

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061719\
 Data File : VU032805.D
 Acq On : 17 Jun 2019 23:56
 Operator : JC/SP
 Sample : K3363-02
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JT6

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	38	rVB	7672	6735	0.05%	0.021%
2	1.396	88	95	107	rVB2	213896	234333	1.58%	0.748%
3	1.675	174	182	197	rVV	97181	120118	0.81%	0.383%
4	1.743	197	203	216	rVB	10590	13359	0.09%	0.043%
5	2.273	356	368	392	rVB3	402731	750062	5.06%	2.394%
6	2.547	451	453	456	rVB	545	262	0.00%	0.001%
7	2.617	468	475	488	rVB2	2666	4392	0.03%	0.014%
8	2.695	491	499	510	rBV3	5093	8295	0.06%	0.026%
9	2.762	517	520	523	rBV	319	275	0.00%	0.001%
10	2.875	552	555	561	rVB4	448	380	0.00%	0.001%
11	2.907	561	565	570	rBV2	197	251	0.00%	0.001%
12	2.977	570	587	612	rBV	288437	528128	3.56%	1.686%
13	3.174	645	648	651	rVV2	402	345	0.00%	0.001%
14	3.206	656	658	667	rVB3	672	763	0.01%	0.002%
15	3.399	715	718	719	rVV	453	238	0.00%	0.001%
16	3.421	723	725	727	rVV2	438	249	0.00%	0.001%
17	3.431	727	728	733	rVB2	342	239	0.00%	0.001%
18	3.627	785	789	790	rBV	368	274	0.00%	0.001%
19	3.785	835	838	844	rVB2	295	249	0.00%	0.001%
20	3.868	860	864	867	rBV3	339	273	0.00%	0.001%
21	4.042	913	918	920	rBV2	267	288	0.00%	0.001%
22	4.087	928	932	935	rBV4	329	235	0.00%	0.001%
23	4.215	940	972	1022	rBV	6096291	14820553	100.00%	47.309%
24	4.640	1088	1104	1127	rBV	154408	356743	2.41%	1.139%
25	5.148	1257	1262	1265	rVB2	346	269	0.00%	0.001%
26	5.331	1295	1319	1348	rBV2	308131	909997	6.14%	2.905%
27	5.547	1374	1386	1399	rBV	6181	12863	0.09%	0.041%
28	5.813	1466	1469	1475	rBV4	355	350	0.00%	0.001%
29	5.881	1476	1490	1514	rBV	279268	547167	3.69%	1.747%
30	6.180	1566	1583	1610	rBV	2743618	5167912	34.87%	16.497%
31	6.325	1615	1628	1647	rVB	208656	415259	2.80%	1.326%
32	6.421	1651	1658	1668	rVB	5487	9608	0.06%	0.031%
33	6.527	1686	1691	1696	rBV3	2149	3190	0.02%	0.010%
34	6.698	1731	1744	1777	rBV	710452	1252154	8.45%	3.997%

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 Title : VOC Analysis

35	6.955	1822	1824	1827	rBV2	549	275	0.00%	0.001%
36	7.222	1894	1907	1924	rBV	119328	212405	1.43%	0.678%
37	7.415	1955	1967	1991	rBV	138256	237532	1.60%	0.758%
38	7.559	1999	2012	2028	rBV	429613	742938	5.01%	2.372%
39	7.698	2050	2055	2067	rVB8	2049	3625	0.02%	0.012%
40	7.762	2072	2075	2089	rVB6	1115	1805	0.01%	0.006%
41	7.842	2089	2100	2122	rBV2	99381	172040	1.16%	0.549%
42	8.000	2146	2149	2152	rVB3	449	315	0.00%	0.001%
43	8.022	2153	2156	2160	rBV2	451	386	0.00%	0.001%
44	8.148	2184	2195	2212	rBV	75690	124413	0.84%	0.397%
45	8.225	2212	2219	2222	rVV4	10559	14212	0.10%	0.045%
46	8.257	2223	2229	2234	rVV3	29973	44492	0.30%	0.142%
47	8.305	2234	2244	2264	rVV	317842	550560	3.71%	1.757%
48	8.408	2266	2276	2301	rVV	500997	798458	5.39%	2.549%
49	8.521	2303	2311	2329	rVB	31971	54356	0.37%	0.174%
50	8.752	2376	2383	2384	rBV2	279	323	0.00%	0.001%
51	8.762	2384	2386	2389	rVV3	362	228	0.00%	0.001%
52	8.897	2414	2428	2449	rBV	348711	552596	3.73%	1.764%
53	9.083	2470	2486	2513	rBV	425989	702477	4.74%	2.242%
54	9.225	2527	2530	2534	rVB2	455	348	0.00%	0.001%
55	9.366	2566	2574	2579	rVB7	676	932	0.01%	0.003%
56	9.511	2616	2619	2621	rVB	377	255	0.00%	0.001%
57	9.601	2637	2647	2662	rBV4	4762	9442	0.06%	0.030%
58	9.762	2688	2697	2712	rVV2	17147	27017	0.18%	0.086%
59	9.852	2722	2725	2728	rBV2	415	304	0.00%	0.001%
60	9.903	2736	2741	2746	rBV4	350	534	0.00%	0.002%
61	10.231	2838	2843	2846	rBV4	358	357	0.00%	0.001%
62	10.257	2846	2851	2853	rBV3	316	283	0.00%	0.001%
63	10.424	2891	2903	2928	rVB	302205	490686	3.31%	1.566%
64	10.678	2979	2982	2986	rBV3	456	278	0.00%	0.001%
65	10.714	2989	2993	2997	rVB4	368	313	0.00%	0.001%
66	10.771	3008	3011	3015	rBV2	286	231	0.00%	0.001%
67	10.881	3042	3045	3049	rBV2	356	253	0.00%	0.001%
68	10.926	3054	3059	3061	rBV4	324	290	0.00%	0.001%
69	11.013	3082	3086	3087	rBV3	357	322	0.00%	0.001%
70	11.099	3110	3113	3117	rVB2	503	320	0.00%	0.001%
71	11.151	3126	3129	3132	rBV2	333	246	0.00%	0.001%

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72	11.202	3141	3145	3153	rVB3	489	581	0.00%	0.002%
73	11.321	3179	3182	3184	rBV3	400	294	0.00%	0.001%
74	11.395	3202	3205	3208	rVB2	515	323	0.00%	0.001%
75	11.418	3208	3212	3217	rBV2	325	408	0.00%	0.001%
76	11.479	3219	3231	3255	rBV	438605	699715	4.72%	2.234%
77	11.707	3300	3302	3307	rVB4	367	271	0.00%	0.001%
78	11.855	3335	3348	3372	rBV	424034	705720	4.76%	2.253%
79	12.112	3424	3428	3431	rBV4	441	305	0.00%	0.001%
80	12.148	3437	3439	3442	rBV3	374	239	0.00%	0.001%
81	12.164	3442	3444	3449	rVB3	570	396	0.00%	0.001%
82	12.186	3449	3451	3454	rBV2	308	231	0.00%	0.001%
83	12.247	3466	3470	3478	rVB4	699	787	0.01%	0.003%
84	12.289	3479	3483	3488	rBV2	646	521	0.00%	0.002%
85	12.315	3488	3491	3495	rBV3	480	377	0.00%	0.001%
86	12.408	3516	3520	3523	rBV	355	280	0.00%	0.001%
87	12.456	3533	3535	3538	rBV2	412	253	0.00%	0.001%
88	12.652	3592	3596	3601	rBV3	375	277	0.00%	0.001%
89	12.967	3692	3694	3697	rVB3	442	228	0.00%	0.001%
90	13.032	3712	3714	3718	rVB3	737	474	0.00%	0.002%
91	13.456	3844	3846	3850	rBV2	410	247	0.00%	0.001%
92	13.543	3871	3873	3878	rVB3	484	328	0.00%	0.001%
93	13.591	3885	3888	3891	rBV2	602	403	0.00%	0.001%
94	13.707	3921	3924	3928	rBV2	524	436	0.00%	0.001%
95	13.784	3945	3948	3952	rBV2	451	408	0.00%	0.001%
96	13.938	3994	3996	4000	rBV2	370	250	0.00%	0.001%
97	14.363	4126	4128	4132	rBV4	437	321	0.00%	0.001%
98	14.398	4136	4139	4142	rVV2	611	425	0.00%	0.001%
99	14.623	4207	4209	4210	rBV	595	263	0.00%	0.001%
100	15.141	4368	4370	4373	rBV2	680	393	0.00%	0.001%

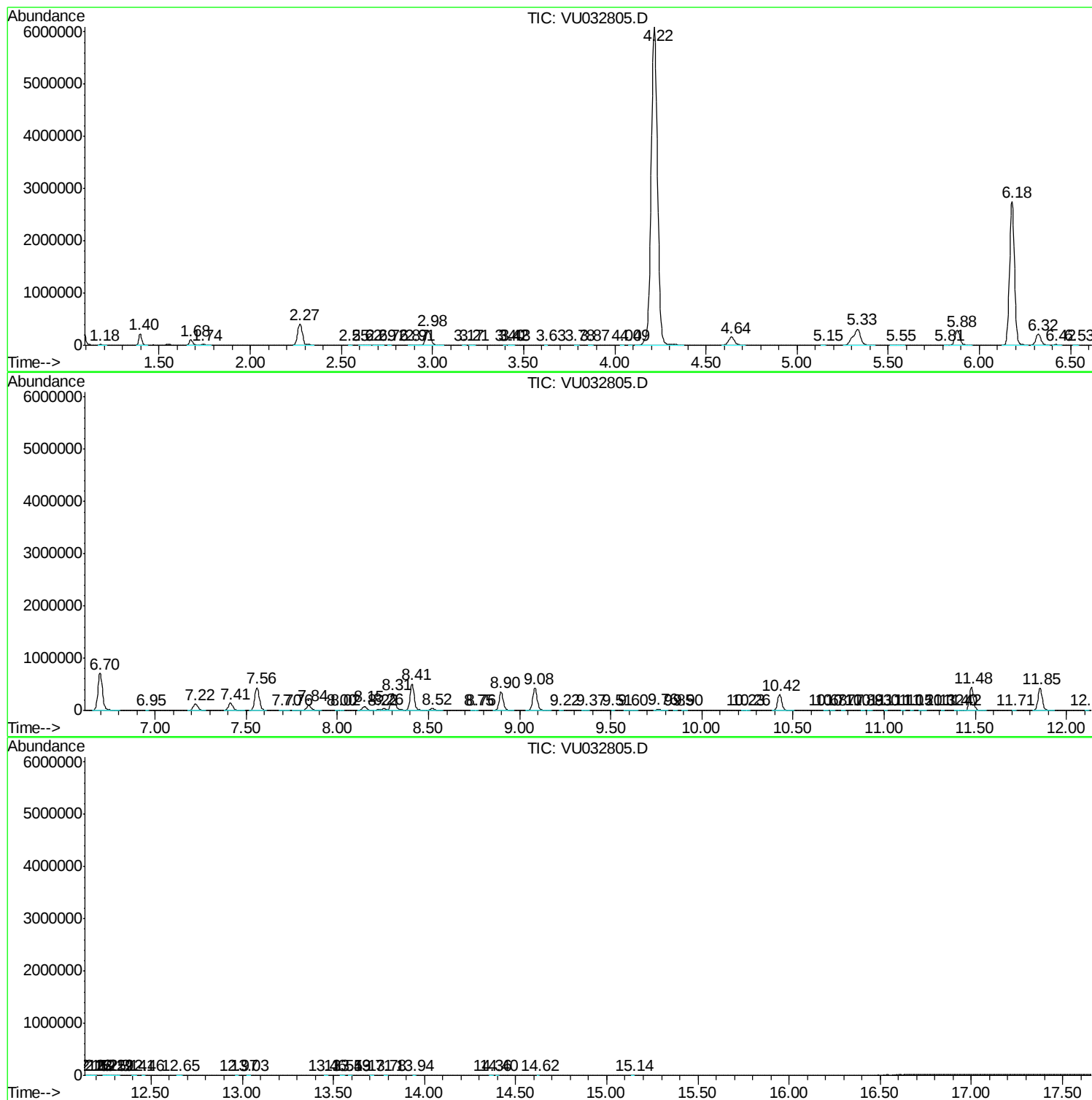
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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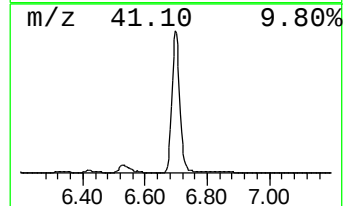
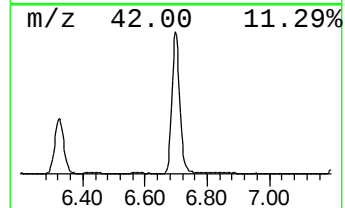
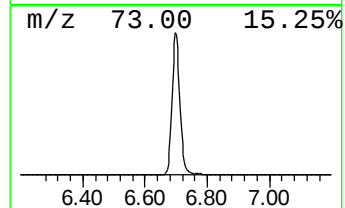
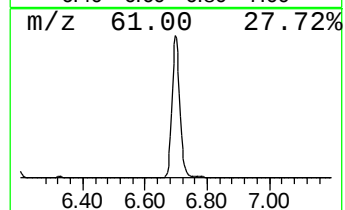
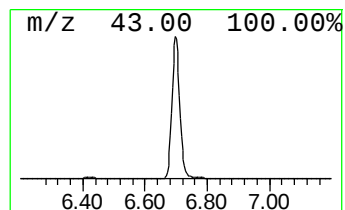
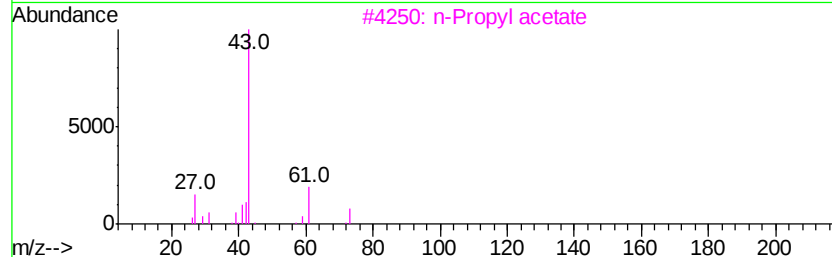
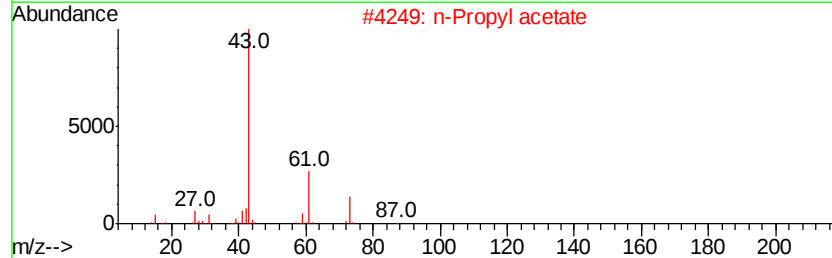
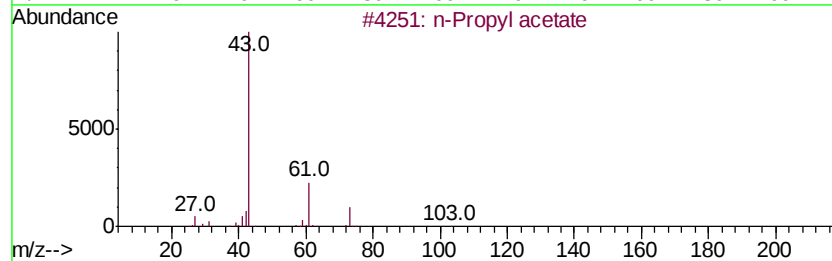
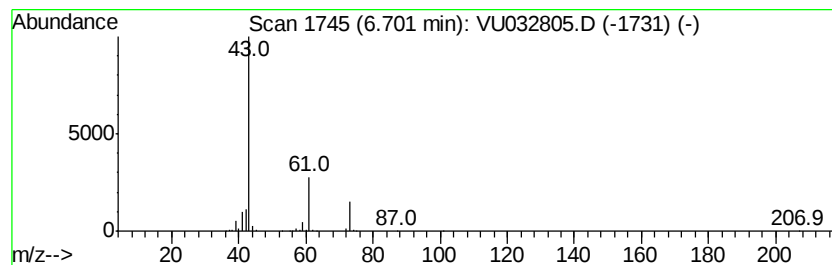
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	114.42 ug/L	1252150	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		Isobutylamine	73	C4H11N	000078-81-9	9



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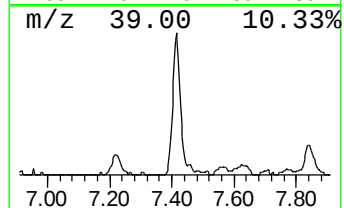
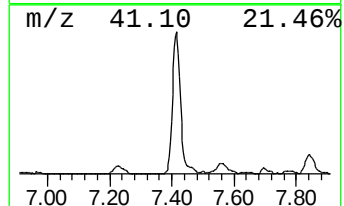
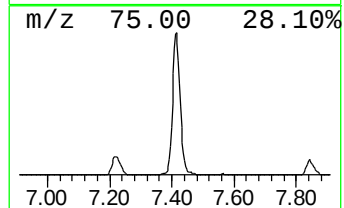
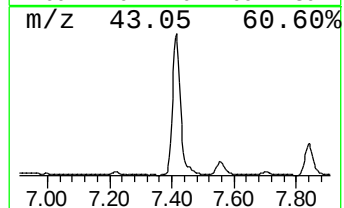
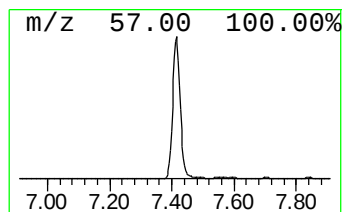
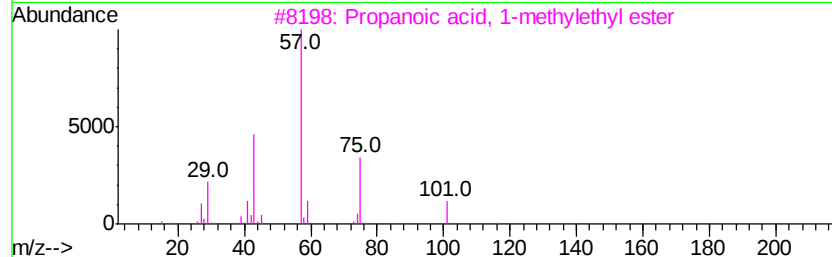
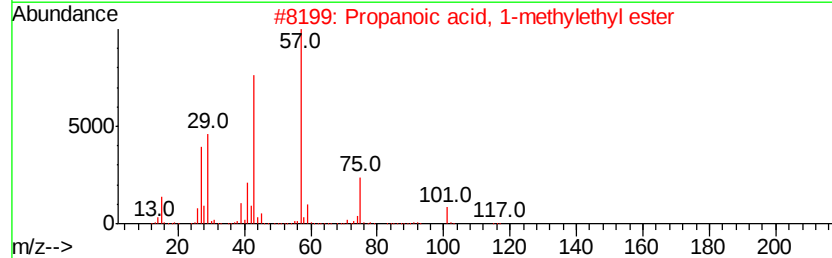
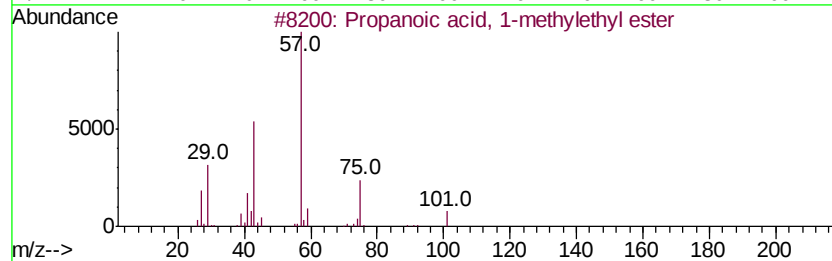
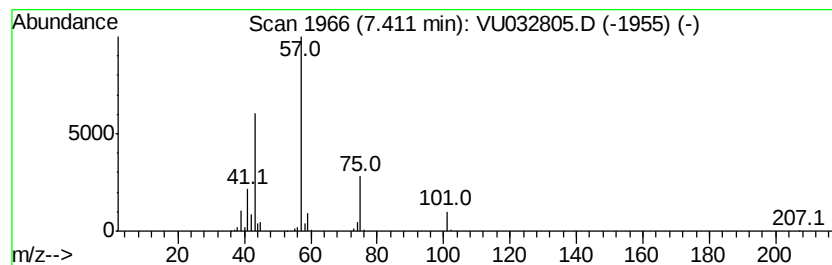
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	21.71 ug/L	237532	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	83
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	42
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40



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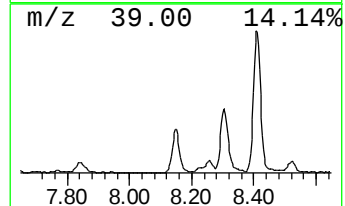
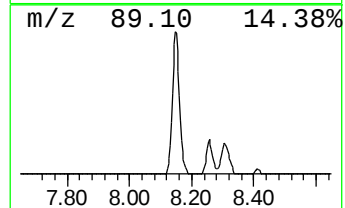
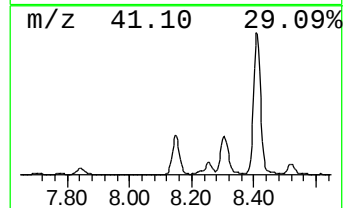
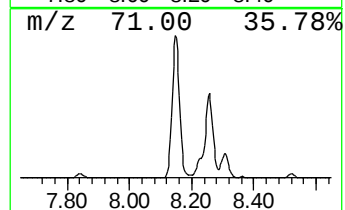
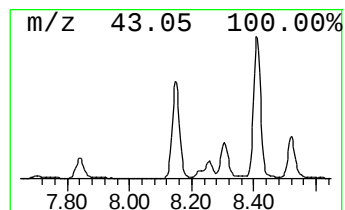
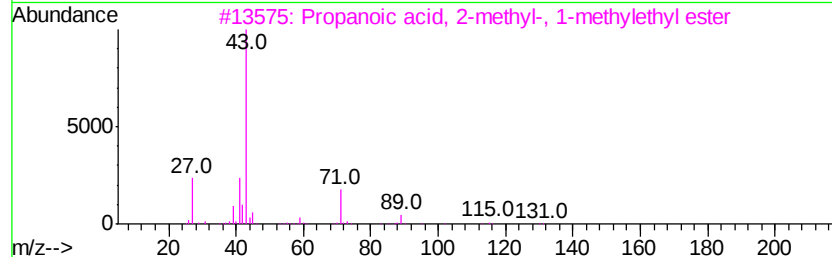
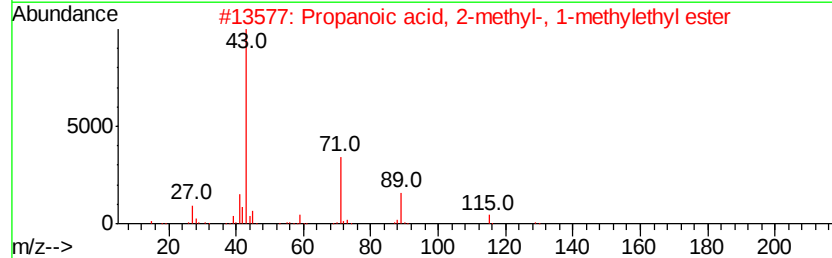
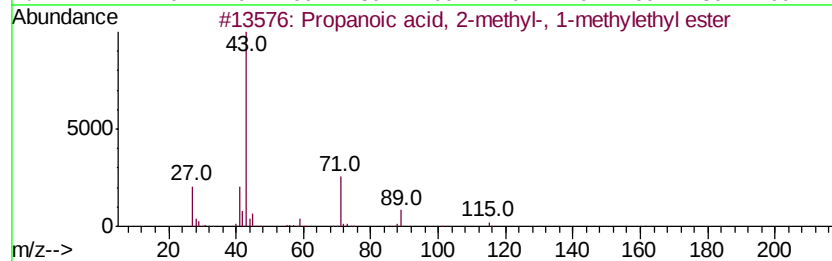
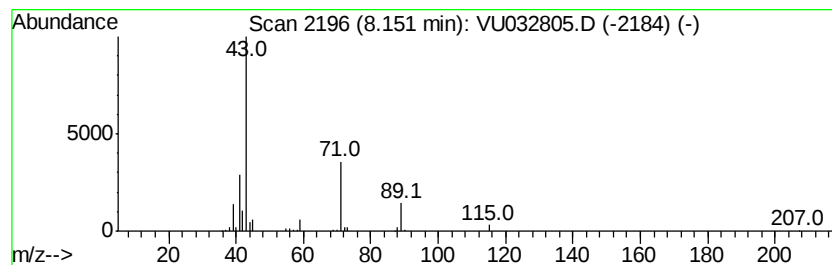
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	8.86 ug/L	124413	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	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-, 1-met...	130	C7H14O2	000617-50-5	72	
5	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	53	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032805.D
Acq On : 17 Jun 2019 23:56
Operator : JC/SP
Sample : K3363-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JT6

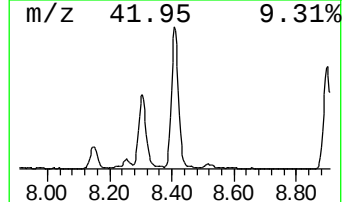
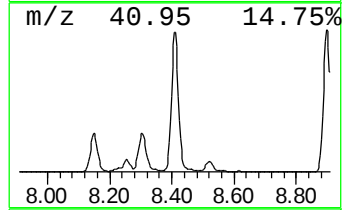
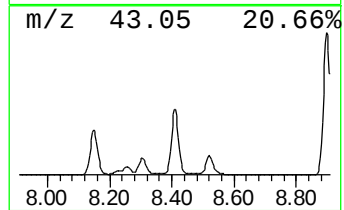
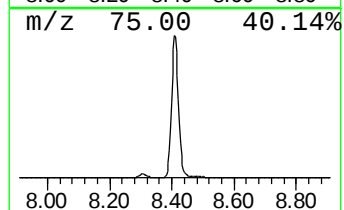
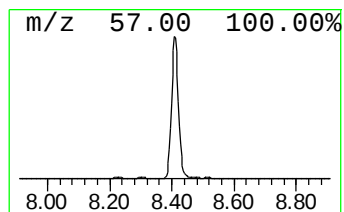
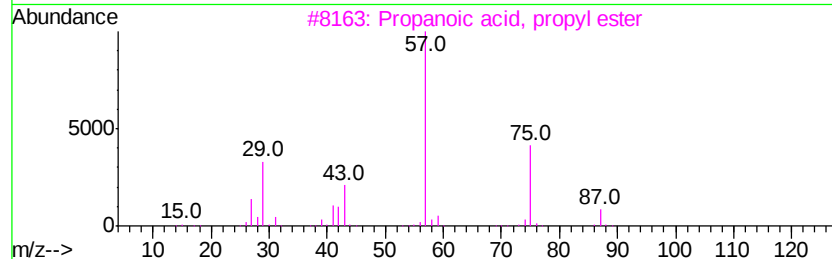
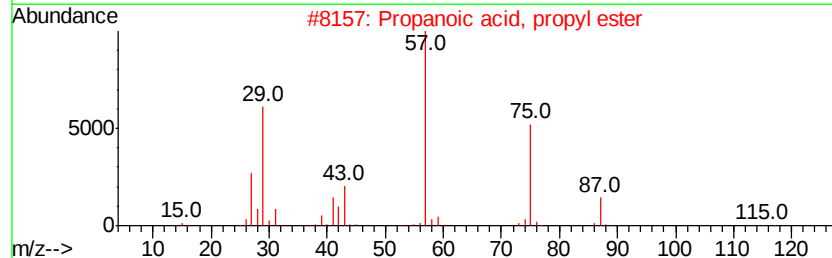
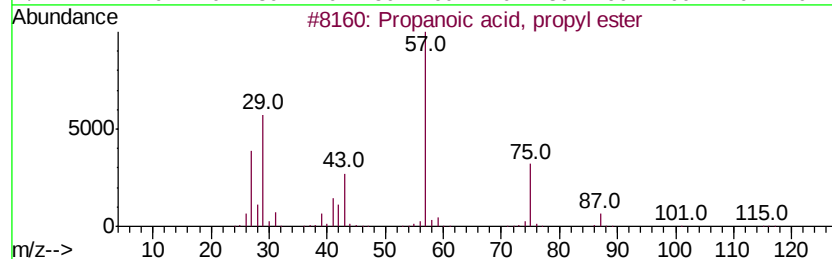
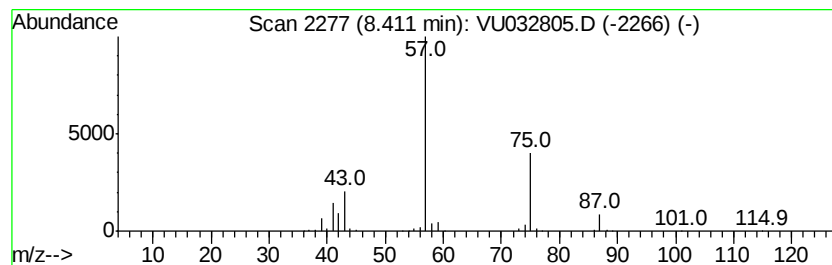
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Quant Title : VOC Analysis

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	56.83 ug/L	798458	Chlorobenzene-d5	9.08

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032805.D
Acq On : 17 Jun 2019 23:56
Operator : JC/SP
Sample : K3363-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JT6

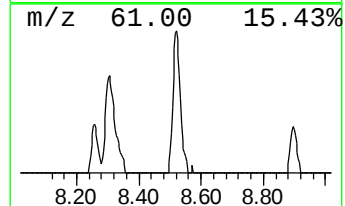
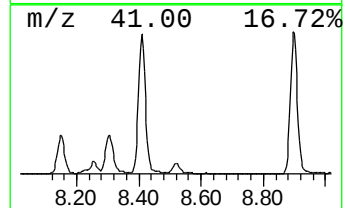
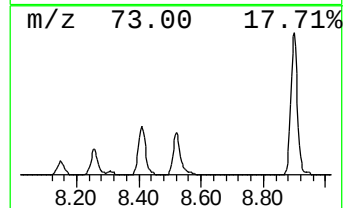
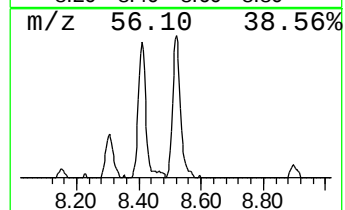
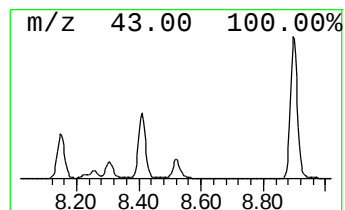
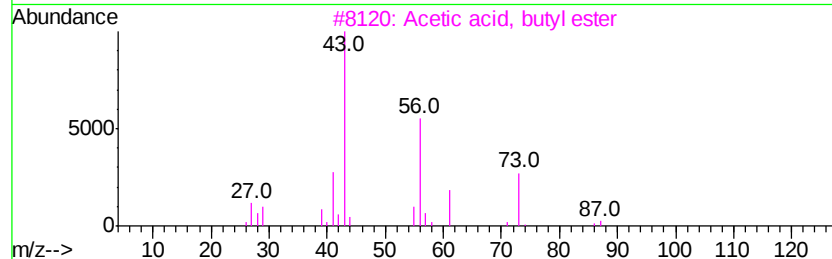
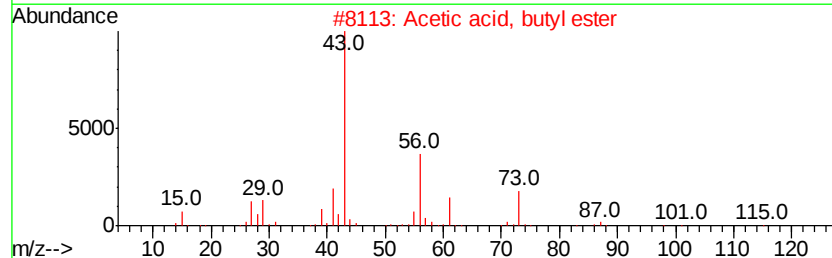
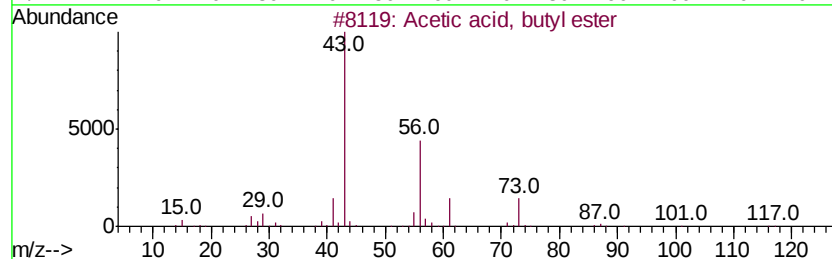
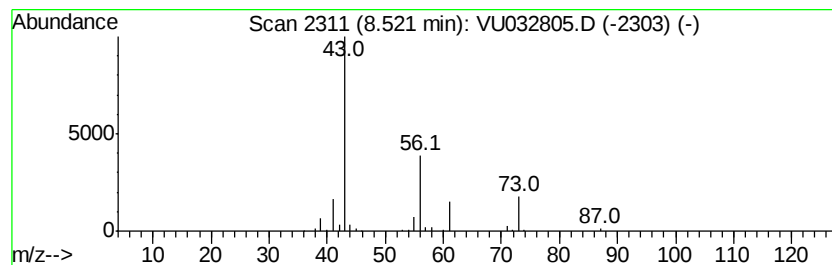
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Quant Title : VOC Analysis

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	3.87 ug/L	54356	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	56
4		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
5		Isobutylamine	73	C4H11N	000078-81-9	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032805.D
Acq On : 17 Jun 2019 23:56
Operator : JC/SP
Sample : K3363-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JT6

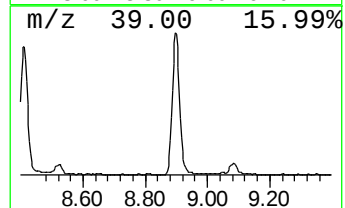
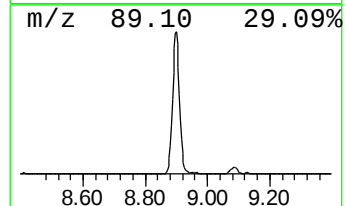
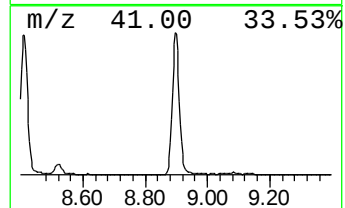
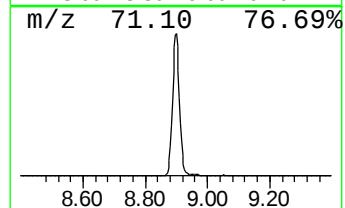
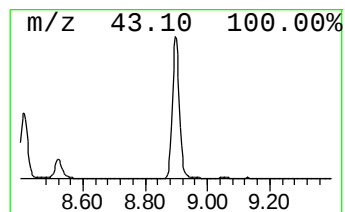
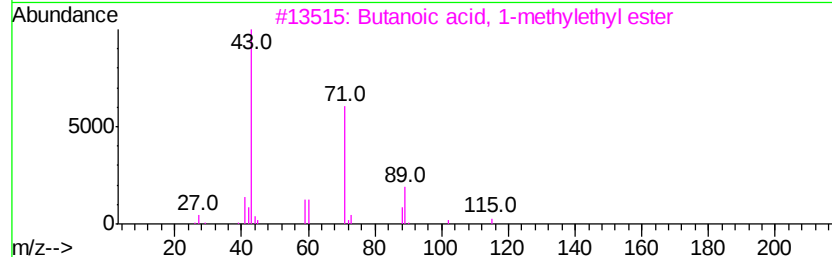
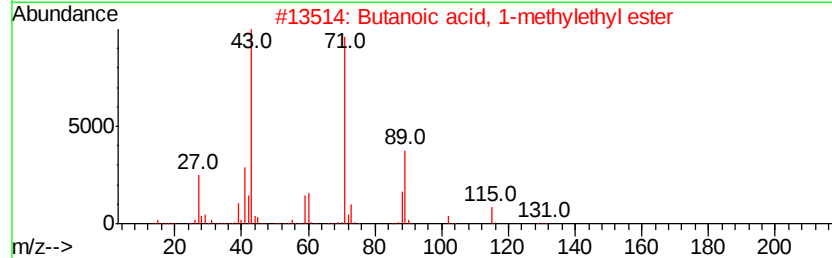
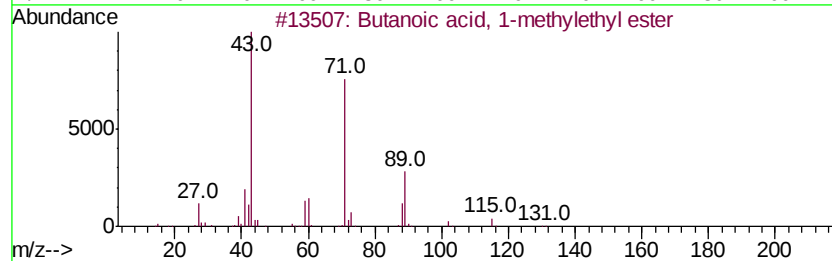
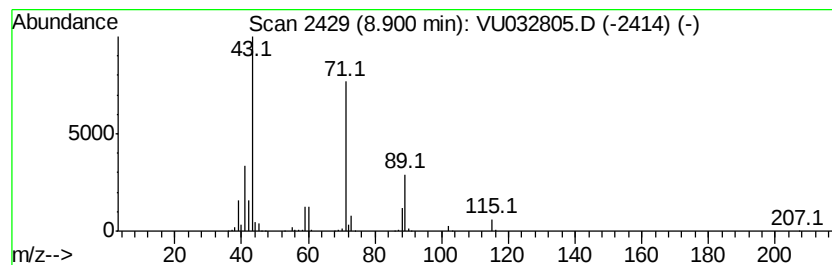
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	39.33 ug/L	552596	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		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
5		Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061719\
Data File : VU032805.D
Acq On : 17 Jun 2019 23:56
Operator : JC/SP
Sample : K3363-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JT6

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	114.4	ug/L	1252150	1	5.88	547167	50.0
Propanoic acid, 1...	7.41	21.7	ug/L	237532	1	5.88	547167	50.0
Propanoic acid, 2...	8.15	8.9	ug/L	124413	2	9.08	702477	50.0
Propanoic acid, p...	8.41	56.8	ug/L	798458	2	9.08	702477	50.0
Acetic acid, buty...	8.52	3.9	ug/L	54356	2	9.08	702477	50.0
Butanoic acid, 1-...	8.90	39.3	ug/L	552596	2	9.08	702477	50.0