

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061719\
 Data File : VU032790.D
 Acq On : 17 Jun 2019 18:13
 Operator : JC/SP
 Sample : K3324-02
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JW1

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\SOMULM061719WMA.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	23	28	36	rBV2	8380	8244	0.54%	0.075%
2	1.396	87	95	104	rBV	104138	104941	6.93%	0.956%
3	1.675	174	182	196	rVB	85430	107212	7.08%	0.977%
4	2.267	355	366	376	rBV	172577	261742	17.29%	2.385%
5	2.315	377	381	396	rVB2	13798	21580	1.43%	0.197%
6	2.524	444	446	451	rVB3	420	333	0.02%	0.003%
7	2.617	469	475	483	rBV4	1189	1707	0.11%	0.016%
8	2.694	490	499	509	rVB2	10137	17295	1.14%	0.158%
9	2.830	537	541	548	rVB3	639	731	0.05%	0.007%
10	2.875	552	555	558	rVB	324	227	0.01%	0.002%
11	2.939	572	575	577	rBV2	321	255	0.02%	0.002%
12	3.122	629	632	638	rVB3	335	339	0.02%	0.003%
13	3.177	645	649	655	rVB4	475	439	0.03%	0.004%
14	3.264	674	676	683	rVB2	296	285	0.02%	0.003%
15	3.341	697	700	702	rBV2	406	262	0.02%	0.002%
16	3.408	707	721	736	rVV3	3695	9632	0.64%	0.088%
17	3.537	757	761	762	rBV	329	239	0.02%	0.002%
18	3.617	782	786	789	rVV2	342	321	0.02%	0.003%
19	3.643	789	794	799	rVB4	572	670	0.04%	0.006%
20	3.694	808	810	813	rVV3	456	281	0.02%	0.003%
21	3.714	813	816	821	rVV2	333	277	0.02%	0.003%
22	3.945	884	888	890	rVV2	302	238	0.02%	0.002%
23	3.958	890	892	903	rVB3	411	575	0.04%	0.005%
24	4.167	945	957	989	rBV2	91893	260121	17.19%	2.370%
25	4.640	1088	1104	1123	rBV	141472	329699	21.78%	3.005%
26	4.829	1157	1163	1166	rBV3	304	294	0.02%	0.003%
27	4.849	1166	1169	1172	rBV4	336	291	0.02%	0.003%
28	4.871	1172	1176	1180	rBV3	543	564	0.04%	0.005%
29	5.022	1220	1223	1228	rVB	294	227	0.01%	0.002%
30	5.051	1228	1232	1235	rBV2	437	416	0.03%	0.004%
31	5.071	1235	1238	1240	rBV	408	271	0.02%	0.002%
32	5.138	1255	1259	1265	rVB3	223	239	0.02%	0.002%
33	5.212	1275	1282	1286	rBV2	437	562	0.04%	0.005%
34	5.331	1296	1319	1344	rBV2	276409	818046	54.05%	7.455%

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Integration Parameters: LSCINT.P

Integrator: RTE
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 Title : VOC Analysis

35	5.546	1375	1386	1399	rBV	6399	14023	0.93%	0.128%
36	5.781	1453	1459	1462	rBV3	380	428	0.03%	0.004%
37	5.878	1474	1489	1513	rBV	275766	539947	35.67%	4.920%
38	6.180	1570	1583	1600	rBV	118516	227670	15.04%	2.075%
39	6.325	1613	1628	1646	rBV	190976	382549	25.28%	3.486%
40	6.418	1649	1657	1677	rVB2	8357	18672	1.23%	0.170%
41	6.530	1684	1692	1698	rBV	3365	5610	0.37%	0.051%
42	6.569	1699	1704	1712	rBV2	5079	8491	0.56%	0.077%
43	6.698	1731	1744	1776	rBV	863878	1513523	100.00%	13.793%
44	7.058	1854	1856	1859	rVB2	484	310	0.02%	0.003%
45	7.099	1865	1869	1874	rBV3	372	410	0.03%	0.004%
46	7.222	1892	1907	1924	rBV	111641	200272	13.23%	1.825%
47	7.370	1949	1953	1954	rBV4	456	389	0.03%	0.004%
48	7.415	1955	1967	1995	rVB	151564	265707	17.56%	2.421%
49	7.559	1999	2012	2027	rBV	374786	648313	42.83%	5.908%
50	7.694	2047	2054	2064	rBV6	1968	3717	0.25%	0.034%
51	7.842	2089	2100	2120	rBV3	92953	162835	10.76%	1.484%
52	8.035	2159	2160	2164	rVB2	479	283	0.02%	0.003%
53	8.067	2164	2170	2172	rBV3	636	516	0.03%	0.005%
54	8.148	2180	2195	2209	rBV	88574	145707	9.63%	1.328%
55	8.222	2209	2218	2223	rBV3	27860	44149	2.92%	0.402%
56	8.305	2235	2244	2265	rVB	324654	539794	35.66%	4.919%
57	8.408	2265	2276	2294	rBV	639913	984361	65.04%	8.970%
58	8.517	2303	2310	2332	rVB	45775	76563	5.06%	0.698%
59	8.649	2346	2351	2354	rVB5	538	470	0.03%	0.004%
60	8.726	2373	2375	2379	rBV2	608	437	0.03%	0.004%
61	8.800	2396	2398	2403	rVB2	380	306	0.02%	0.003%
62	8.897	2416	2428	2456	rBV	435579	679834	44.92%	6.195%
63	9.083	2470	2486	2505	rBV	418597	693348	45.81%	6.318%
64	9.222	2525	2529	2532	rVB3	555	396	0.03%	0.004%
65	9.247	2532	2537	2540	rBV3	641	799	0.05%	0.007%
66	9.373	2573	2576	2582	rVB5	825	640	0.04%	0.006%
67	9.562	2631	2635	2636	rBV	434	324	0.02%	0.003%
68	9.601	2638	2647	2663	rVB3	6325	11539	0.76%	0.105%
69	9.710	2678	2681	2686	rBV3	420	294	0.02%	0.003%
70	9.762	2686	2697	2713	rBV	26040	42031	2.78%	0.383%
71	9.839	2718	2721	2725	rBV2	288	224	0.01%	0.002%

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72	9.874	2728	2732	2735	rBV3	441	386	0.03%	0.004%
73	10.019	2773	2777	2779	rBV2	486	418	0.03%	0.004%
74	10.122	2803	2809	2812	rBV4	443	558	0.04%	0.005%
75	10.154	2815	2819	2823	rVV2	443	381	0.03%	0.003%
76	10.257	2844	2851	2854	rBV4	588	704	0.05%	0.006%
77	10.337	2871	2876	2882	rVB3	358	439	0.03%	0.004%
78	10.424	2890	2903	2926	rBV	288808	469693	31.03%	4.280%
79	10.575	2947	2950	2954	rVB3	623	492	0.03%	0.004%
80	10.656	2973	2975	2978	rVB3	413	229	0.02%	0.002%
81	10.688	2982	2985	2987	rBV2	391	285	0.02%	0.003%
82	10.755	3004	3006	3012	rVV5	387	311	0.02%	0.003%
83	10.842	3030	3033	3036	rBV2	378	278	0.02%	0.003%
84	11.051	3095	3098	3103	rBV2	347	353	0.02%	0.003%
85	11.106	3111	3115	3119	rBV2	549	410	0.03%	0.004%
86	11.141	3125	3126	3130	rBV2	326	229	0.02%	0.002%
87	11.180	3136	3138	3144	rVB2	414	306	0.02%	0.003%
88	11.238	3153	3156	3159	rVB2	612	383	0.03%	0.003%
89	11.257	3159	3162	3167	rVB2	369	314	0.02%	0.003%
90	11.479	3219	3231	3255	rBV	426320	684770	45.24%	6.240%
91	11.771	3319	3322	3332	rVB3	584	677	0.04%	0.006%
92	11.855	3336	3348	3373	rBV	389005	645228	42.63%	5.880%
93	12.180	3445	3449	3454	rBV4	627	701	0.05%	0.006%
94	12.241	3466	3468	3471	rVB	661	290	0.02%	0.003%
95	12.376	3507	3510	3513	rBV	424	338	0.02%	0.003%
96	12.553	3563	3565	3568	rBV	510	232	0.02%	0.002%
97	13.234	3774	3777	3781	rVB4	489	347	0.02%	0.003%
98	13.289	3791	3794	3797	rBV2	503	326	0.02%	0.003%
99	14.765	4250	4253	4255	rBV	659	457	0.03%	0.004%
100	15.099	4354	4357	4358	rBV2	884	491	0.03%	0.004%

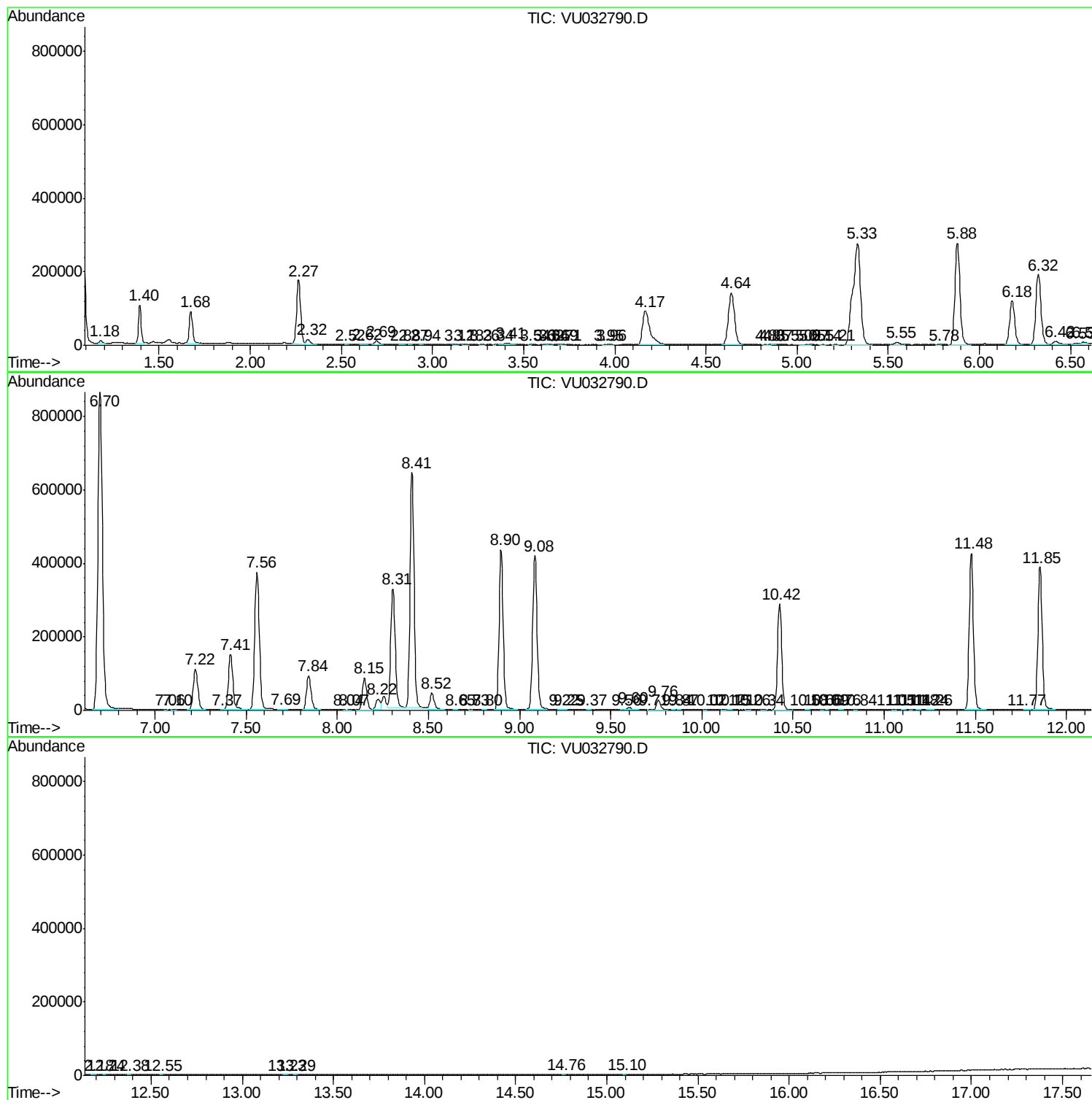
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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



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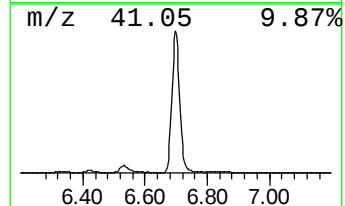
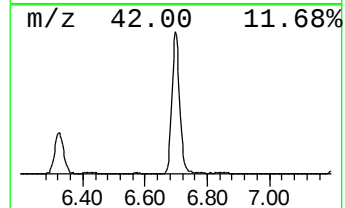
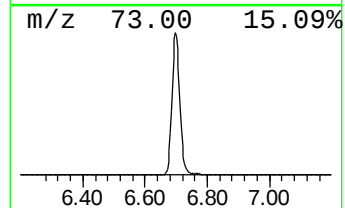
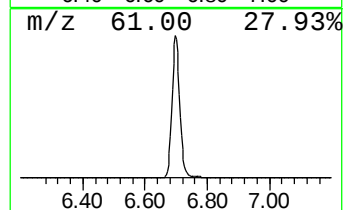
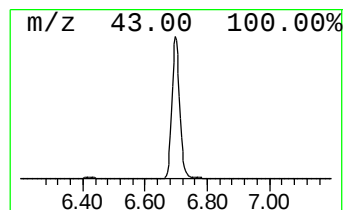
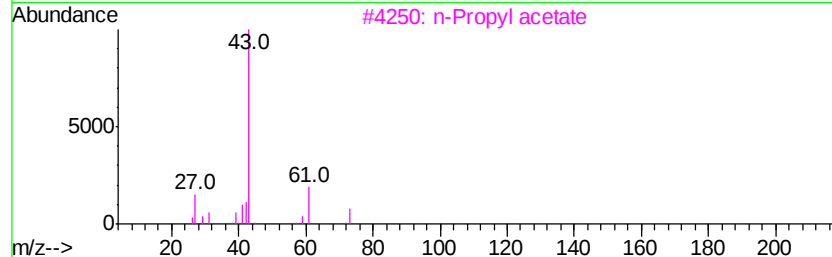
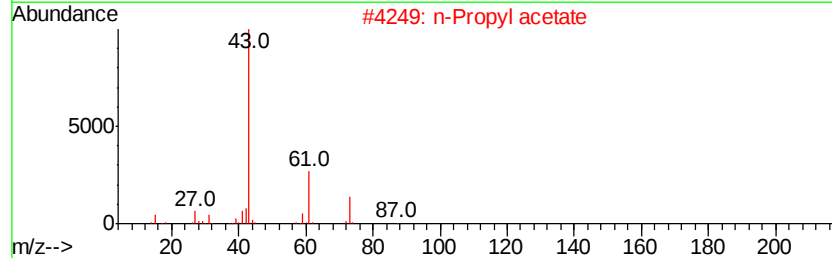
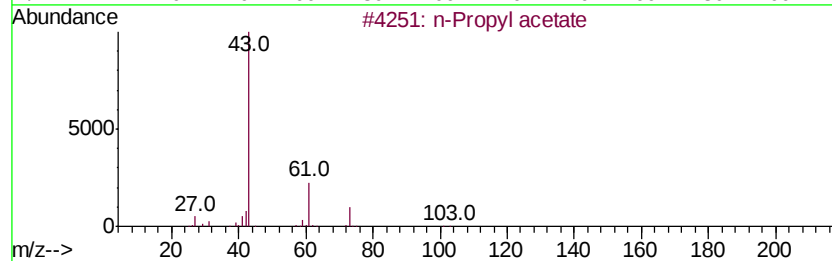
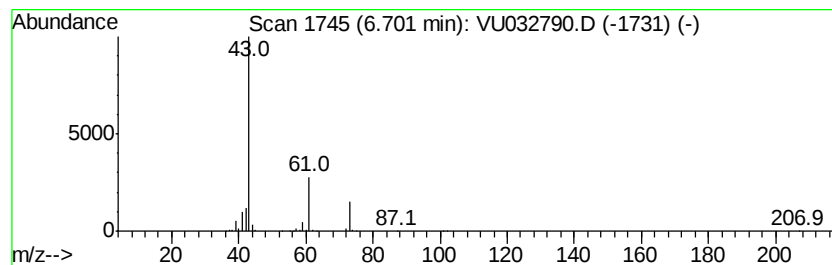
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	140.16 ug/L	1513520	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	78
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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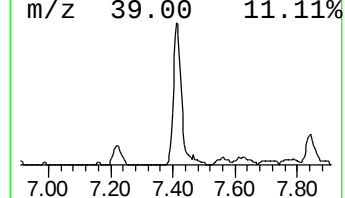
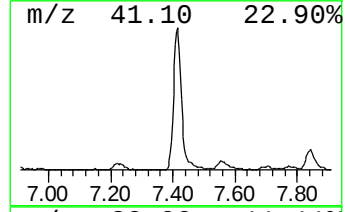
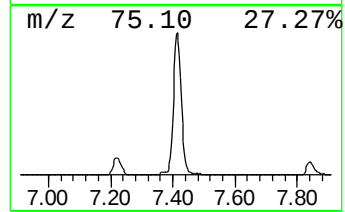
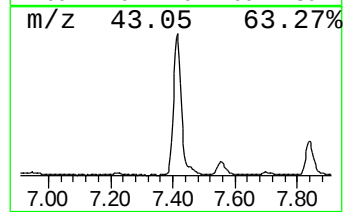
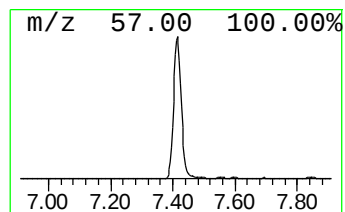
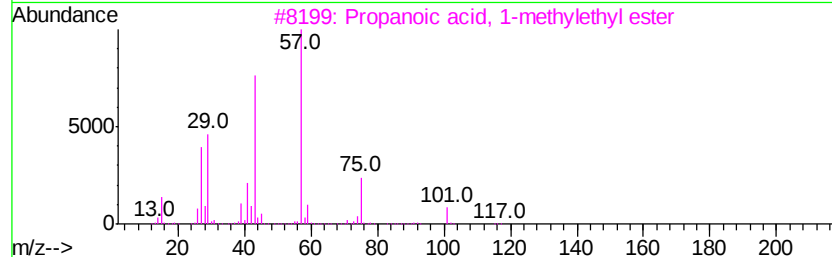
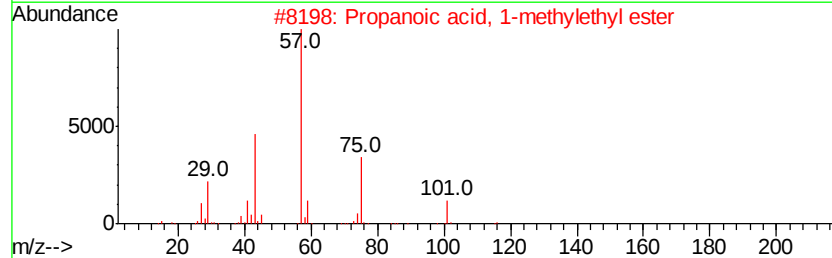
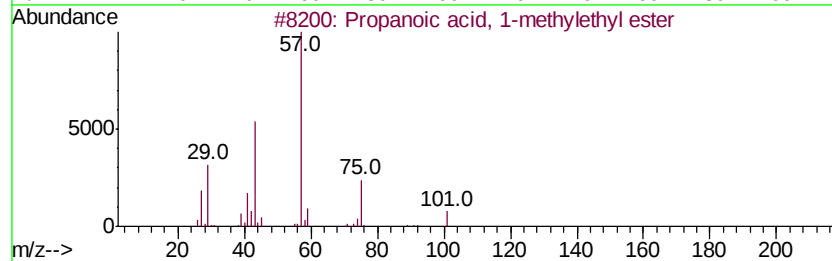
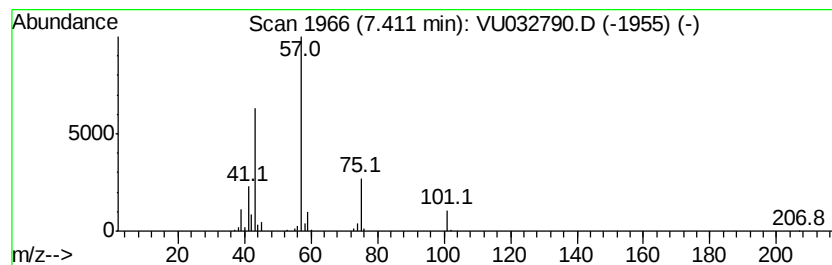
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Quant Title : VOC Analysis

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	24.60 ug/L	265707	1,4-Difluorobenzene	5.88

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2		000637-78-5	86
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2		000637-78-5	83
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2		000637-78-5	78
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2		000637-78-5	53
5	Propanoic acid, propyl ester	116	C6H12O2		000106-36-5	45



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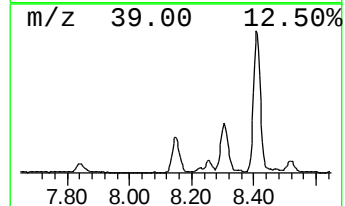
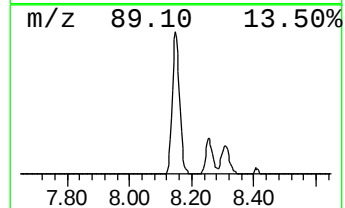
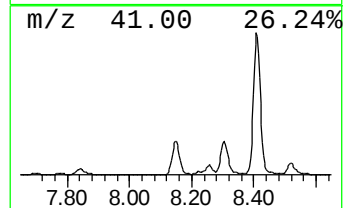
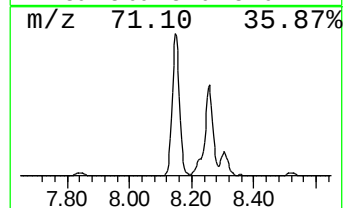
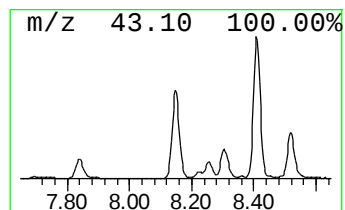
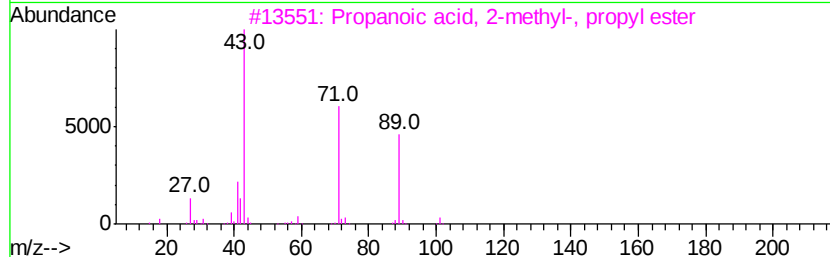
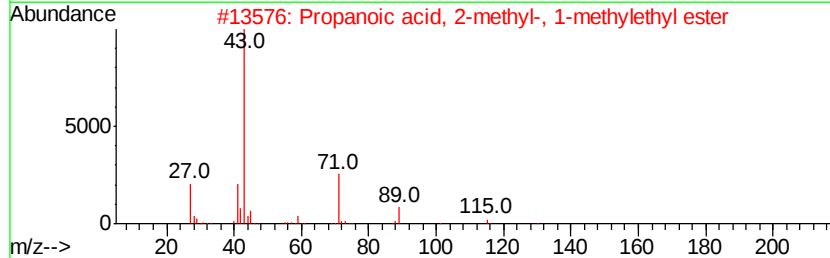
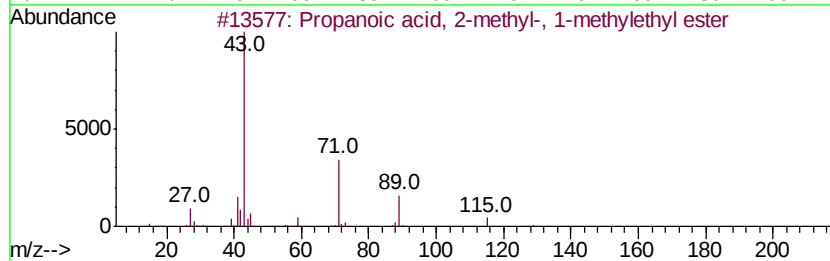
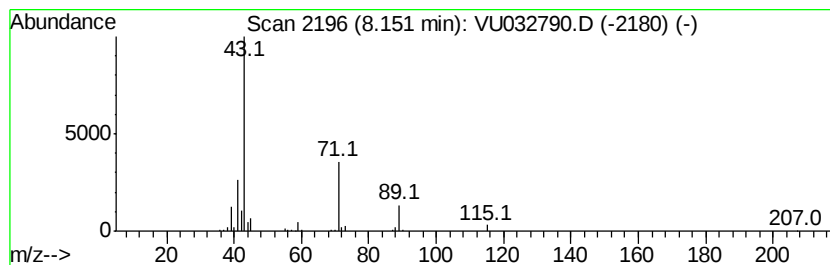
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	10.51 ug/L	145707	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3		Propanoic acid, 2-methyl-, propv...	130	C7H14O2	000644-49-5	64
4		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032790.D
Acq On : 17 Jun 2019 18:13
Operator : JC/SP
Sample : K3324-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JW1

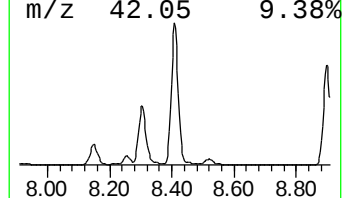
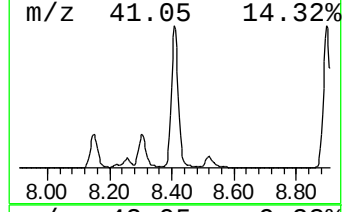
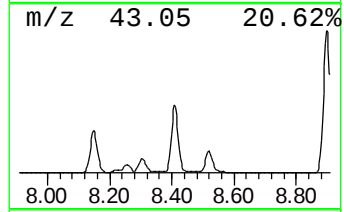
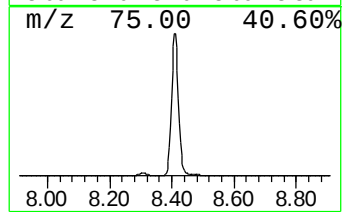
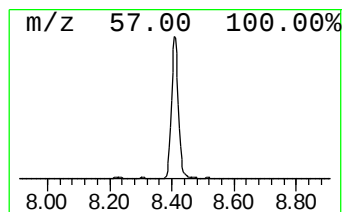
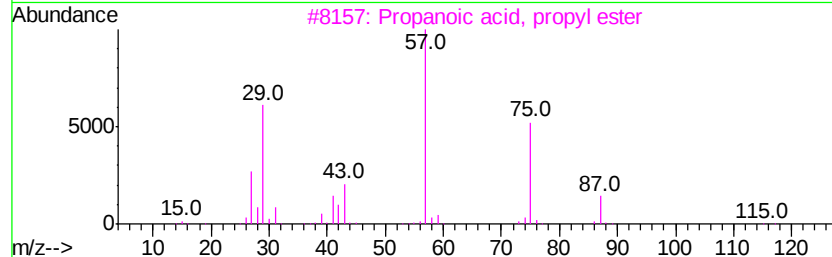
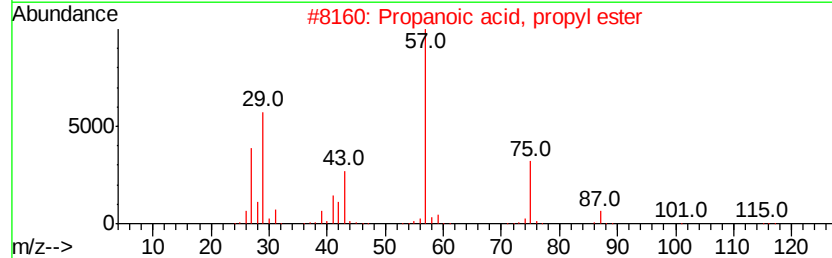
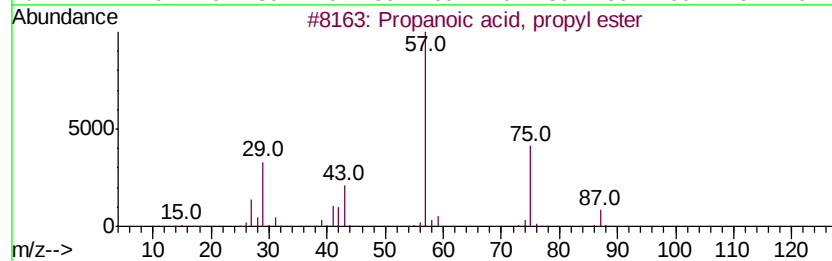
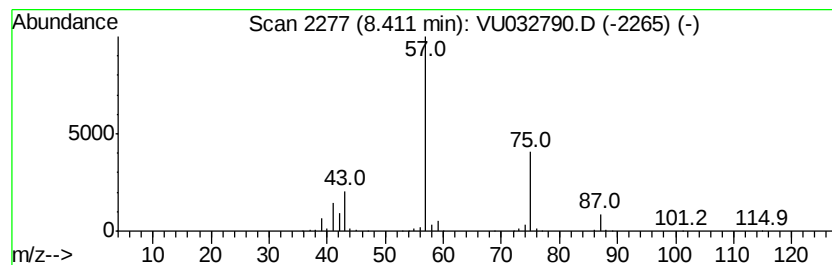
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Quant Title : VOC Analysis

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	70.99 ug/L	984361	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\VU061719\
Data File : VU032790.D
Acq On : 17 Jun 2019 18:13
Operator : JC/SP
Sample : K3324-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW1

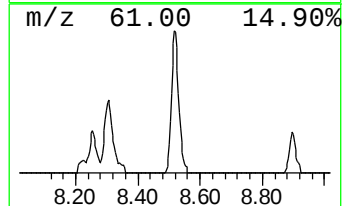
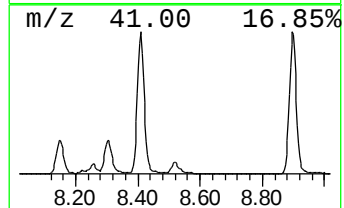
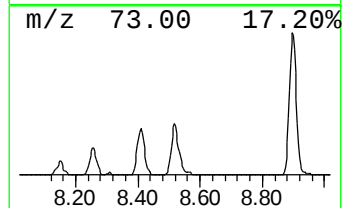
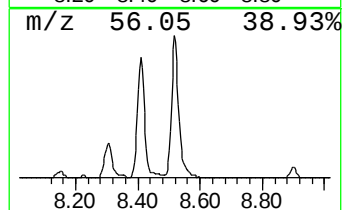
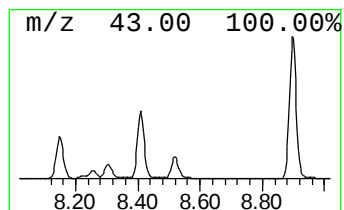
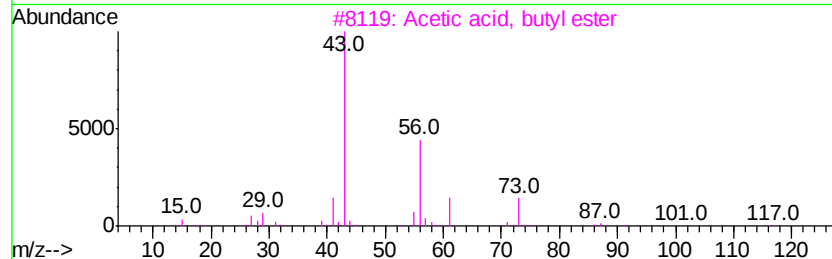
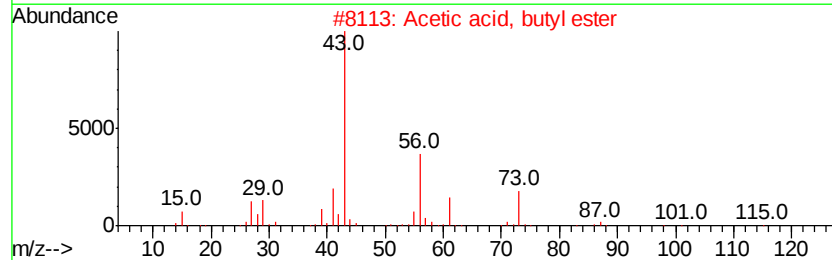
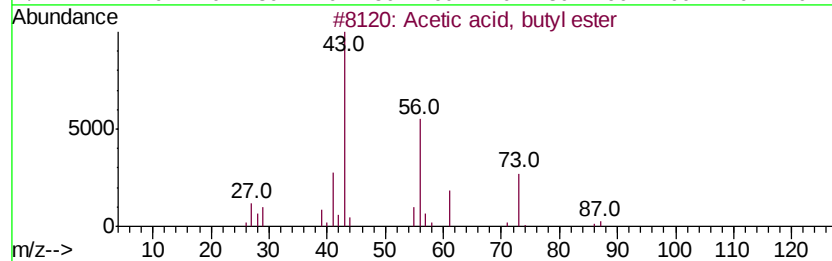
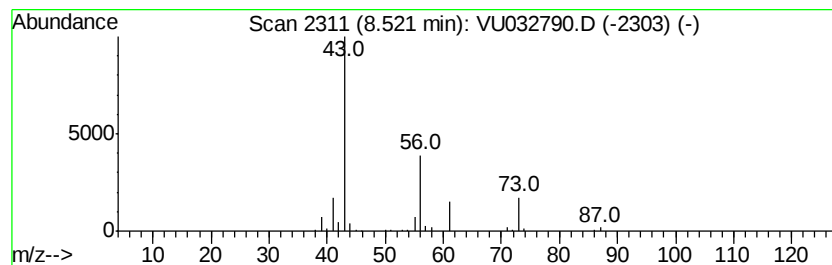
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Quant Title : VOC Analysis

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	5.52 ug/L	76563	Chlorobenzene-d5	9.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72		
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64		
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64		
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56		
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36		



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032790.D
Acq On : 17 Jun 2019 18:13
Operator : JC/SP
Sample : K3324-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW1

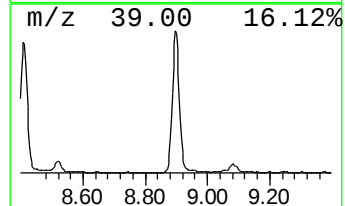
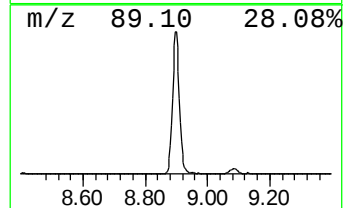
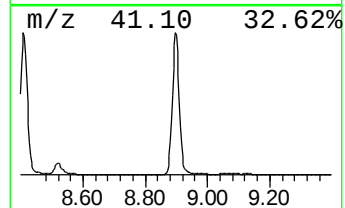
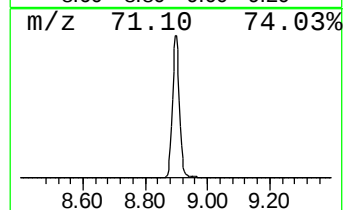
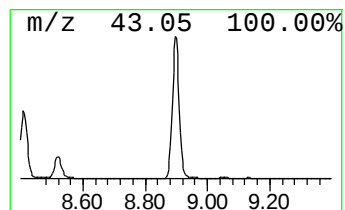
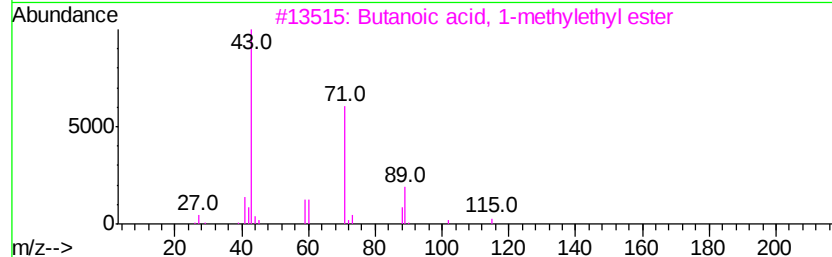
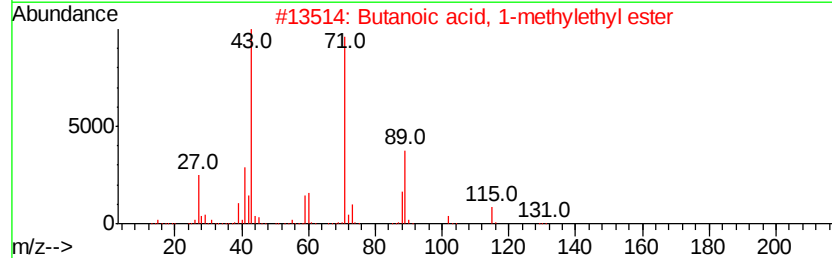
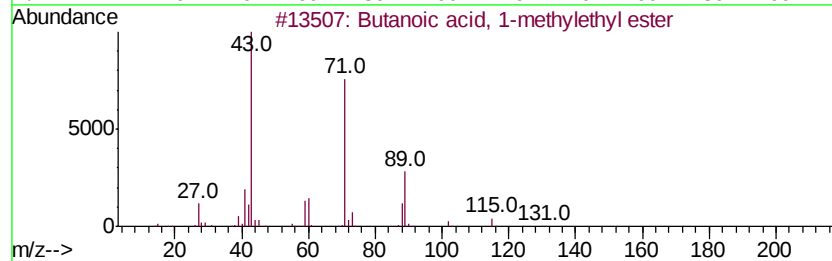
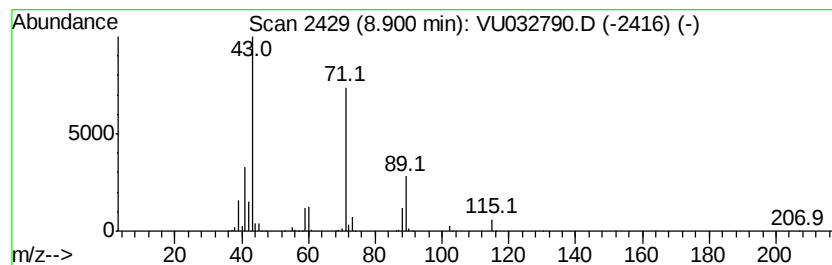
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Quant Title : VOC Analysis

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	49.03 ug/L	679834	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032790.D
Acq On : 17 Jun 2019 18:13
Operator : JC/SP
Sample : K3324-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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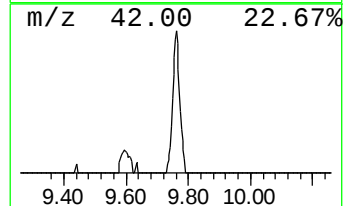
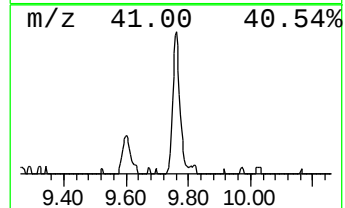
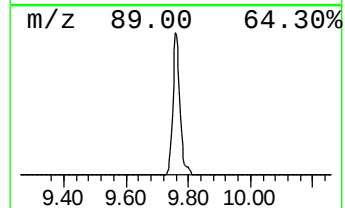
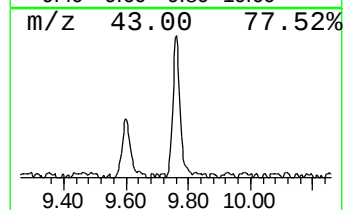
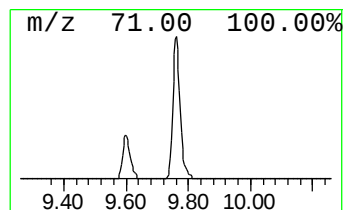
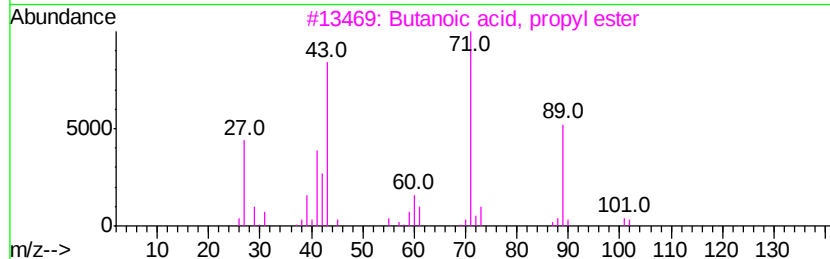
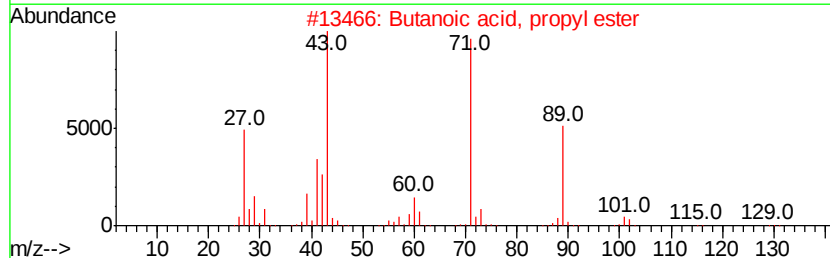
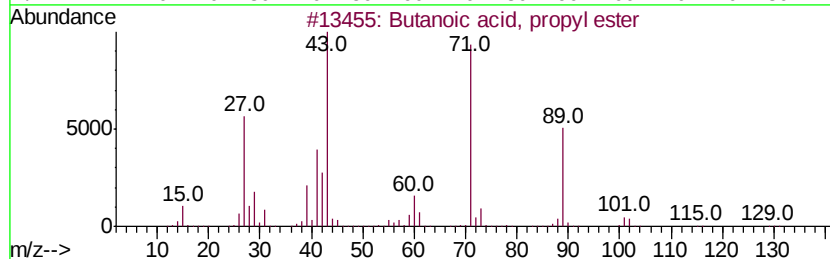
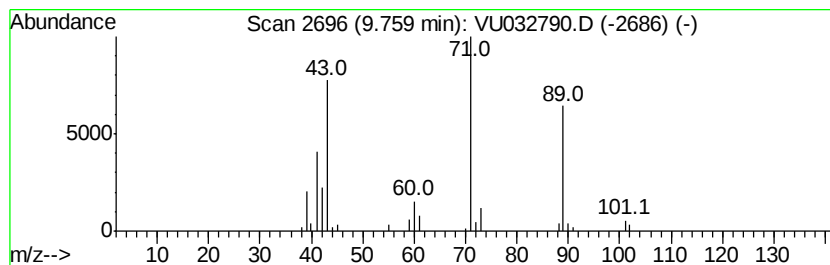
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	3.03 ug/L	42031	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
3		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
4		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
5		Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061719\
Data File : VU032790.D
Acq On : 17 Jun 2019 18:13
Operator : JC/SP
Sample : K3324-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.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	140.2	ug/L	1513520	1	5.88	539947	50.0
Propanoic acid, 1...	7.41	24.6	ug/L	265707	1	5.88	539947	50.0
Propanoic acid, 2...	8.15	10.5	ug/L	145707	2	9.08	693348	50.0
Propanoic acid, p...	8.41	71.0	ug/L	984361	2	9.08	693348	50.0
Acetic acid, buty...	8.52	5.5	ug/L	76563	2	9.08	693348	50.0
Butanoic acid, 1-...	8.90	49.0	ug/L	679834	2	9.08	693348	50.0
Butanoic acid, pr...	9.76	3.0	ug/L	42031	2	9.08	693348	50.0