

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
 Data File : VU032818.D
 Acq On : 18 Jun 2019 12:51
 Operator : JC/SP
 Sample : K3363-19
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JR0

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	24	28	34	rVB	6305	5302	0.38%	0.053%
2	1.396	88	95	105	rBV	97158	101914	7.36%	1.015%
3	1.675	175	182	194	rVB	84070	102837	7.43%	1.024%
4	2.267	356	366	376	rVB	164996	243019	17.56%	2.420%
5	2.441	417	420	423	rBV4	691	537	0.04%	0.005%
6	2.614	464	474	484	rBV5	1526	3024	0.22%	0.030%
7	2.695	489	499	513	rVB2	7413	13000	0.94%	0.129%
8	2.820	529	538	541	rBV3	742	996	0.07%	0.010%
9	3.087	616	621	626	rBV3	451	497	0.04%	0.005%
10	3.116	627	630	634	rVB2	279	229	0.02%	0.002%
11	3.177	646	649	652	rBV3	481	318	0.02%	0.003%
12	3.209	656	659	662	rBV3	338	262	0.02%	0.003%
13	3.231	662	666	671	rVB3	432	495	0.04%	0.005%
14	3.264	671	676	680	rBV3	492	580	0.04%	0.006%
15	3.383	710	713	716	rVB	414	335	0.02%	0.003%
16	3.402	716	719	720	rBV2	376	231	0.02%	0.002%
17	3.431	725	728	730	rBV	402	274	0.02%	0.003%
18	3.505	747	751	753	rBV2	353	231	0.02%	0.002%
19	3.534	757	760	763	rVB	453	304	0.02%	0.003%
20	3.553	763	766	768	rBV	386	255	0.02%	0.003%
21	3.694	804	810	813	rVV3	311	329	0.02%	0.003%
22	3.958	887	892	893	rVV	289	259	0.02%	0.003%
23	3.971	894	896	902	rVB2	487	267	0.02%	0.003%
24	4.051	915	921	923	rBV2	311	364	0.03%	0.004%
25	4.167	944	957	990	rBV	88518	232918	16.83%	2.320%
26	4.350	1012	1014	1017	rVB3	507	253	0.02%	0.003%
27	4.379	1021	1023	1027	rBV2	379	285	0.02%	0.003%
28	4.579	1080	1085	1088	rBV3	339	338	0.02%	0.003%
29	4.640	1088	1104	1125	rBV	140236	328079	23.70%	3.268%
30	4.868	1171	1175	1178	rBV2	676	517	0.04%	0.005%
31	4.887	1178	1181	1192	rVB5	720	916	0.07%	0.009%
32	4.952	1196	1201	1206	rBV2	188	263	0.02%	0.003%
33	4.984	1207	1211	1214	rVB2	379	292	0.02%	0.003%
34	5.051	1226	1232	1235	rBV3	330	270	0.02%	0.003%

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35	5.093	1242	1245	1250	rBV2	300	280	0.02%	0.003%
36	5.331	1294	1319	1345	rBV2	266196	807795	58.36%	8.046%
37	5.550	1378	1387	1401	rVB4	5528	11413	0.82%	0.114%
38	5.643	1413	1416	1421	rBB3	423	359	0.03%	0.004%
39	5.749	1443	1449	1452	rVB3	305	278	0.02%	0.003%
40	5.881	1470	1490	1511	rBV	270090	533238	38.53%	5.311%
41	6.186	1574	1585	1597	rVB4	4674	8991	0.65%	0.090%
42	6.325	1614	1628	1645	rBV	188256	374941	27.09%	3.734%
43	6.421	1651	1658	1672	rVB3	5686	11424	0.83%	0.114%
44	6.534	1685	1693	1698	rBV3	2689	4255	0.31%	0.042%
45	6.575	1700	1706	1713	rVV	4117	6872	0.50%	0.068%
46	6.698	1731	1744	1780	rBV	778072	1384121	100.00%	13.786%
47	7.048	1850	1853	1858	rVB3	491	397	0.03%	0.004%
48	7.080	1858	1863	1865	rBV3	598	474	0.03%	0.005%
49	7.112	1870	1873	1878	rVB2	335	254	0.02%	0.003%
50	7.222	1894	1907	1922	rBV	94670	170118	12.29%	1.694%
51	7.347	1943	1946	1947	rBV2	445	245	0.02%	0.002%
52	7.366	1947	1952	1955	rVV3	833	749	0.05%	0.007%
53	7.415	1955	1967	1997	rVB	138787	242264	17.50%	2.413%
54	7.559	1998	2012	2029	rBV	351063	603136	43.58%	6.007%
55	7.775	2070	2079	2086	rBV5	1151	1526	0.11%	0.015%
56	7.842	2089	2100	2116	rBV2	82234	143162	10.34%	1.426%
57	8.019	2151	2155	2158	rVB4	623	507	0.04%	0.005%
58	8.045	2158	2163	2165	rBV	359	349	0.03%	0.003%
59	8.148	2184	2195	2210	rVV	75397	125860	9.09%	1.254%
60	8.225	2210	2219	2223	rVV3	17569	27789	2.01%	0.277%
61	8.257	2224	2229	2235	rVV2	31916	48013	3.47%	0.478%
62	8.305	2235	2244	2265	rVV	314612	540839	39.07%	5.387%
63	8.411	2266	2277	2300	rVV	561809	895113	64.67%	8.915%
64	8.521	2303	2311	2329	rVB	37728	63911	4.62%	0.637%
65	8.710	2366	2370	2373	rVB2	492	340	0.02%	0.003%
66	8.733	2373	2377	2382	rVB3	263	257	0.02%	0.003%
67	8.759	2382	2385	2387	rBV2	428	328	0.02%	0.003%
68	8.900	2415	2429	2448	rBV	372494	594426	42.95%	5.921%
69	9.083	2471	2486	2510	rBV	404005	664059	47.98%	6.614%
70	9.244	2531	2536	2539	rBV2	435	372	0.03%	0.004%
71	9.331	2560	2563	2566	rVV2	489	323	0.02%	0.003%

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72	9.366	2570	2574	2576	rBV4	379	308	0.02%	0.003%
73	9.382	2576	2579	2587	rVB5	506	566	0.04%	0.006%
74	9.460	2599	2603	2607	rBV3	408	362	0.03%	0.004%
75	9.482	2607	2610	2614	rVV2	541	400	0.03%	0.004%
76	9.514	2617	2620	2628	rBV3	273	238	0.02%	0.002%
77	9.601	2637	2647	2659	rBV3	5961	9914	0.72%	0.099%
78	9.762	2685	2697	2708	rBV2	20343	32461	2.35%	0.323%
79	9.849	2722	2724	2728	rVB2	524	307	0.02%	0.003%
80	9.884	2733	2735	2739	rVV3	321	248	0.02%	0.002%
81	9.929	2747	2749	2758	rVB3	440	436	0.03%	0.004%
82	9.968	2758	2761	2763	rBV2	420	236	0.02%	0.002%
83	10.106	2799	2804	2807	rVV3	452	443	0.03%	0.004%
84	10.234	2841	2844	2849	rVB3	468	441	0.03%	0.004%
85	10.427	2890	2904	2921	rBV	288153	464883	33.59%	4.630%
86	10.771	3008	3011	3017	rVB2	387	299	0.02%	0.003%
87	10.810	3017	3023	3026	rBV2	234	252	0.02%	0.003%
88	10.926	3057	3059	3063	rVB2	408	268	0.02%	0.003%
89	11.479	3218	3231	3254	rBV	399293	629601	45.49%	6.271%
90	11.559	3254	3256	3259	rVV2	592	303	0.02%	0.003%
91	11.614	3270	3273	3277	rVB5	791	592	0.04%	0.006%
92	11.649	3281	3284	3289	rVB3	738	584	0.04%	0.006%
93	11.784	3324	3326	3329	rBV3	475	347	0.03%	0.003%
94	11.855	3335	3348	3367	rBV	354727	585412	42.29%	5.831%
95	12.148	3436	3439	3442	rBV3	432	283	0.02%	0.003%
96	12.411	3517	3521	3527	rBV4	306	374	0.03%	0.004%
97	13.147	3748	3750	3754	rVB3	474	295	0.02%	0.003%
98	14.086	4040	4042	4046	rBV2	408	266	0.02%	0.003%
99	14.546	4183	4185	4189	rBV2	482	374	0.03%	0.004%
100	15.163	4373	4377	4380	rBV2	896	822	0.06%	0.008%

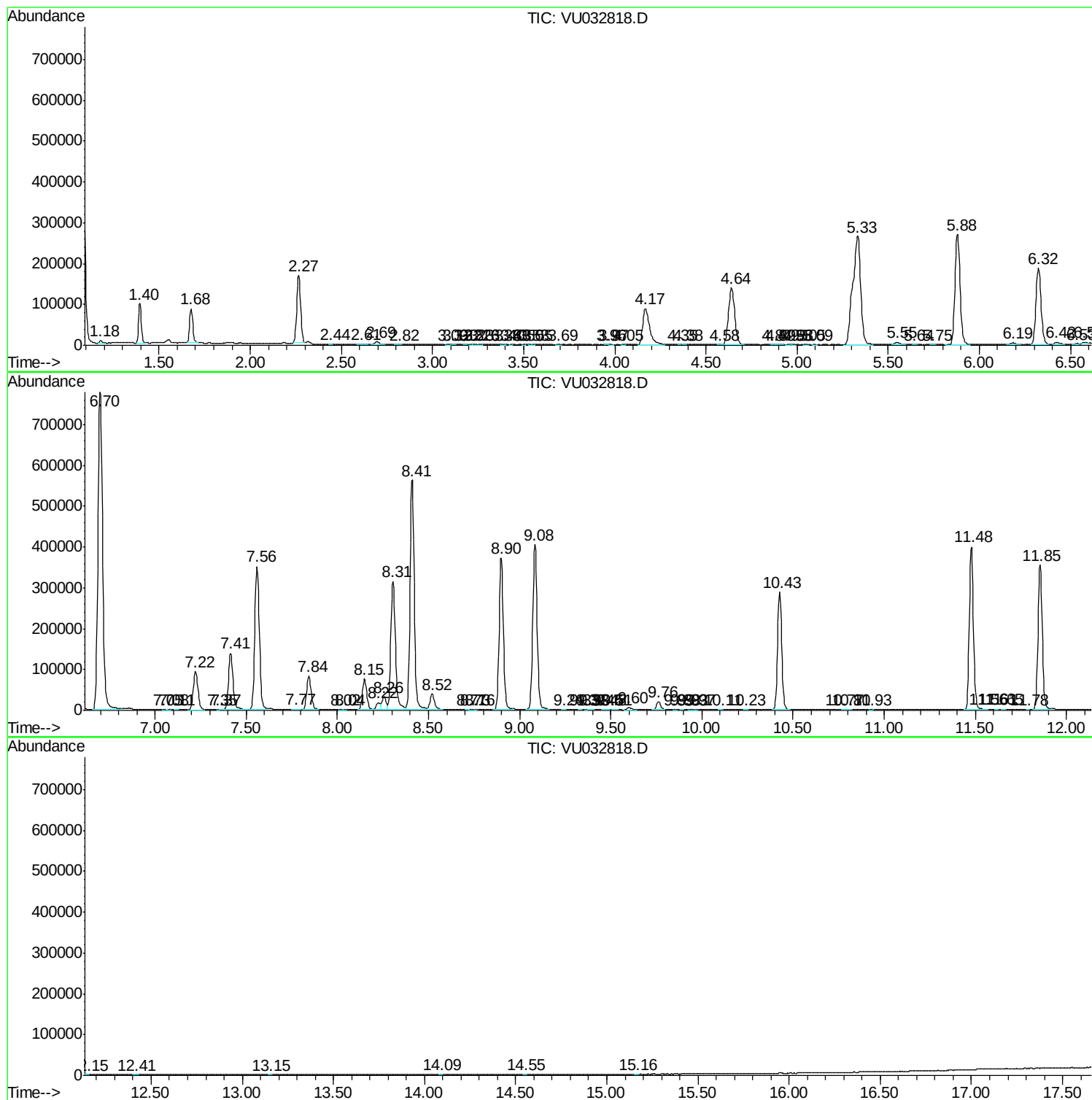
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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



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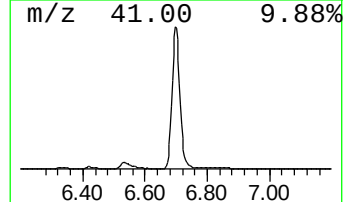
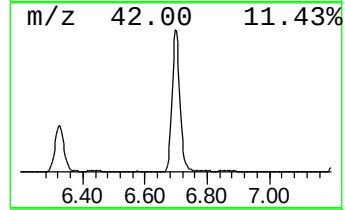
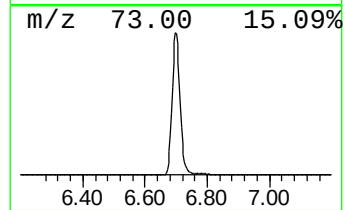
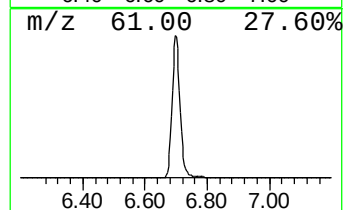
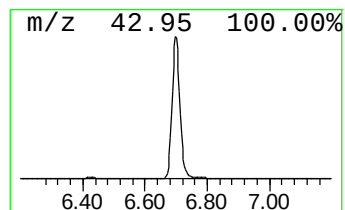
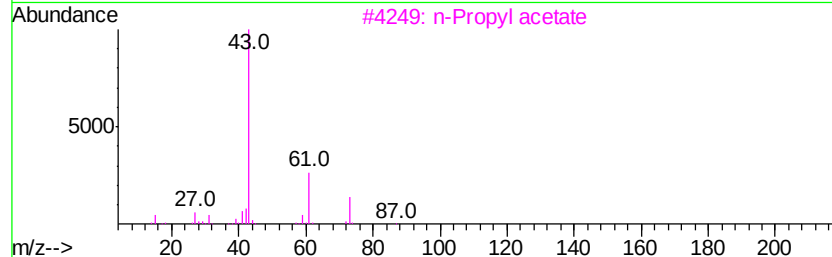
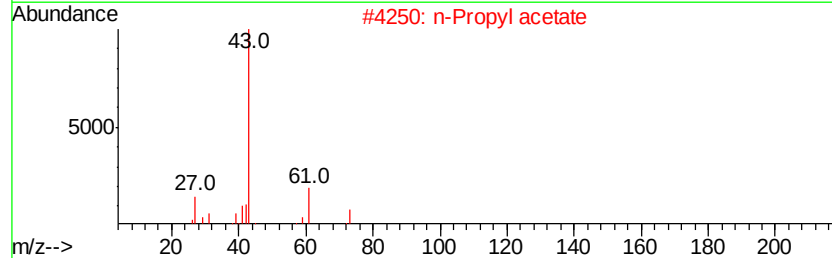
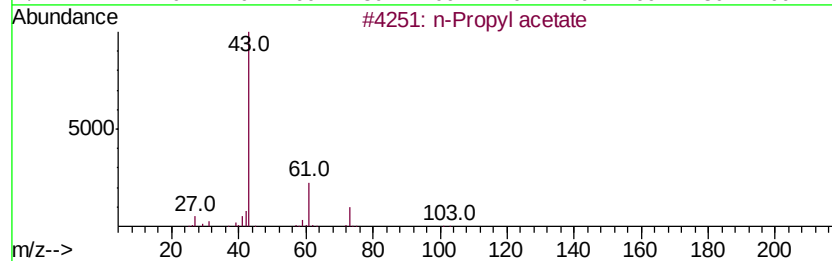
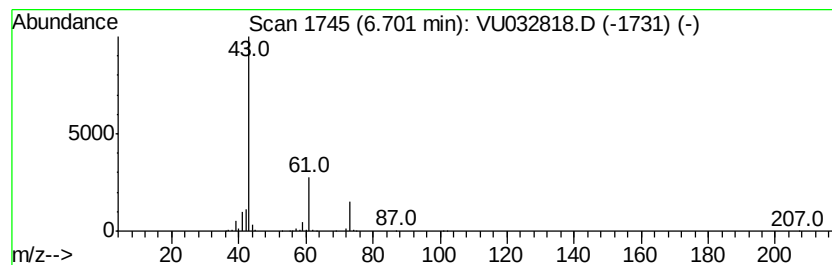
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	129.79 ug/L	1384120	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		Isopropyl acetate	102	C5H10O2	000108-21-4	9



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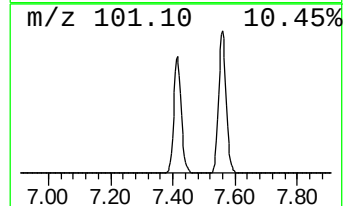
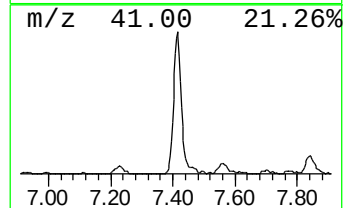
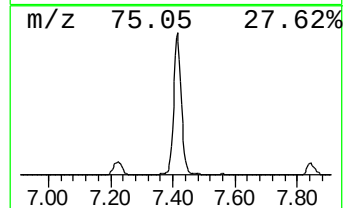
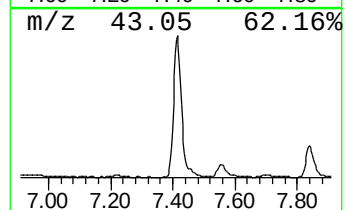
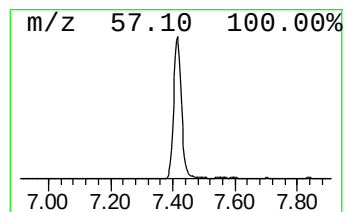
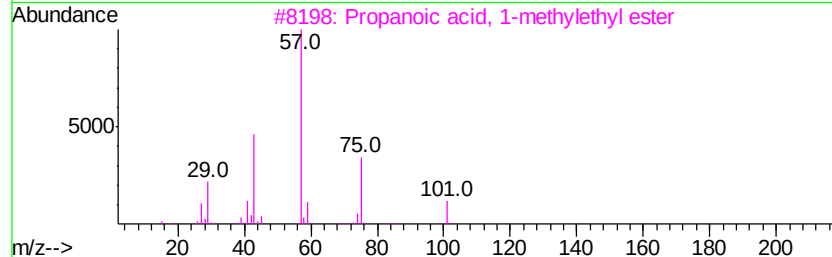
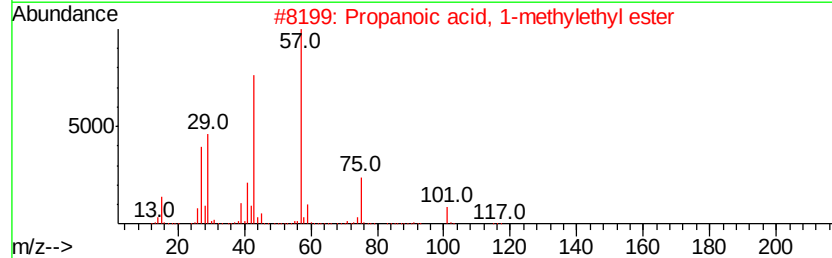
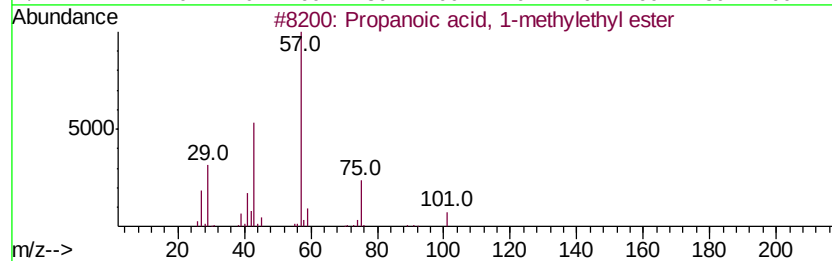
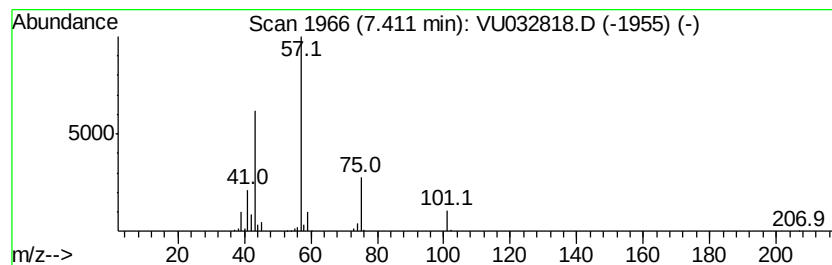
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Quant Title : VOC Analysis

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	22.72 ug/L	242264	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	86
2		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45



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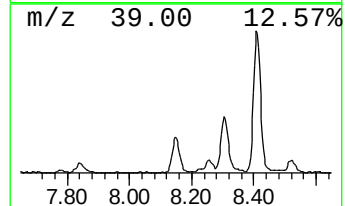
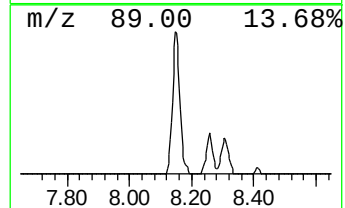
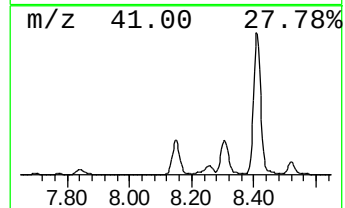
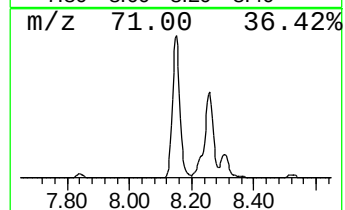
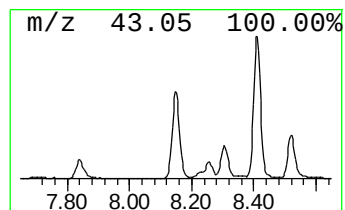
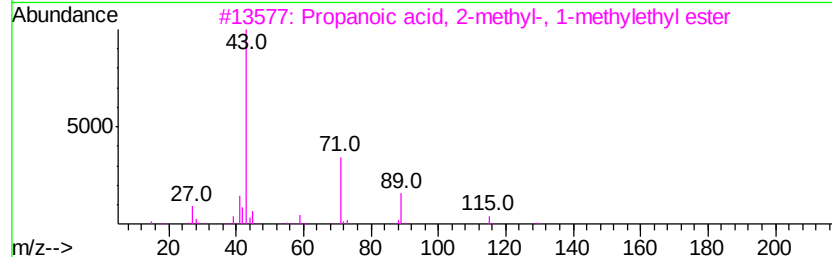
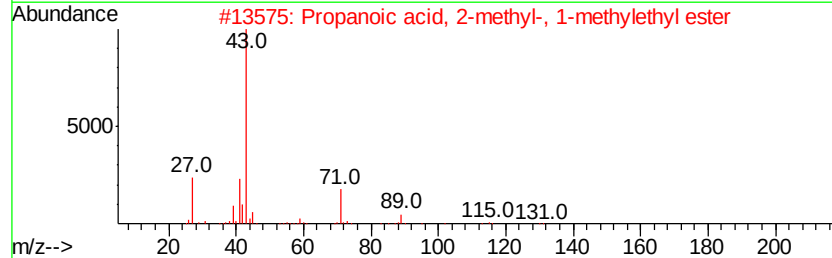
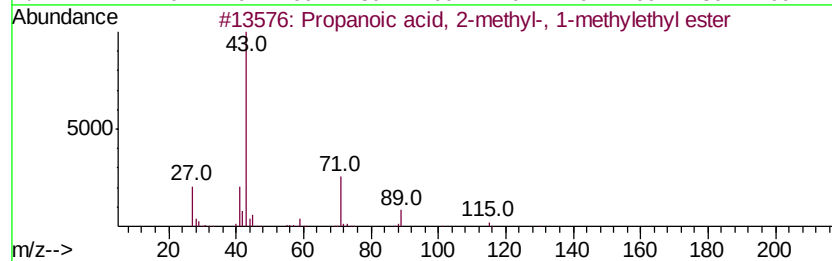
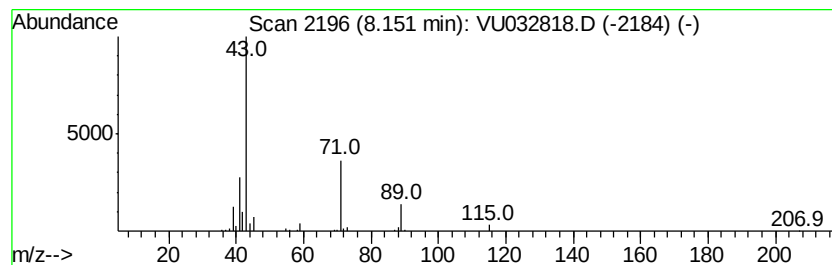
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Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.48 ug/L	125860	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-, 1-met...	130	C7H14O2	000617-50-5	83
4		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	56



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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JR0

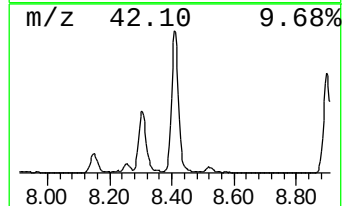
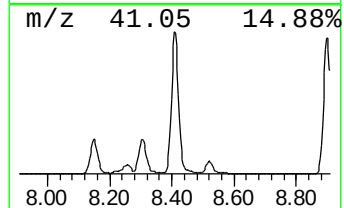
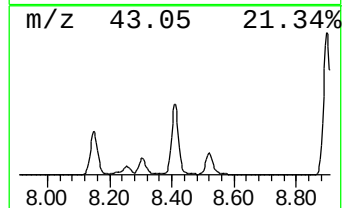
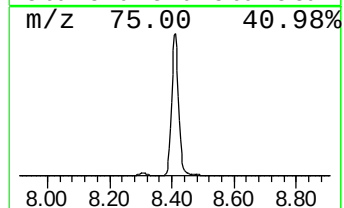
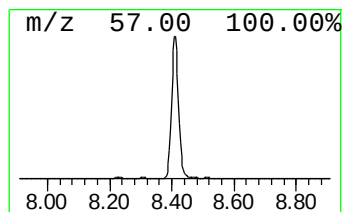
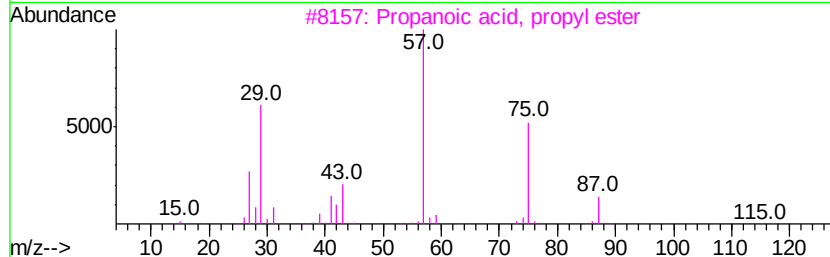
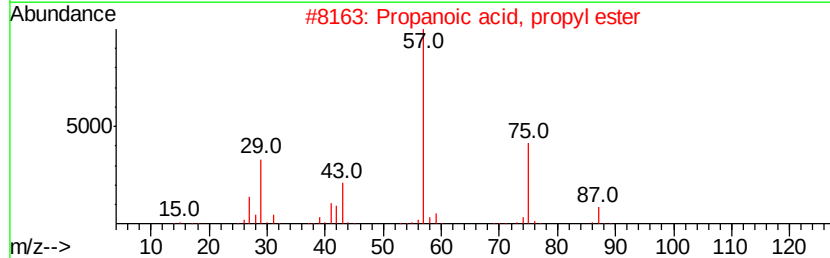
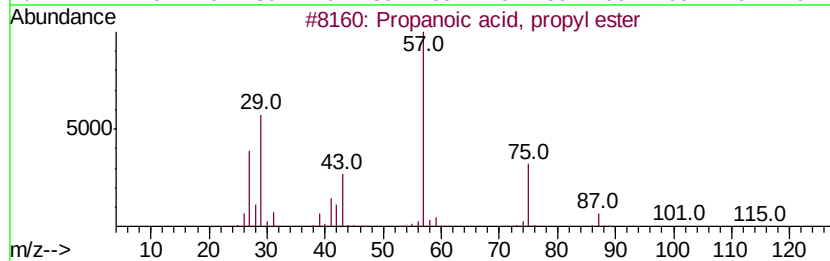
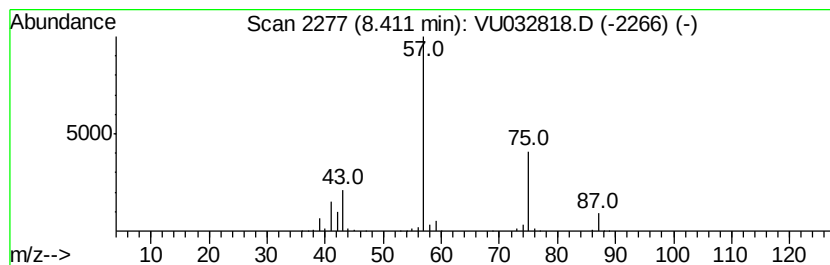
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Quant Title : VOC Analysis

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	67.40 ug/L	895113	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	25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032818.D
Acq On : 18 Jun 2019 12:51
Operator : JC/SP
Sample : K3363-19
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR0

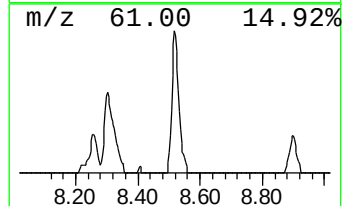
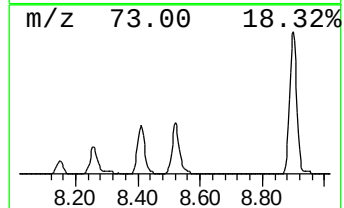
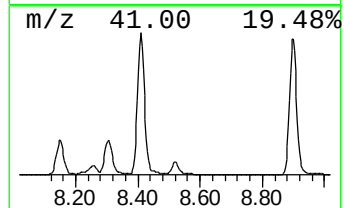
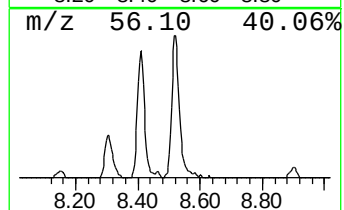
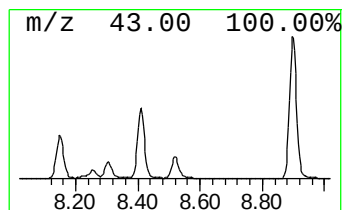
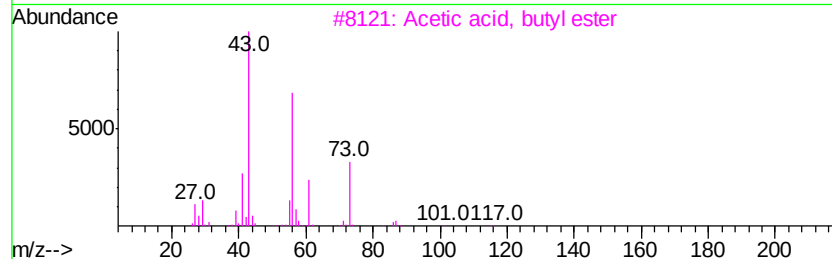
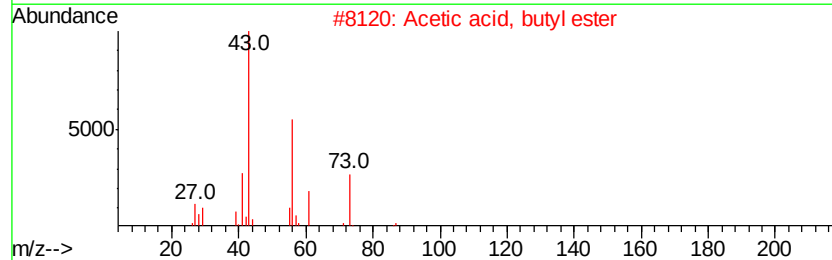
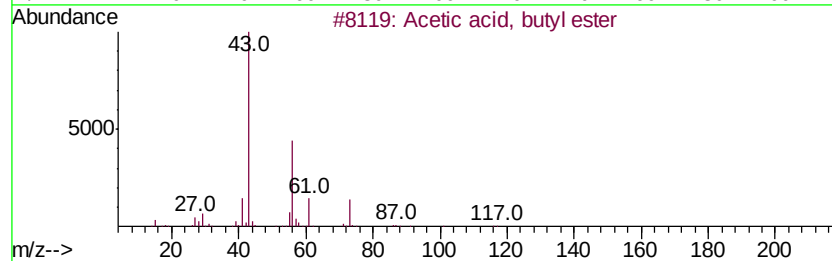
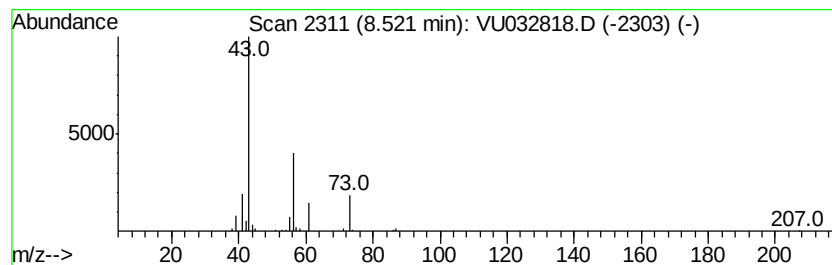
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Quant Title : VOC Analysis

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	4.81 ug/L	63911	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
3		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
4		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
5		1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	23



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032818.D
Acq On : 18 Jun 2019 12:51
Operator : JC/SP
Sample : K3363-19
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR0

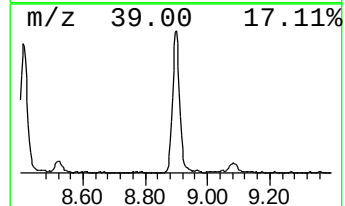
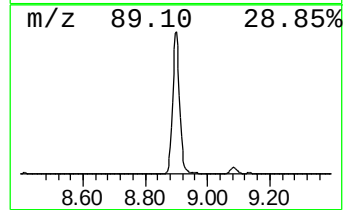
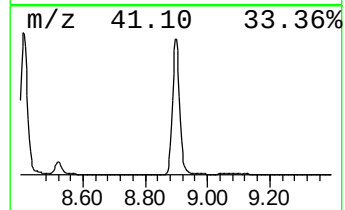
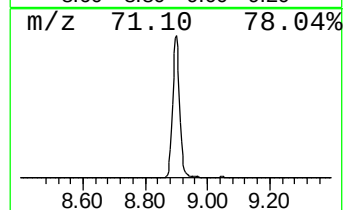
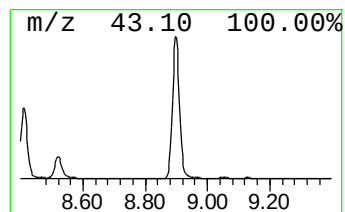
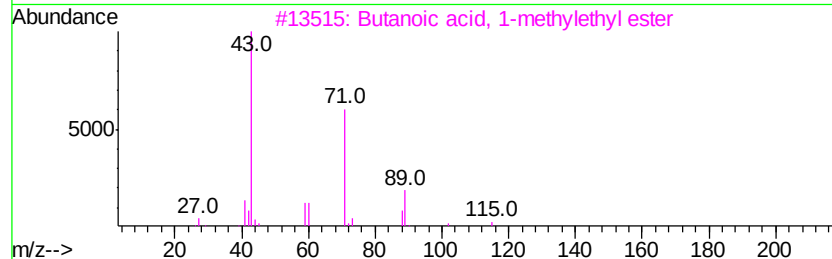
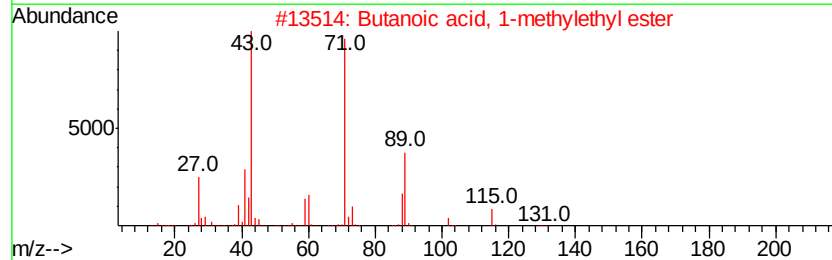
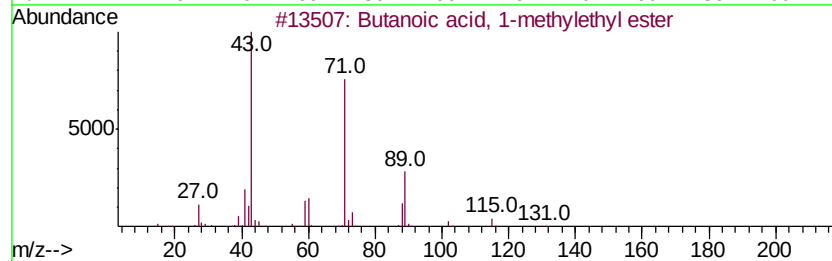
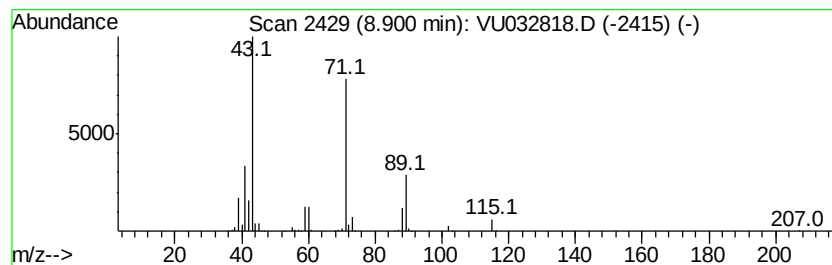
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	44.76 ug/L	594426	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
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-, propy...	130	C7H14O2	000644-49-5	72
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032818.D
Acq On : 18 Jun 2019 12:51
Operator : JC/SP
Sample : K3363-19
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR0

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	129.8	ug/L	1384120	1	5.88	533238	50.0
Propanoic acid, 1...	7.41	22.7	ug/L	242264	1	5.88	533238	50.0
Propanoic acid, 2...	8.15	9.5	ug/L	125860	2	9.08	664059	50.0
Propanoic acid, p...	8.41	67.4	ug/L	895113	2	9.08	664059	50.0
Acetic acid, buty...	8.52	4.8	ug/L	63911	2	9.08	664059	50.0
Butanoic acid, 1-...	8.90	44.8	ug/L	594426	2	9.08	664059	50.0