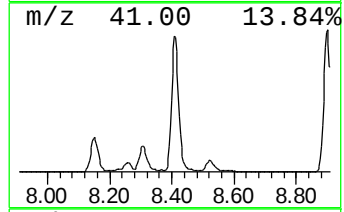
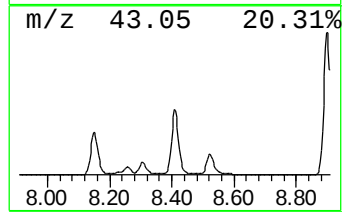
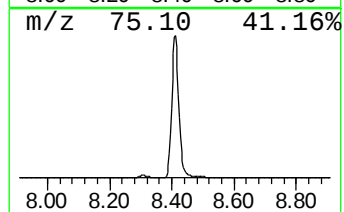
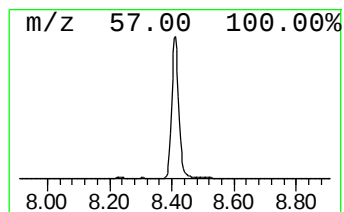
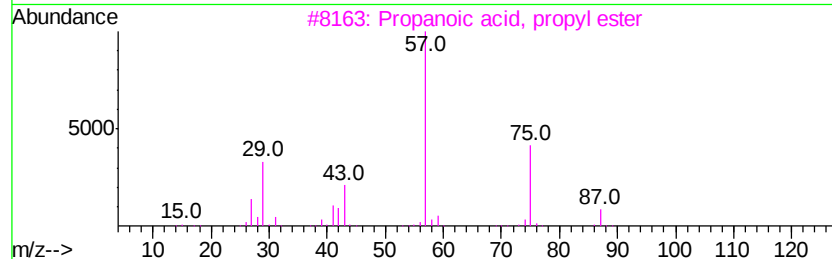
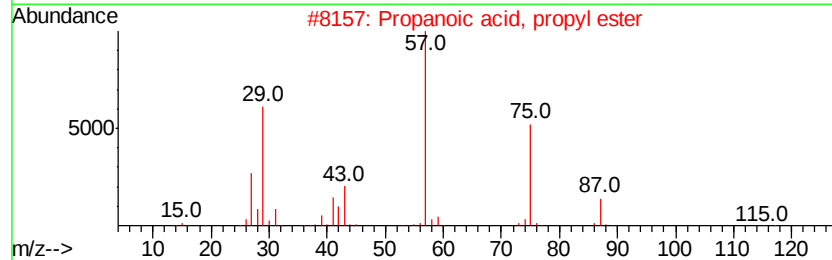
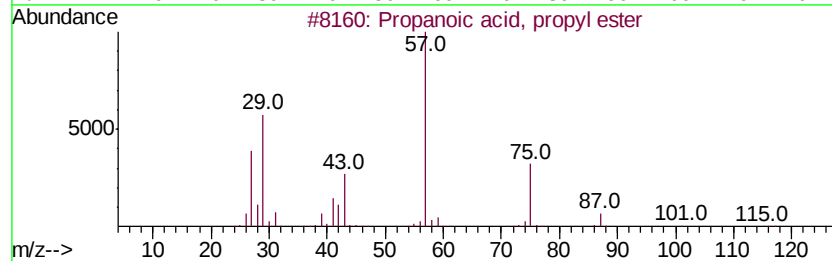
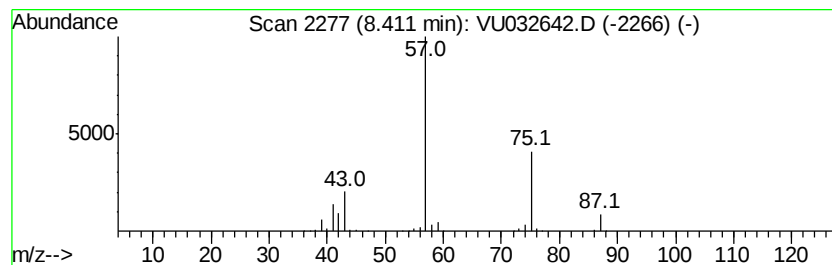
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	80.07 ug/L	829106	Chlorobenzene-d5	9.08

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	78
5		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032642.D
Acq On : 12 Jun 2019 11:30
Operator : JC/SP
Sample : VLEB01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

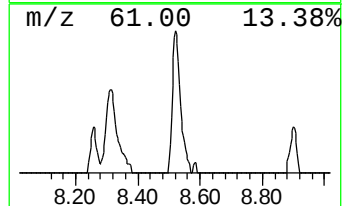
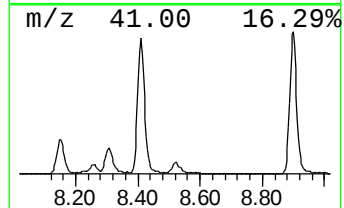
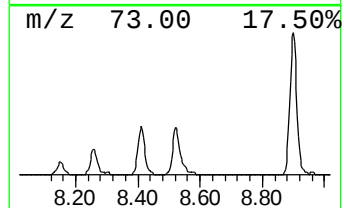
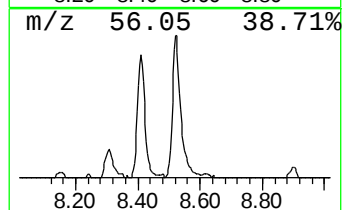
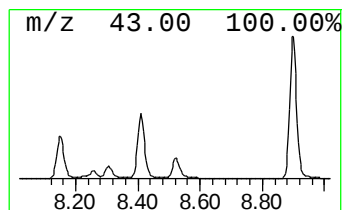
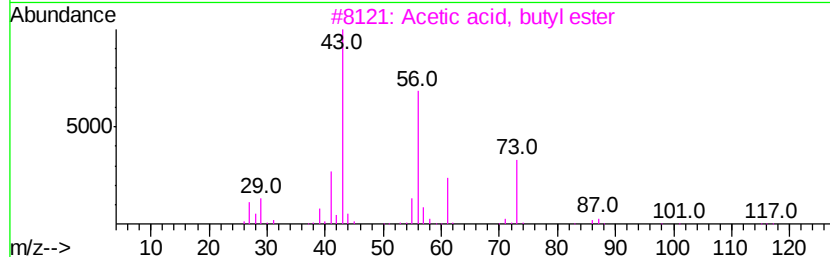
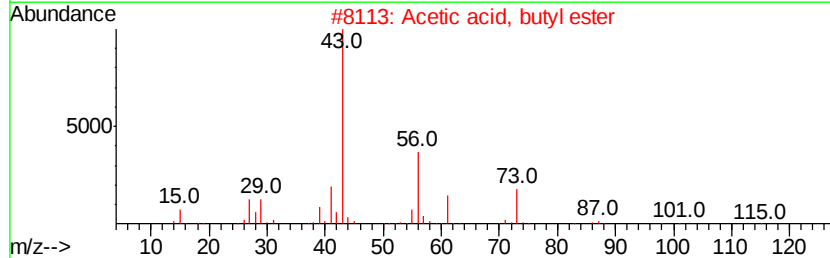
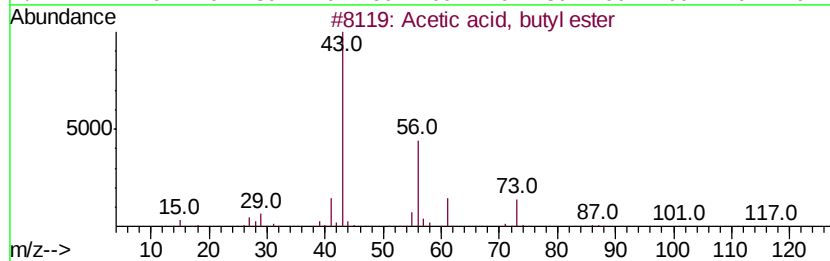
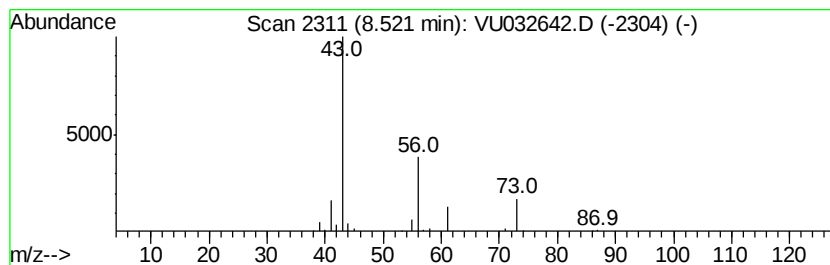
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	5.81 ug/L	60119	Chlorobenzene-d5	9.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	83
2	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	83
3	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	72
4	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	64
5	Isobutyl acetate			116	C6H12O2	000110-19-0	25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032642.D
Acq On : 12 Jun 2019 11:30
Operator : JC/SP
Sample : VLEB01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

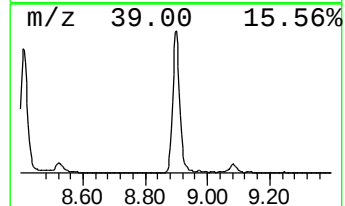
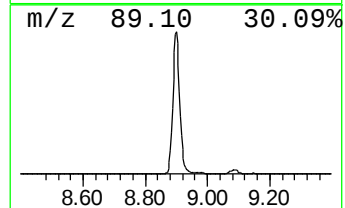
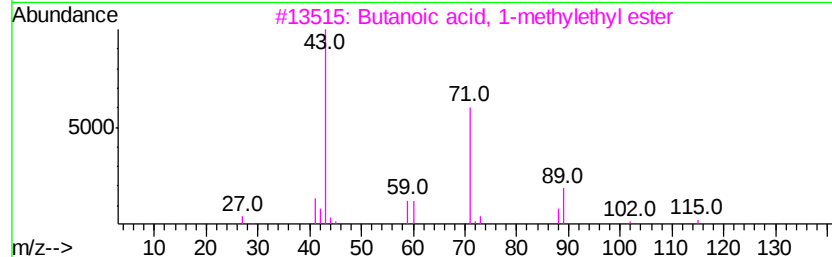
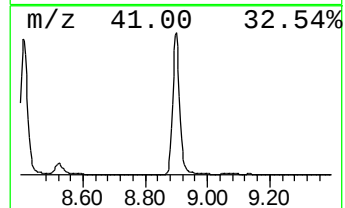
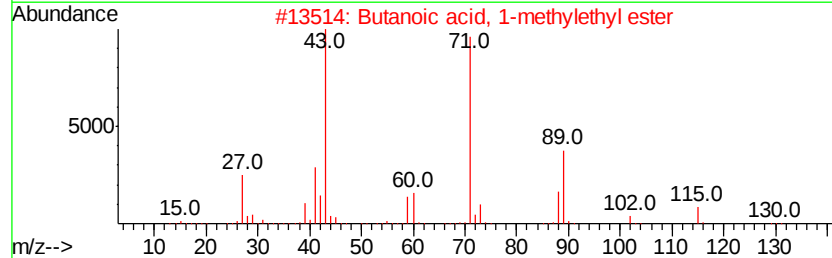
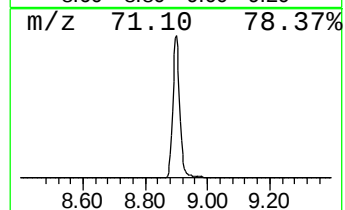
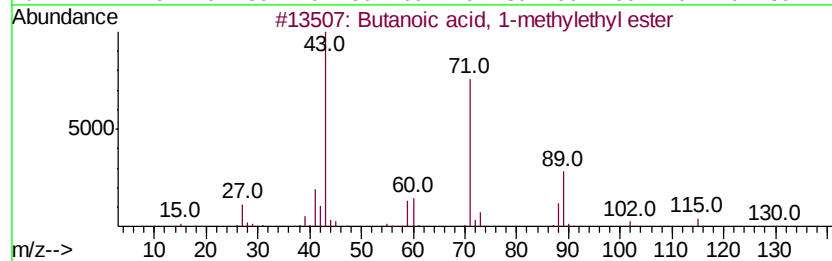
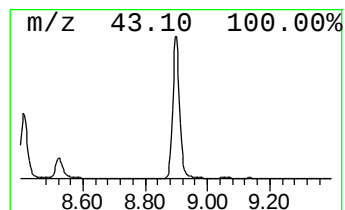
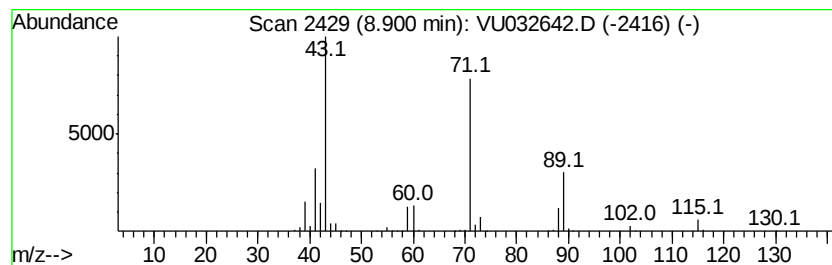
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	55.31 ug/L	572740	Chlorobenzene-d5	9.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	95
2			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
3			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
4			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	59
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032642.D
Acq On : 12 Jun 2019 11:30
Operator : JC/SP
Sample : VLEB01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

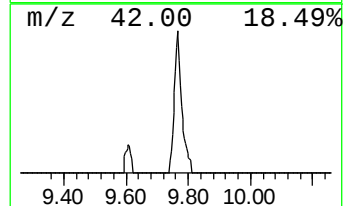
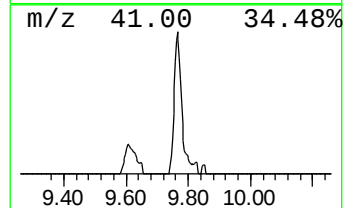
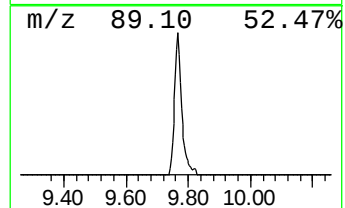
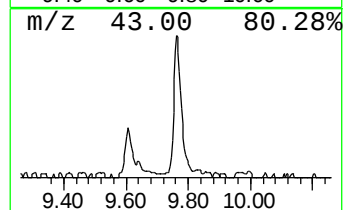
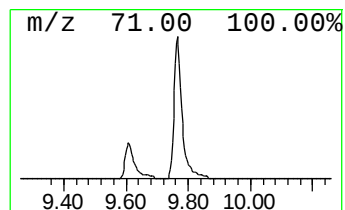
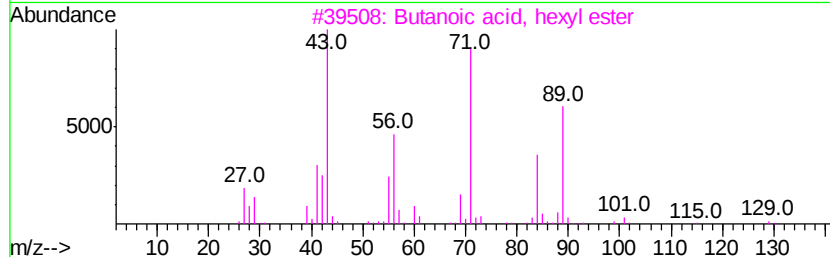
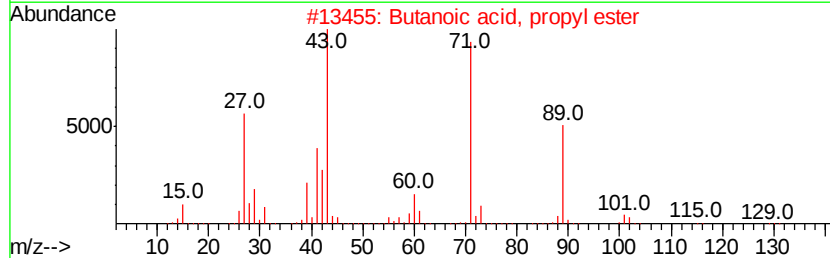
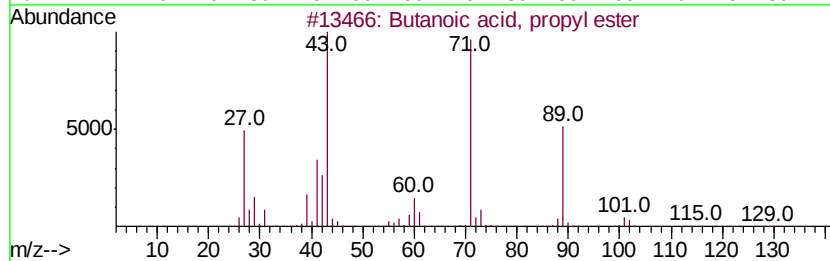
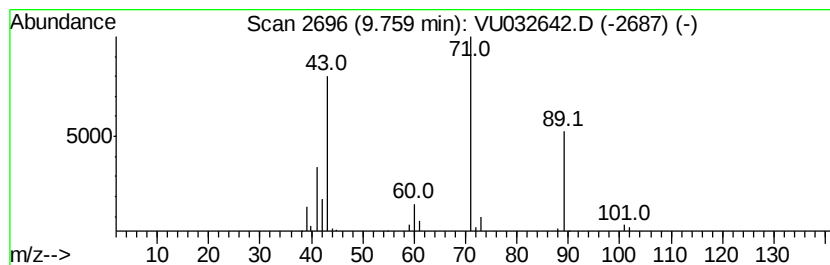
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	3.30 ug/L	34221	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
2		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
3		Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	83
4		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061219\
Data File : VU032642.D
Acq On : 12 Jun 2019 11:30
Operator : JC/SP
Sample : VLEB01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.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	6.70	144.4	ug/L	1195960	1	5.88	413960	50.0
Propanoic acid, 1...	7.41	25.9	ug/L	214681	1	5.88	413960	50.0
Propanoic acid, 2...	8.15	12.0	ug/L	123819	2	9.08	517725	50.0
Propanoic acid, p...	8.41	80.1	ug/L	829106	2	9.08	517725	50.0
Acetic acid, buty...	8.52	5.8	ug/L	60119	2	9.08	517725	50.0
Butanoic acid, 1-...	8.90	55.3	ug/L	572740	2	9.08	517725	50.0
Butanoic acid, pr...	9.76	3.3	ug/L	34221	2	9.08	517725	50.0