

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061719\
 Data File : VU032792.D
 Acq On : 17 Jun 2019 18:58
 Operator : JC/SP
 Sample : K3324-07
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JR3

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	8360	8043	0.58%	0.078%
2	1.395	88	95	106	rVB	98874	102806	7.36%	0.998%
3	1.550	138	143	151	rVB3	9622	12398	0.89%	0.120%
4	1.675	175	182	195	rVB	84420	103548	7.41%	1.006%
5	2.267	355	366	377	rBV	170755	256026	18.32%	2.486%
6	2.550	451	454	457	rBV2	521	380	0.03%	0.004%
7	2.614	468	474	482	rBV5	932	1551	0.11%	0.015%
8	2.694	491	499	513	rVB2	5614	9612	0.69%	0.093%
9	2.743	513	514	518	rVB3	381	184	0.01%	0.002%
10	2.788	525	528	531	rVB2	600	376	0.03%	0.004%
11	2.813	531	536	538	rBV2	466	405	0.03%	0.004%
12	2.974	583	586	592	rBV3	304	236	0.02%	0.002%
13	3.177	647	649	652	rVB3	468	260	0.02%	0.003%
14	3.202	652	657	660	rBV2	261	324	0.02%	0.003%
15	3.292	682	685	690	rVB2	291	256	0.02%	0.002%
16	3.321	690	694	696	rBV4	460	349	0.02%	0.003%
17	3.360	701	706	710	rVB4	541	640	0.05%	0.006%
18	3.382	710	713	715	rBV2	330	231	0.02%	0.002%
19	3.450	730	734	737	rBV3	355	310	0.02%	0.003%
20	3.534	756	760	763	rBV2	240	226	0.02%	0.002%
21	3.620	784	787	790	rVV3	376	323	0.02%	0.003%
22	3.691	806	809	814	rVB3	320	275	0.02%	0.003%
23	3.804	840	844	846	rBV3	267	197	0.01%	0.002%
24	3.890	868	871	874	rVB2	520	393	0.03%	0.004%
25	3.910	874	877	878	rBV	288	180	0.01%	0.002%
26	3.981	896	899	904	rBV2	265	290	0.02%	0.003%
27	4.167	944	957	992	rBV	84736	225000	16.10%	2.185%
28	4.389	1023	1026	1028	rBV2	312	199	0.01%	0.002%
29	4.550	1069	1076	1077	rBV3	483	516	0.04%	0.005%
30	4.640	1087	1104	1127	rBV	140029	324686	23.23%	3.153%
31	4.771	1143	1145	1148	rVB2	497	313	0.02%	0.003%
32	4.874	1172	1177	1182	rBV3	562	542	0.04%	0.005%
33	4.997	1209	1215	1220	rBV3	641	691	0.05%	0.007%
34	5.070	1235	1238	1240	rBV2	283	226	0.02%	0.002%

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 Title : VOC Analysis

35	5.180	1266	1272	1274	rBV2	348	287	0.02%	0.003%
36	5.231	1281	1288	1292	rBV2	625	890	0.06%	0.009%
37	5.331	1296	1319	1345	rBV2	270690	810060	57.96%	7.867%
38	5.443	1352	1354	1357	rVB2	508	260	0.02%	0.003%
39	5.550	1376	1387	1401	rVV2	6114	12755	0.91%	0.124%
40	5.723	1437	1441	1444	rBV3	386	265	0.02%	0.003%
41	5.807	1464	1467	1472	rVB4	480	285	0.02%	0.003%
42	5.878	1476	1489	1508	rBV	278025	548275	39.23%	5.324%
43	6.183	1575	1584	1595	rVB7	6311	12512	0.90%	0.122%
44	6.324	1614	1628	1649	rVV	188491	372516	26.66%	3.618%
45	6.418	1649	1657	1676	rVB2	6631	14304	1.02%	0.139%
46	6.575	1699	1706	1714	rBV2	4999	8845	0.63%	0.086%
47	6.697	1731	1744	1779	rBV	787043	1397507	100.00%	13.571%
48	7.222	1895	1907	1930	rVV	109440	194809	13.94%	1.892%
49	7.414	1955	1967	1991	rBV	144637	245805	17.59%	2.387%
50	7.559	1999	2012	2028	rBV	369999	644220	46.10%	6.256%
51	7.694	2050	2054	2056	rBV4	1221	1008	0.07%	0.010%
52	7.842	2089	2100	2117	rBV2	92569	160234	11.47%	1.556%
53	8.025	2154	2157	2161	rBV2	381	237	0.02%	0.002%
54	8.051	2163	2165	2169	rVB2	526	343	0.02%	0.003%
55	8.148	2183	2195	2211	rBV	81596	135204	9.67%	1.313%
56	8.228	2211	2220	2221	rVV3	9260	10603	0.76%	0.103%
57	8.257	2223	2229	2235	rVV2	31299	48693	3.48%	0.473%
58	8.305	2235	2244	2265	rVV	303500	526350	37.66%	5.111%
59	8.408	2266	2276	2301	rVV	552077	884235	63.27%	8.587%
60	8.517	2302	2310	2328	rVB	38294	66126	4.73%	0.642%
61	8.710	2367	2370	2371	rBV2	512	249	0.02%	0.002%
62	8.900	2417	2429	2463	rVV	386391	613651	43.91%	5.959%
63	9.083	2469	2486	2513	rBV	420438	700173	50.10%	6.799%
64	9.241	2532	2535	2542	rVB6	653	714	0.05%	0.007%
65	9.299	2547	2553	2556	rBV4	701	780	0.06%	0.008%
66	9.334	2562	2564	2568	rBV3	336	249	0.02%	0.002%
67	9.427	2590	2593	2598	rBV3	329	379	0.03%	0.004%
68	9.546	2628	2630	2632	rBV2	349	192	0.01%	0.002%
69	9.601	2639	2647	2656	rBV3	5139	8343	0.60%	0.081%
70	9.713	2676	2682	2684	rBV4	355	362	0.03%	0.004%
71	9.762	2688	2697	2713	rVB	20347	32684	2.34%	0.317%

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72	9.839	2719	2721	2725	rBV3	275	198	0.01%	0.002%
73	10.096	2798	2801	2803	rBV3	294	193	0.01%	0.002%
74	10.270	2849	2855	2857	rBV2	358	371	0.03%	0.004%
75	10.321	2869	2871	2875	rBV3	299	213	0.02%	0.002%
76	10.369	2882	2886	2888	rBV2	270	197	0.01%	0.002%
77	10.427	2888	2904	2921	rBV	283594	457347	32.73%	4.441%
78	10.601	2954	2958	2959	rBV3	612	388	0.03%	0.004%
79	10.729	2996	2998	3003	rVB2	488	263	0.02%	0.003%
80	10.755	3003	3006	3007	rBV	417	225	0.02%	0.002%
81	10.858	3035	3038	3043	rBV2	386	393	0.03%	0.004%
82	10.990	3076	3079	3081	rBV2	296	190	0.01%	0.002%
83	11.112	3113	3117	3122	rBV3	290	328	0.02%	0.003%
84	11.167	3131	3134	3141	rBV4	355	455	0.03%	0.004%
85	11.289	3169	3172	3173	rBV2	428	209	0.01%	0.002%
86	11.350	3188	3191	3194	rBV3	318	256	0.02%	0.002%
87	11.408	3206	3209	3211	rBV	331	229	0.02%	0.002%
88	11.479	3218	3231	3249	rBV	433504	688350	49.26%	6.685%
89	11.855	3335	3348	3373	rBV	389159	636663	45.56%	6.183%
90	12.151	3438	3440	3442	rBV2	339	200	0.01%	0.002%
91	12.192	3449	3453	3459	rBV5	540	744	0.05%	0.007%
92	12.234	3461	3466	3470	rVV4	519	437	0.03%	0.004%
93	12.321	3490	3493	3497	rBV3	508	357	0.03%	0.003%
94	12.376	3508	3510	3513	rVB2	407	222	0.02%	0.002%
95	12.479	3539	3542	3544	rBV	487	284	0.02%	0.003%
96	12.604	3577	3581	3585	rVB4	562	438	0.03%	0.004%
97	12.871	3661	3664	3668	rBV3	455	378	0.03%	0.004%
98	12.987	3696	3700	3707	rBV4	556	708	0.05%	0.007%
99	14.015	4017	4020	4025	rBV4	526	473	0.03%	0.005%
100	14.244	4089	4091	4094	rBV2	399	330	0.02%	0.003%

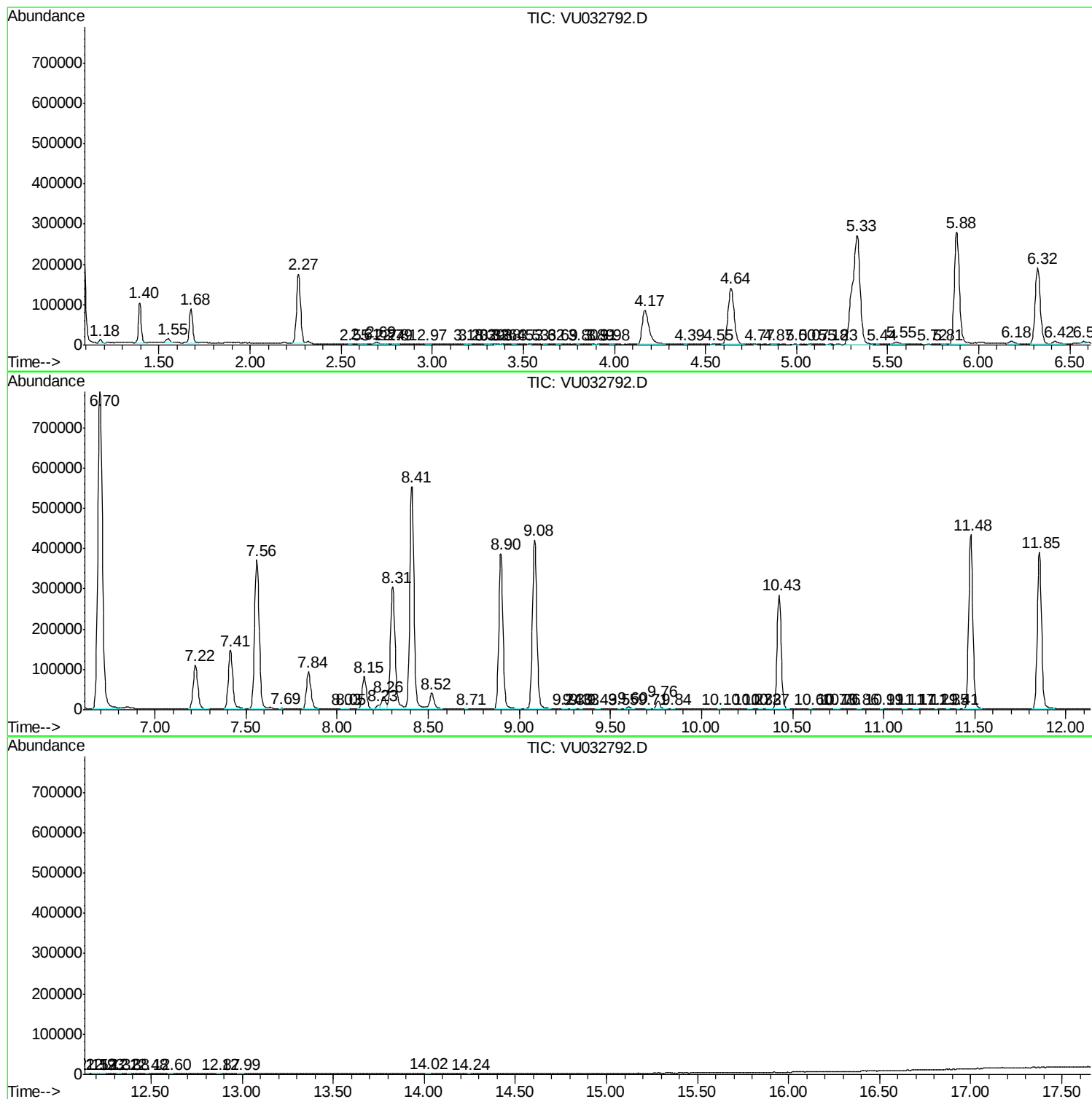
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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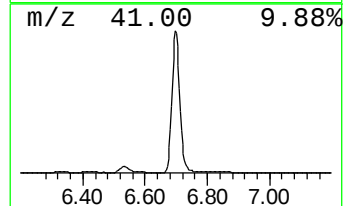
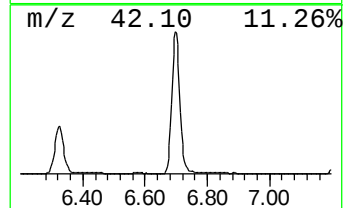
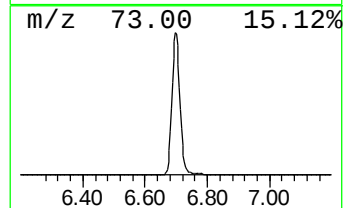
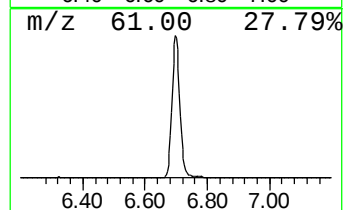
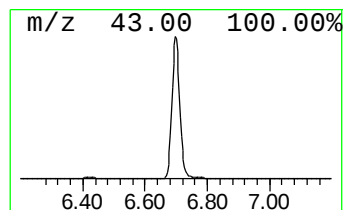
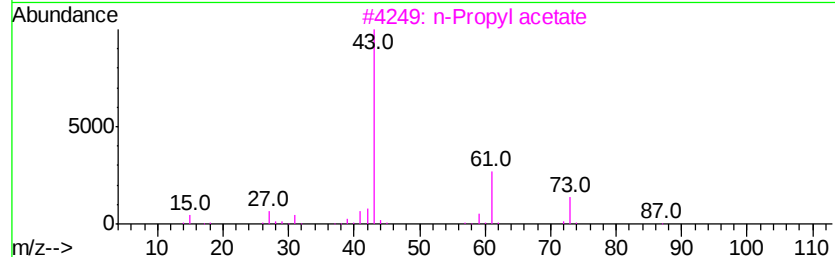
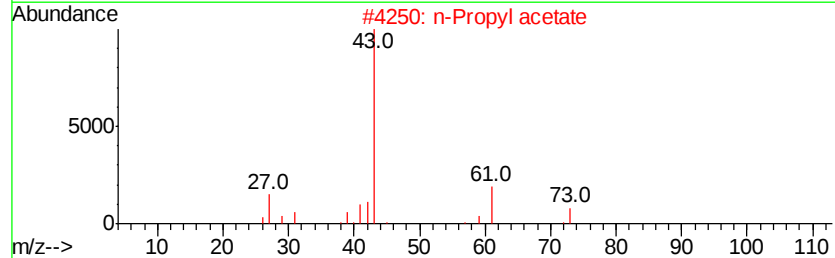
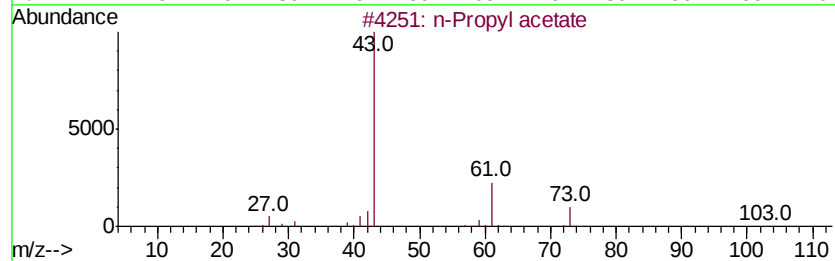
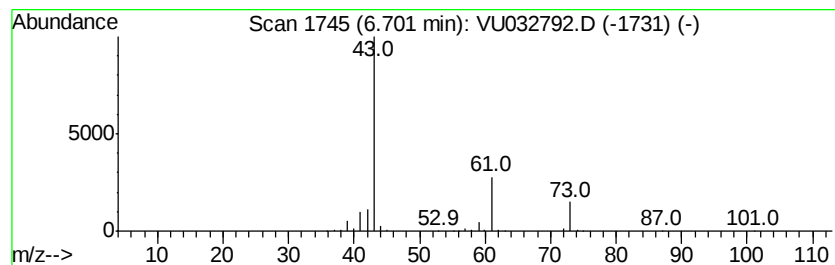
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	127.45 ug/L	1397510	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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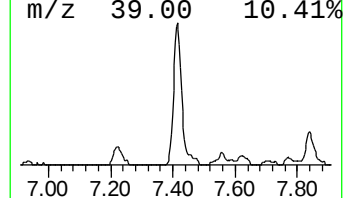
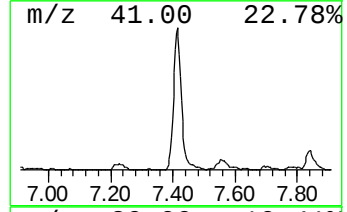
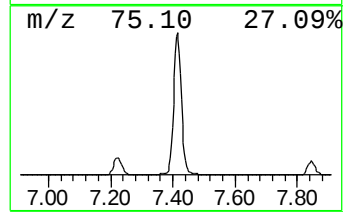
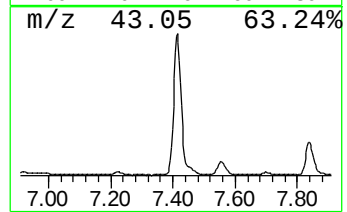
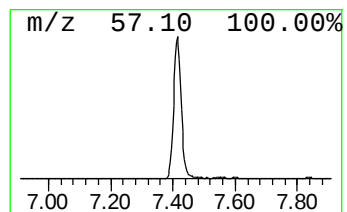
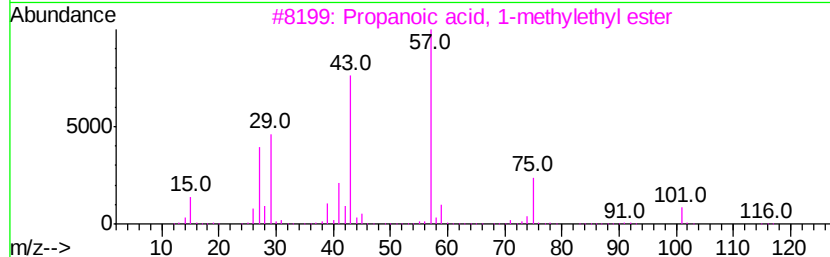
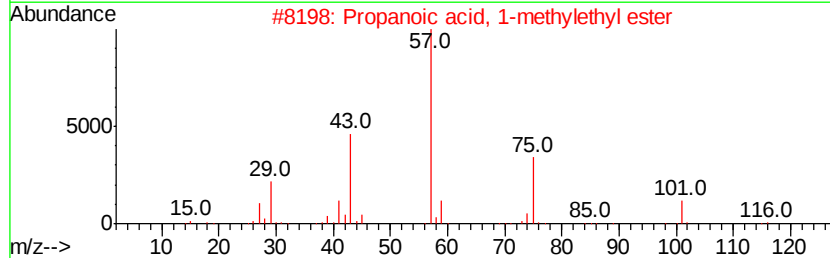
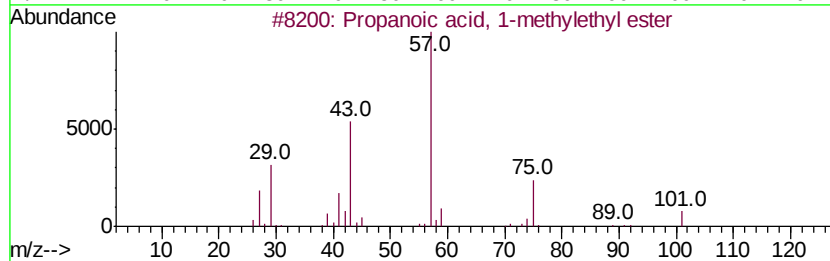
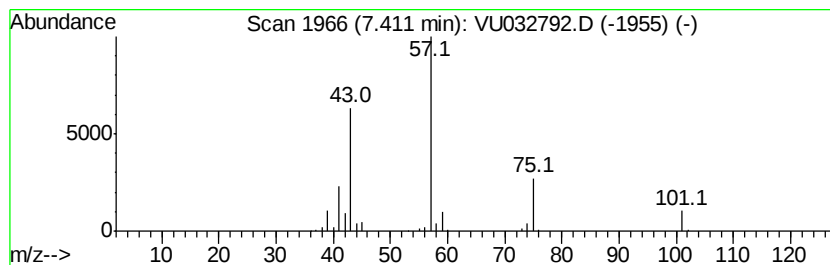
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Quant Title : VOC Analysis

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	22.42 ug/L	245805	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	78
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
4		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40



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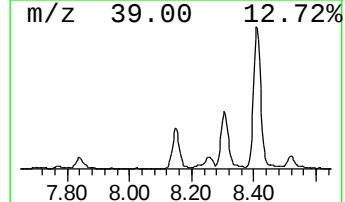
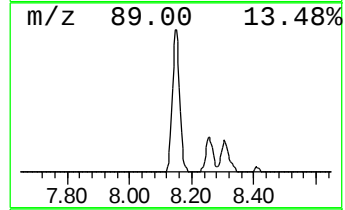
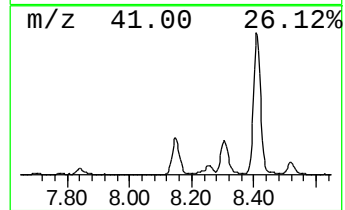
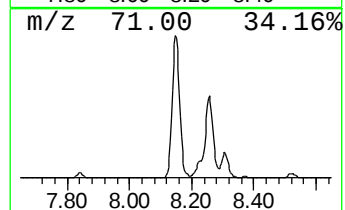
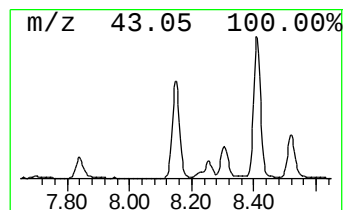
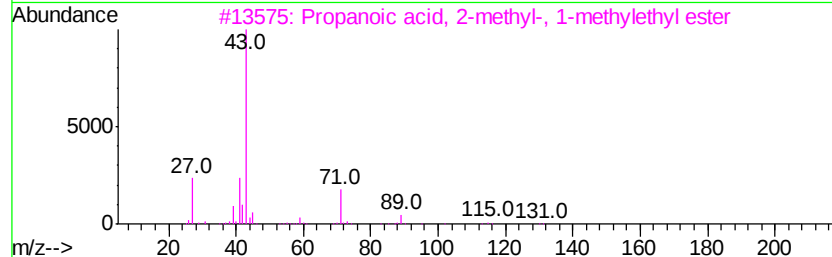
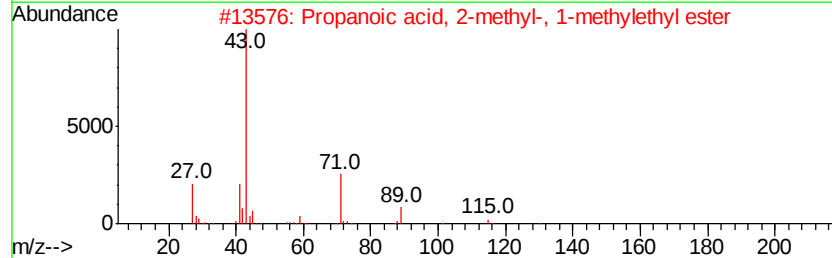
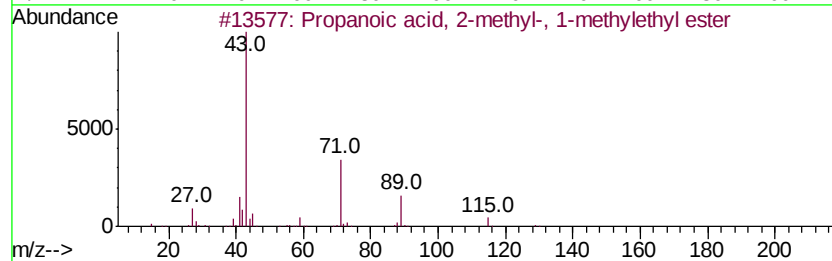
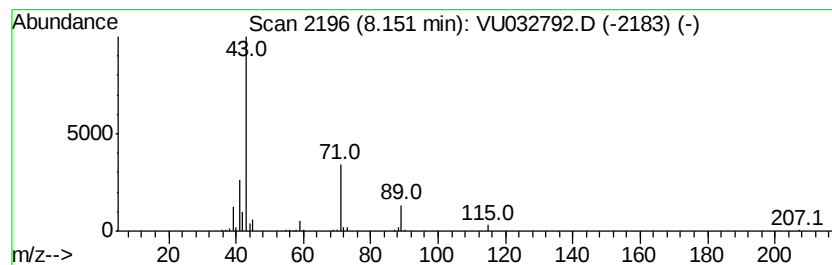
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.66 ug/L	135204	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	72
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032792.D
Acq On : 17 Jun 2019 18:58
Operator : JC/SP
Sample : K3324-07
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JR3

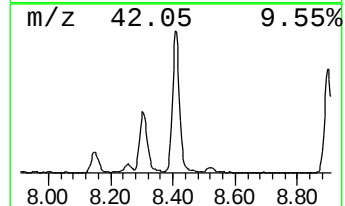
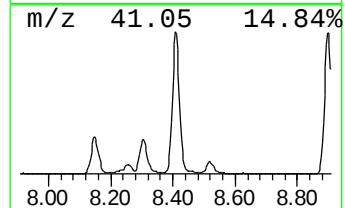
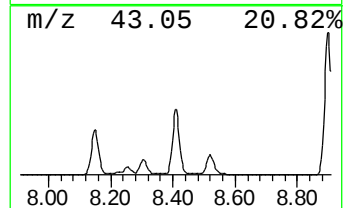
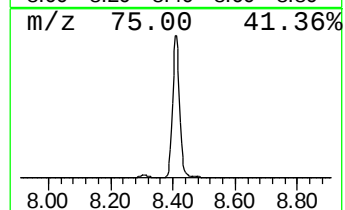
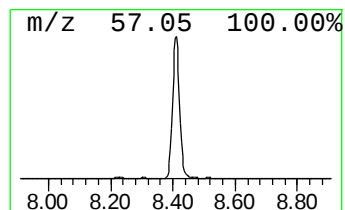
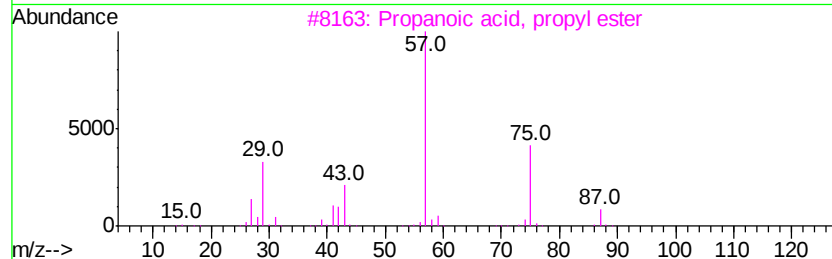
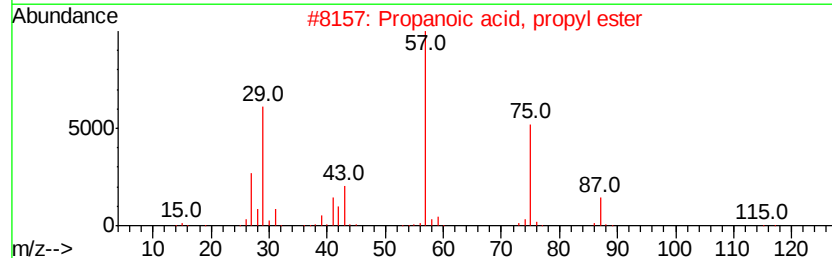
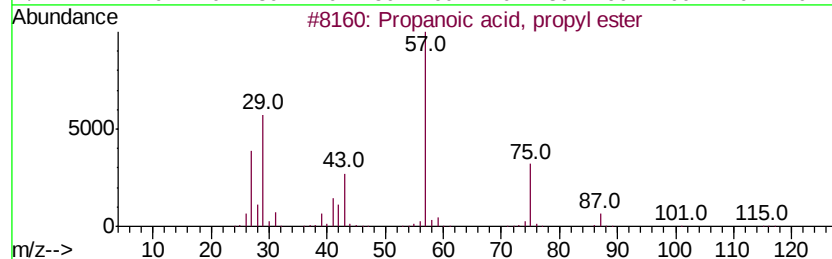
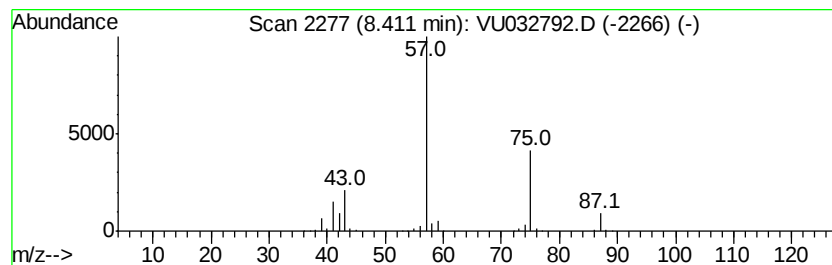
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Quant Title : VOC Analysis

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	63.14 ug/L	884235	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:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061719\
 Data File : VU032792.D
 Acq On : 17 Jun 2019 18:58
 Operator : JC/SP
 Sample : K3324-07
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JR3

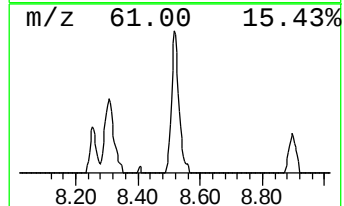
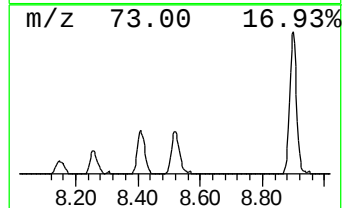
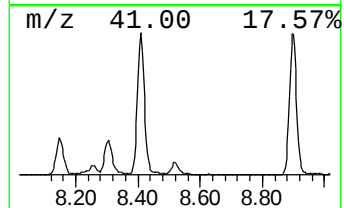
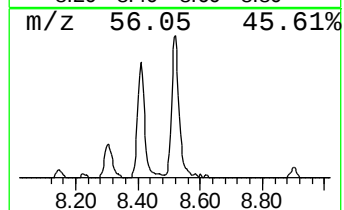
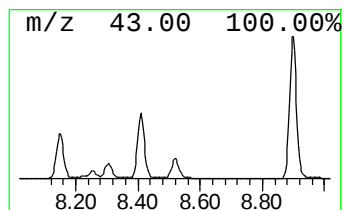
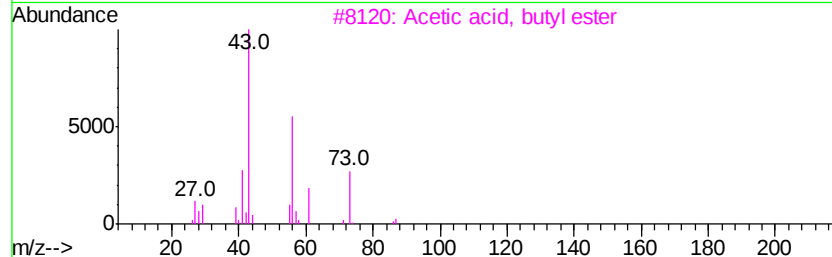
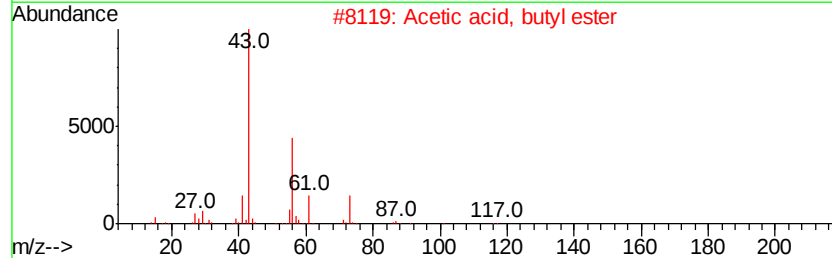
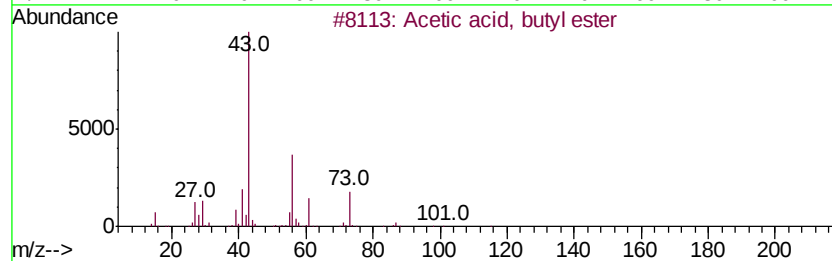
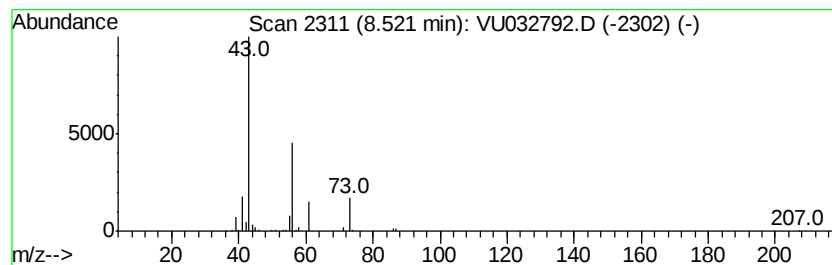
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 Quant Title : VOC Analysis

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	4.72 ug/L	66126	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	83
3		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	45
4		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	45
5		1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032792.D
Acq On : 17 Jun 2019 18:58
Operator : JC/SP
Sample : K3324-07
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR3

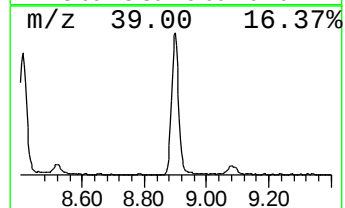
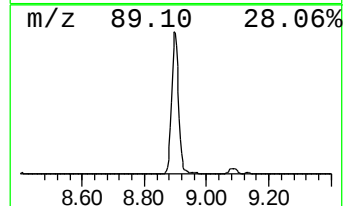
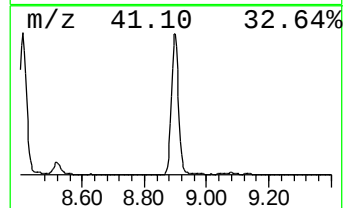
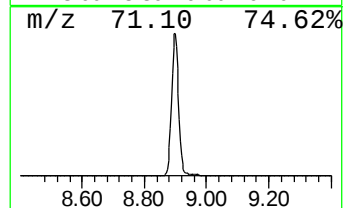
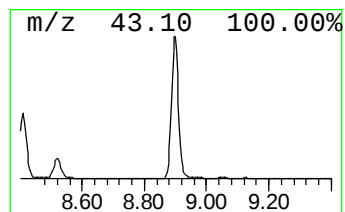
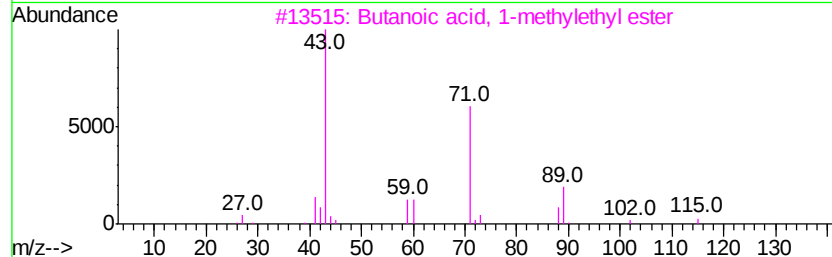
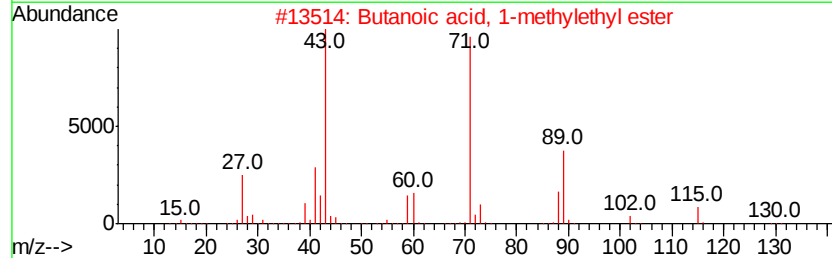
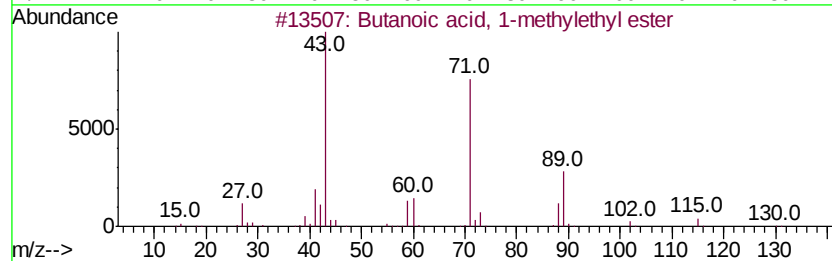
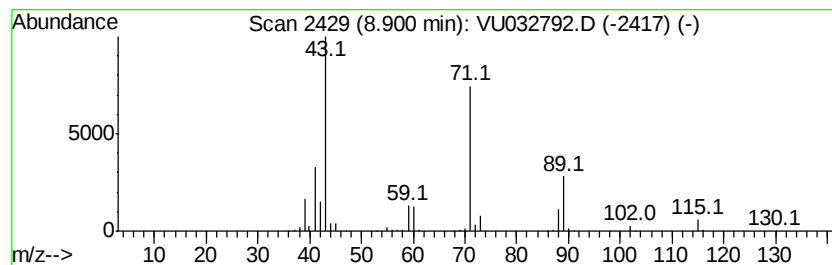
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	43.82 ug/L	613651	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	94
2		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
4		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	64
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061719\
Data File : VU032792.D
Acq On : 17 Jun 2019 18:58
Operator : JC/SP
Sample : K3324-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR3

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	127.5	ug/L	1397510	1	5.88	548275	50.0
Propanoic acid, 1...	7.41	22.4	ug/L	245805	1	5.88	548275	50.0
Propanoic acid, 2...	8.15	9.7	ug/L	135204	2	9.08	700173	50.0
Propanoic acid, p...	8.41	63.1	ug/L	884235	2	9.08	700173	50.0
Acetic acid, buty...	8.52	4.7	ug/L	66126	2	9.08	700173	50.0
Butanoic acid, 1-...	8.90	43.8	ug/L	613651	2	9.08	700173	50.0