

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061719\
 Data File : VU032794.D
 Acq On : 17 Jun 2019 19:44
 Operator : JC/SP
 Sample : K3324-09
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JR5

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	34	rBV2	7196	6622	0.05%	0.027%
2	1.396	88	95	106	rVB2	130925	140952	1.17%	0.567%
3	1.469	112	118	126	rBV	16158	17379	0.14%	0.070%
4	1.675	175	182	197	rVB	85261	104698	0.87%	0.421%
5	2.267	355	366	376	rBV2	182476	286289	2.37%	1.152%
6	2.315	377	381	398	rVB	16895	26424	0.22%	0.106%
7	2.469	425	429	435	rVB4	1411	1626	0.01%	0.007%
8	2.524	440	446	448	rBV2	586	613	0.01%	0.002%
9	2.572	458	461	465	rBV3	403	301	0.00%	0.001%
10	2.617	470	475	485	rVB3	1425	2193	0.02%	0.009%
11	2.694	491	499	510	rVB3	5724	9585	0.08%	0.039%
12	2.977	571	587	606	rBV	60882	110485	0.91%	0.445%
13	3.183	642	651	664	rVB5	2464	5521	0.05%	0.022%
14	3.241	664	669	674	rVB3	573	588	0.00%	0.002%
15	3.408	715	721	726	rBV6	803	1127	0.01%	0.005%
16	3.563	763	769	772	rBV2	269	288	0.00%	0.001%
17	3.672	799	803	807	rBV2	351	334	0.00%	0.001%
18	3.694	807	810	814	rBV3	293	336	0.00%	0.001%
19	3.804	841	844	849	rBV3	331	423	0.00%	0.002%
20	3.852	854	859	868	rBV4	450	858	0.01%	0.003%
21	3.932	881	884	888	rBV3	414	348	0.00%	0.001%
22	3.993	899	903	905	rBV3	631	468	0.00%	0.002%
23	4.215	945	972	1012	rBV	4974201	12096919	100.00%	48.674%
24	4.640	1088	1104	1127	rVB	139896	328195	2.71%	1.321%
25	4.849	1166	1169	1172	rBV3	426	324	0.00%	0.001%
26	4.868	1172	1175	1177	rBV2	502	391	0.00%	0.002%
27	5.013	1215	1220	1225	rVB3	234	266	0.00%	0.001%
28	5.157	1261	1265	1269	rBV	369	280	0.00%	0.001%
29	5.331	1296	1319	1353	rVV2	272387	819004	6.77%	3.295%
30	5.447	1353	1355	1360	rBV3	421	363	0.00%	0.001%
31	5.546	1377	1386	1399	rBV2	5607	12220	0.10%	0.049%
32	5.723	1436	1441	1443	rBV2	487	420	0.00%	0.002%
33	5.784	1456	1460	1462	rBV3	401	345	0.00%	0.001%
34	5.878	1475	1489	1507	rBV	278073	549939	4.55%	2.213%

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 Title : VOC Analysis

35	6.180	1568	1583	1612	rBV	1307618	2488644	20.57%	10.014%
36	6.325	1615	1628	1647	rVV	190296	381135	3.15%	1.534%
37	6.418	1651	1657	1677	rVB	7457	14668	0.12%	0.059%
38	6.572	1699	1705	1713	rBV2	4384	7498	0.06%	0.030%
39	6.698	1731	1744	1771	rBV	779313	1364065	11.28%	5.489%
40	7.083	1863	1864	1870	rVB4	480	289	0.00%	0.001%
41	7.222	1895	1907	1924	rBV	112181	196152	1.62%	0.789%
42	7.415	1956	1967	1992	rVB	143706	246231	2.04%	0.991%
43	7.559	1998	2012	2028	rBV	376528	652245	5.39%	2.624%
44	7.697	2050	2055	2067	rVB9	2175	3374	0.03%	0.014%
45	7.842	2089	2100	2118	rBV2	92827	162250	1.34%	0.653%
46	7.993	2144	2147	2153	rBV4	500	557	0.00%	0.002%
47	8.148	2184	2195	2210	rBV	82309	137422	1.14%	0.553%
48	8.231	2212	2221	2222	rVV5	9706	13815	0.11%	0.056%
49	8.257	2223	2229	2234	rVV2	30716	45175	0.37%	0.182%
50	8.305	2234	2244	2265	rVV	314050	539483	4.46%	2.171%
51	8.408	2265	2276	2302	rVV	529417	842896	6.97%	3.392%
52	8.521	2302	2311	2326	rVB	35593	59513	0.49%	0.239%
53	8.701	2364	2367	2370	rBV3	376	350	0.00%	0.001%
54	8.897	2416	2428	2453	rBV	381856	609857	5.04%	2.454%
55	9.013	2461	2464	2466	rBV3	708	411	0.00%	0.002%
56	9.083	2472	2486	2522	rVB	423198	707812	5.85%	2.848%
57	9.308	2552	2556	2560	rBV2	523	562	0.00%	0.002%
58	9.334	2560	2564	2567	rVV4	620	590	0.00%	0.002%
59	9.350	2567	2569	2572	rVV3	479	341	0.00%	0.001%
60	9.369	2572	2575	2581	rVB4	818	683	0.01%	0.003%
61	9.427	2590	2593	2595	rBV3	428	281	0.00%	0.001%
62	9.601	2636	2647	2658	rBV3	4724	7879	0.07%	0.032%
63	9.713	2680	2682	2686	rBV	361	261	0.00%	0.001%
64	9.762	2687	2697	2713	rVV2	17705	29321	0.24%	0.118%
65	9.842	2720	2722	2726	rVB3	467	270	0.00%	0.001%
66	10.019	2774	2777	2781	rBV3	670	546	0.00%	0.002%
67	10.241	2841	2846	2851	rBV3	575	635	0.01%	0.003%
68	10.308	2863	2867	2874	rVB3	633	645	0.01%	0.003%
69	10.344	2874	2878	2883	rBV2	463	474	0.00%	0.002%
70	10.424	2891	2903	2926	rBV	290049	464095	3.84%	1.867%
71	10.691	2983	2986	2987	rBV	453	256	0.00%	0.001%

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72	10.858	3035	3038	3040	rVV2	333	259	0.00%	0.001%
73	10.874	3040	3043	3047	rVB4	527	414	0.00%	0.002%
74	10.974	3070	3074	3077	rBV4	355	266	0.00%	0.001%
75	11.057	3096	3100	3105	rBV5	394	306	0.00%	0.001%
76	11.173	3133	3136	3140	rBV2	386	272	0.00%	0.001%
77	11.373	3196	3198	3201	rVB2	636	343	0.00%	0.001%
78	11.392	3201	3204	3206	rBV2	578	267	0.00%	0.001%
79	11.411	3206	3210	3215	rVB3	481	407	0.00%	0.002%
80	11.479	3218	3231	3250	rBV	433078	694936	5.74%	2.796%
81	11.623	3273	3276	3278	rBV4	687	474	0.00%	0.002%
82	11.697	3293	3299	3300	rBV5	466	462	0.00%	0.002%
83	11.733	3307	3310	3314	rBV2	455	418	0.00%	0.002%
84	11.855	3334	3348	3370	rBV	384139	640758	5.30%	2.578%
85	12.244	3466	3469	3473	rVB3	561	442	0.00%	0.002%
86	12.408	3516	3520	3522	rBV	383	329	0.00%	0.001%
87	12.591	3573	3577	3579	rBV2	518	348	0.00%	0.001%
88	12.662	3596	3599	3604	rBV4	671	656	0.01%	0.003%
89	12.762	3625	3630	3633	rBV3	512	531	0.00%	0.002%
90	12.852	3655	3658	3661	rBV2	419	342	0.00%	0.001%
91	12.913	3674	3677	3679	rBV3	431	298	0.00%	0.001%
92	13.038	3713	3716	3719	rBV3	413	259	0.00%	0.001%
93	13.186	3758	3762	3766	rBV3	503	426	0.00%	0.002%
94	13.212	3766	3770	3774	rBV3	513	503	0.00%	0.002%
95	13.334	3805	3808	3813	rBV3	401	448	0.00%	0.002%
96	13.630	3896	3900	3904	rVB4	575	572	0.00%	0.002%
97	13.723	3927	3929	3933	rVB4	503	251	0.00%	0.001%
98	13.929	3990	3993	3997	rBV5	450	374	0.00%	0.002%
99	14.025	4020	4023	4028	rVB3	512	334	0.00%	0.001%
100	14.247	4089	4092	4094	rBV	565	356	0.00%	0.001%

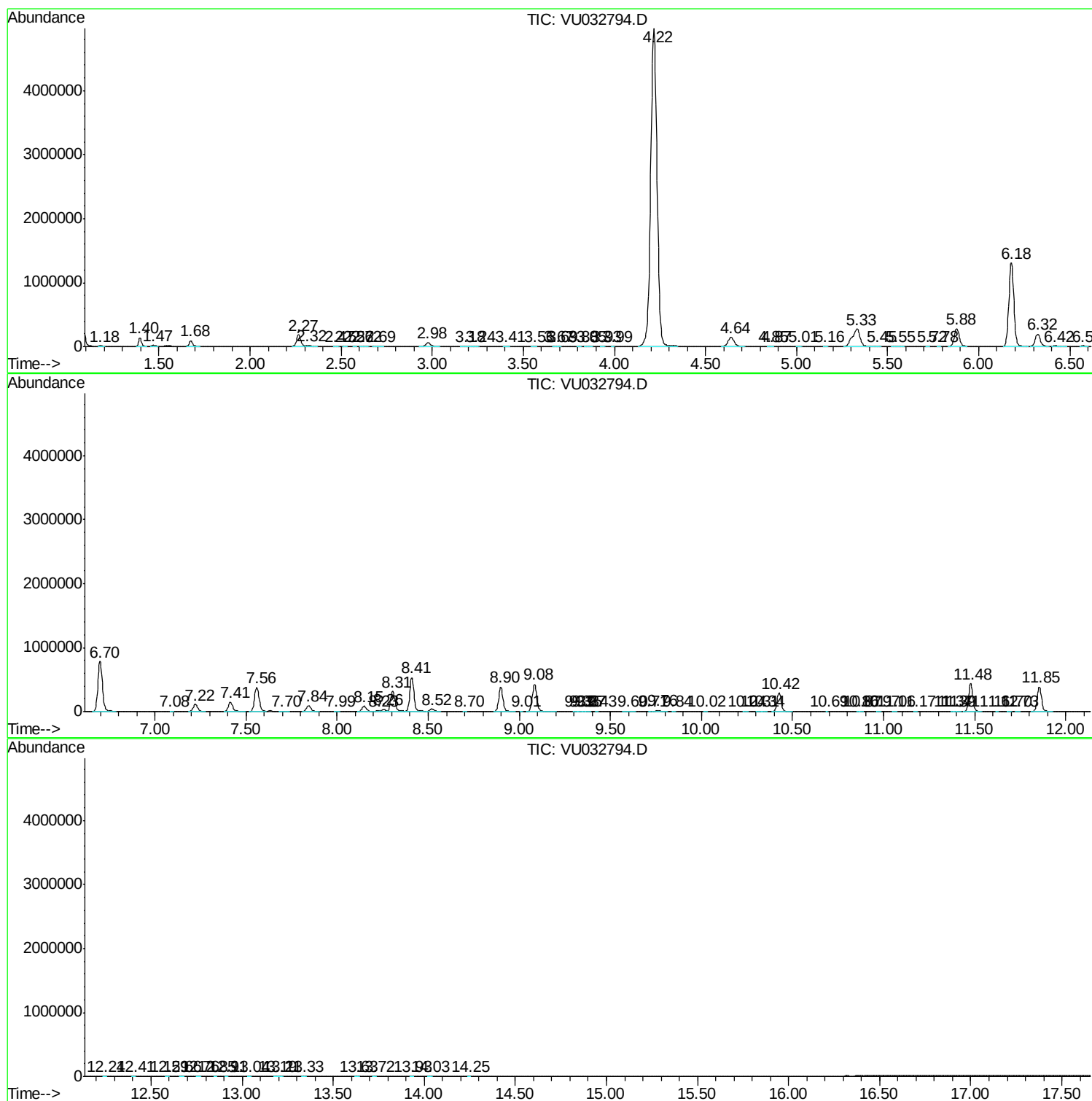
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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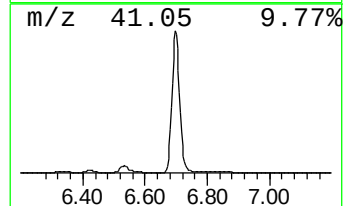
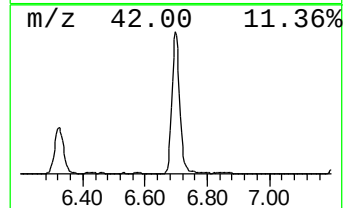
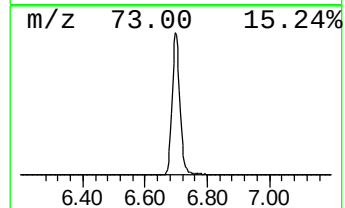
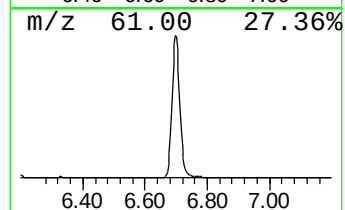
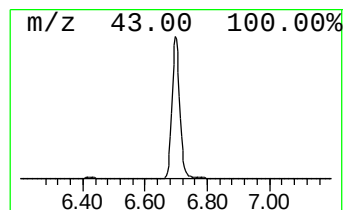
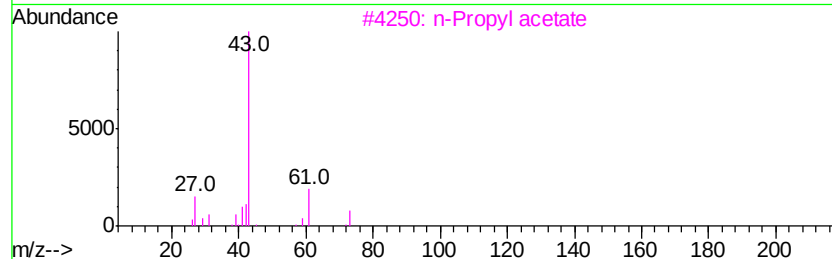
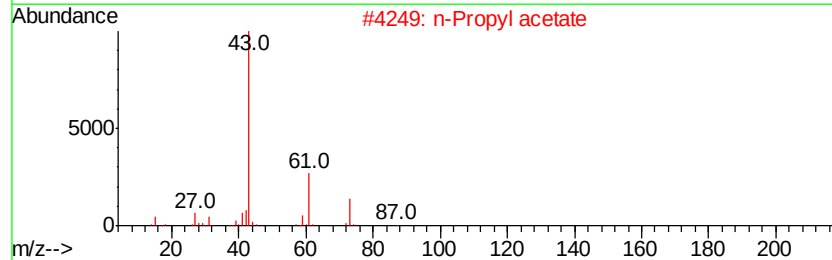
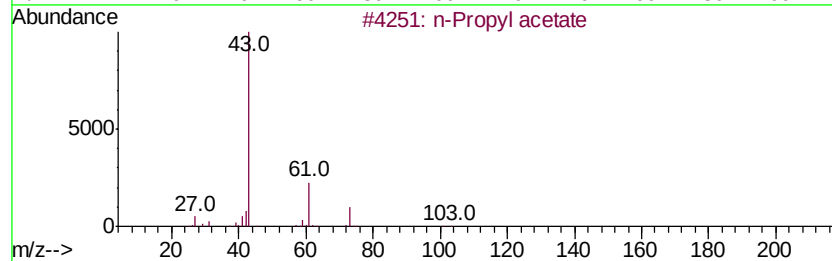
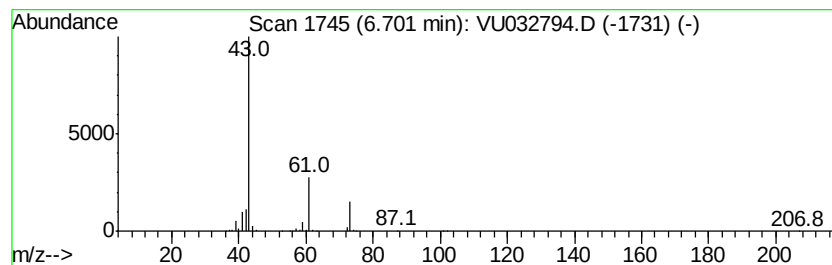
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	124.02 ug/L	1364070	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	64
4		Isopropyl acetate	102	C5H10O2	000108-21-4	36
5		Isopropyl acetate	102	C5H10O2	000108-21-4	33



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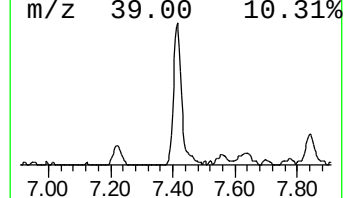
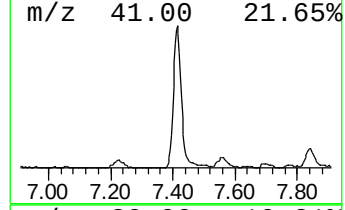
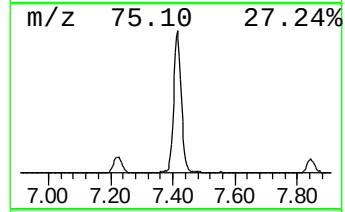
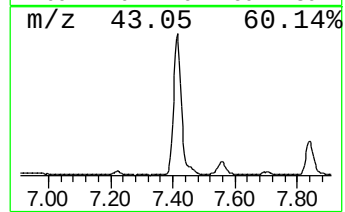
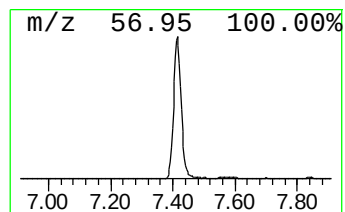
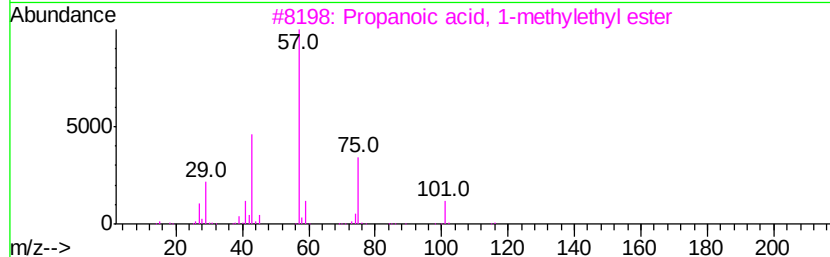
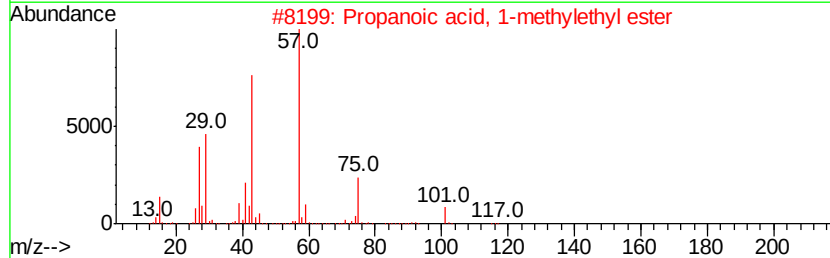
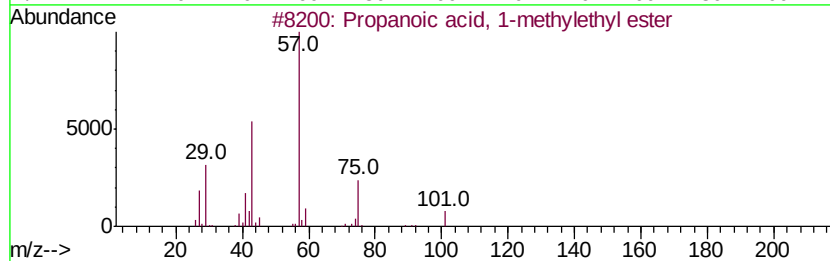
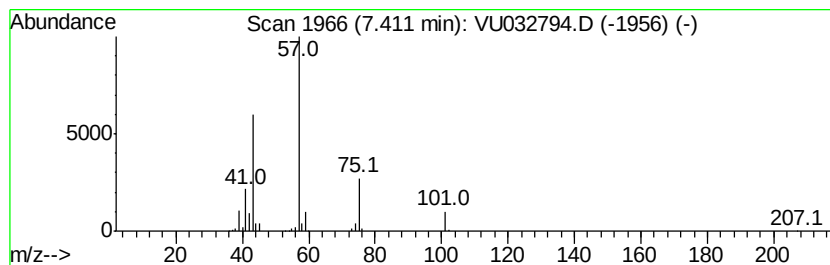
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Quant Title : VOC Analysis

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	22.39 ug/L	246231	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	72
4		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



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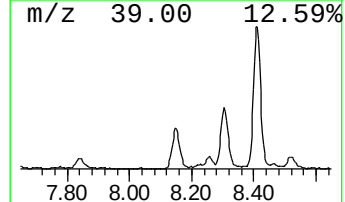
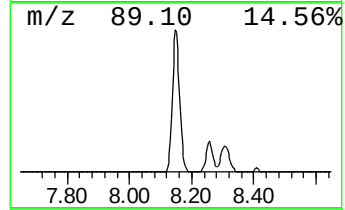
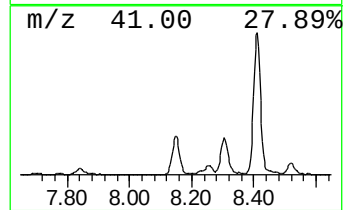
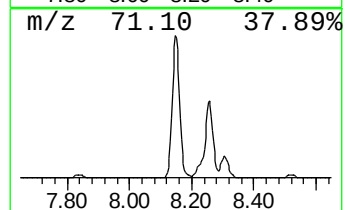
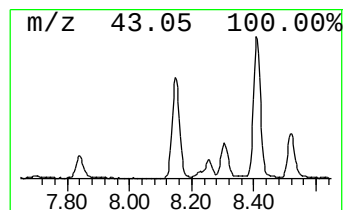
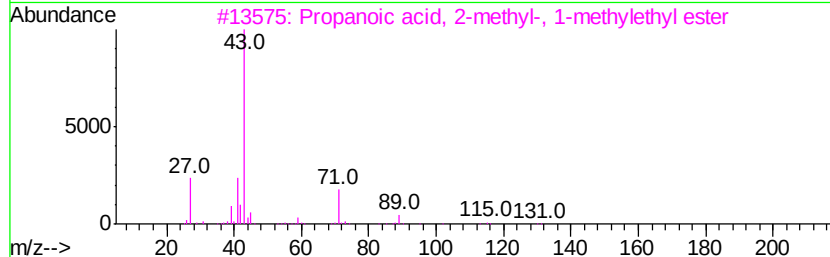
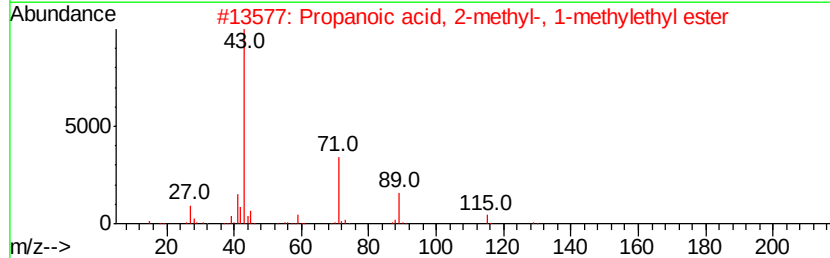
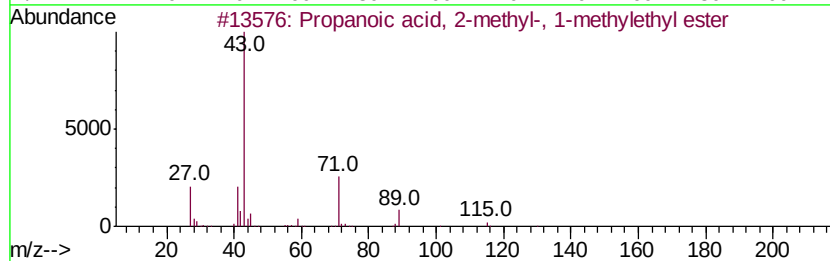
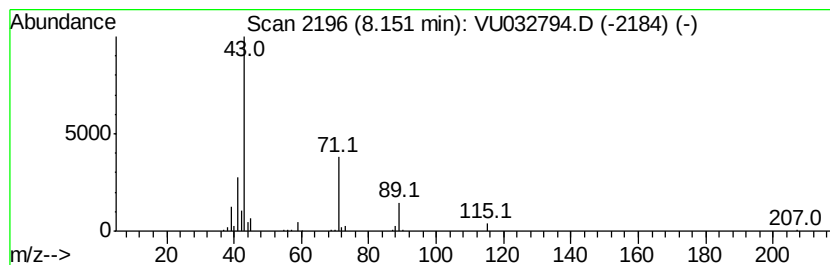
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Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.71 ug/L	137422	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	78		
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64		
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56		



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032794.D
Acq On : 17 Jun 2019 19:44
Operator : JC/SP
Sample : K3324-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JR5

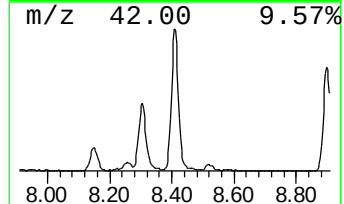
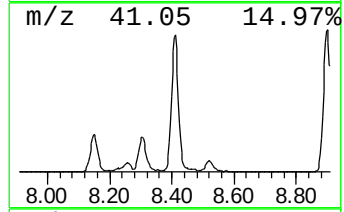
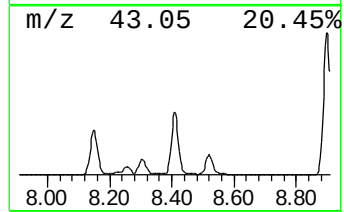
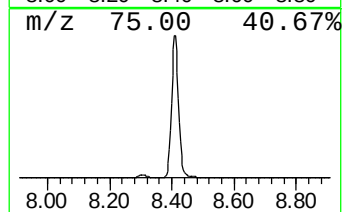
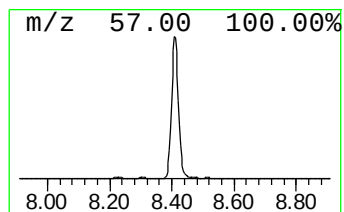
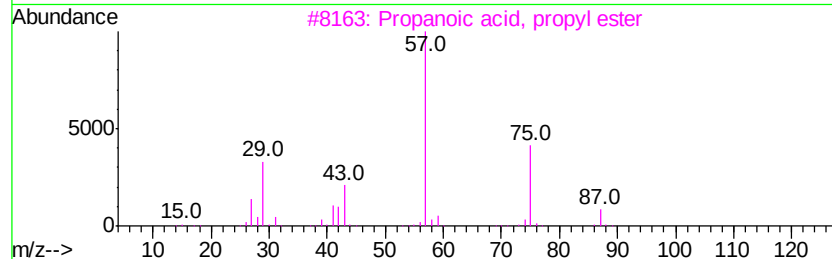
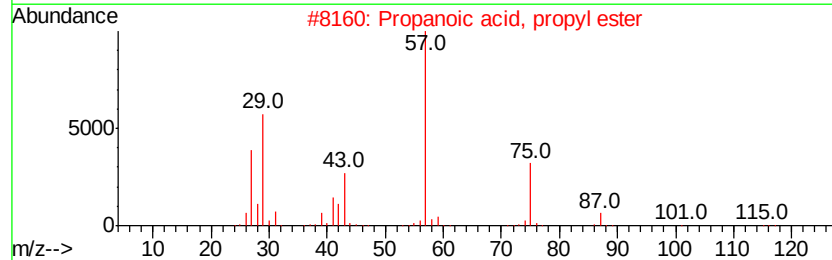
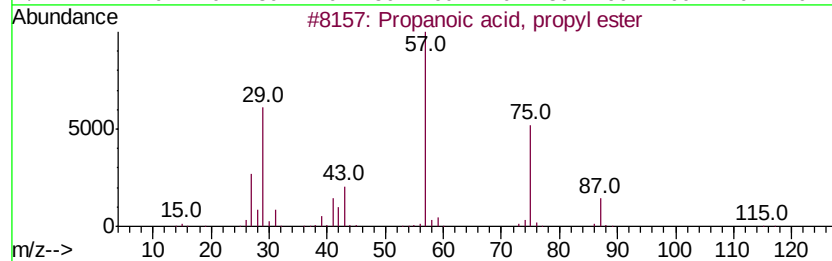
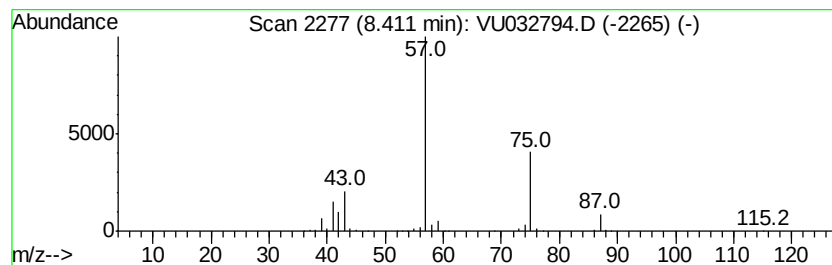
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Quant Title : VOC Analysis

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	59.54 ug/L	842896	Chlorobenzene-d5	9.08

Hit# of	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	25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032794.D
Acq On : 17 Jun 2019 19:44
Operator : JC/SP
Sample : K3324-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR5

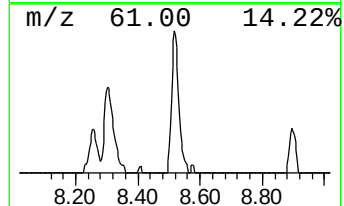
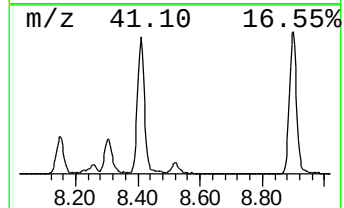
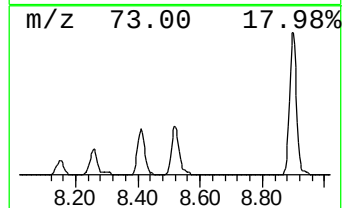
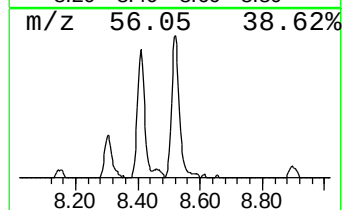
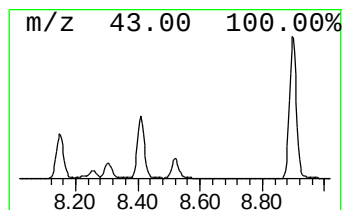
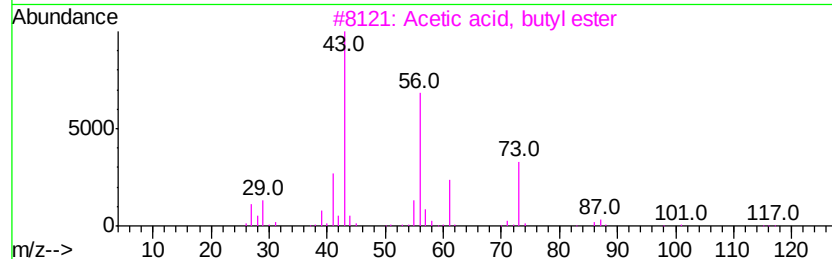
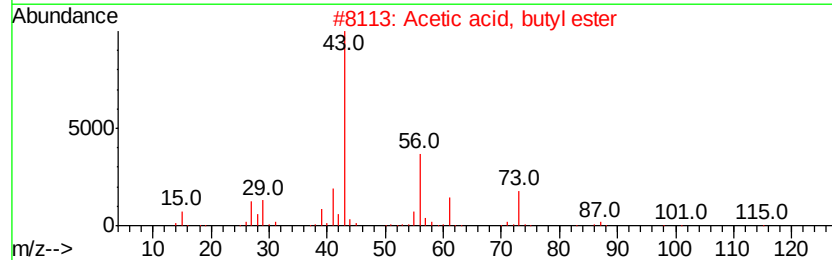
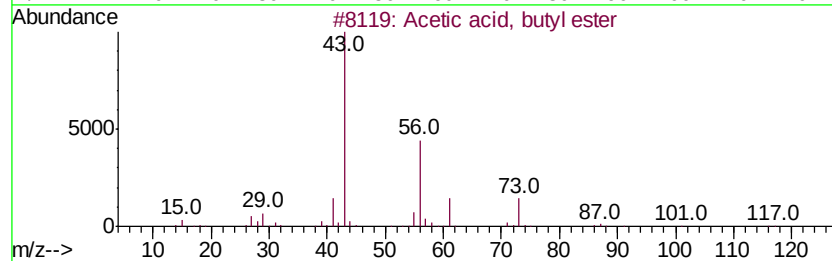
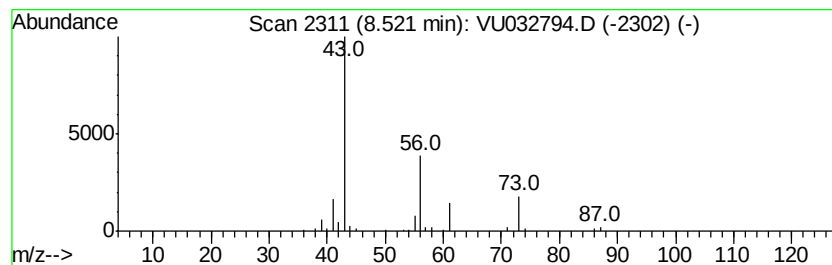
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	4.20 ug/L	59513	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			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
Data File : VU032794.D
Acq On : 17 Jun 2019 19:44
Operator : JC/SP
Sample : K3324-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR5

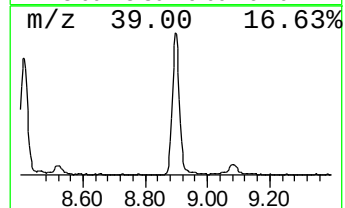
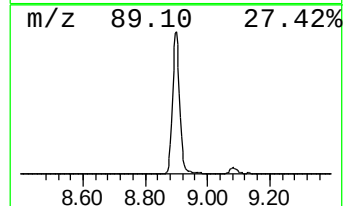
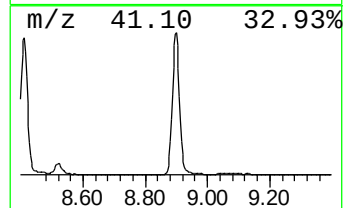
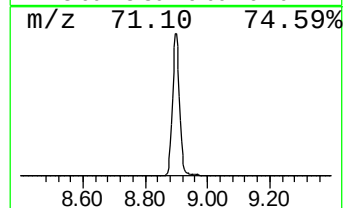
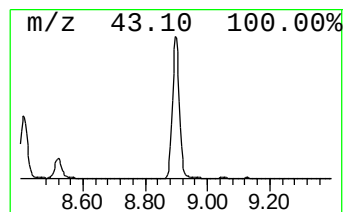
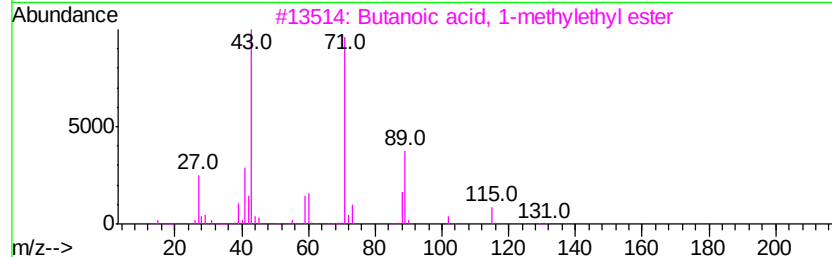
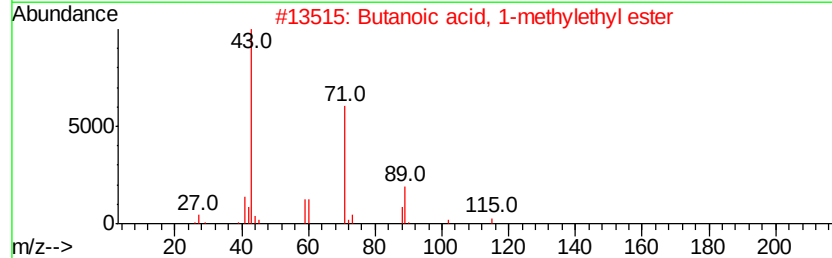
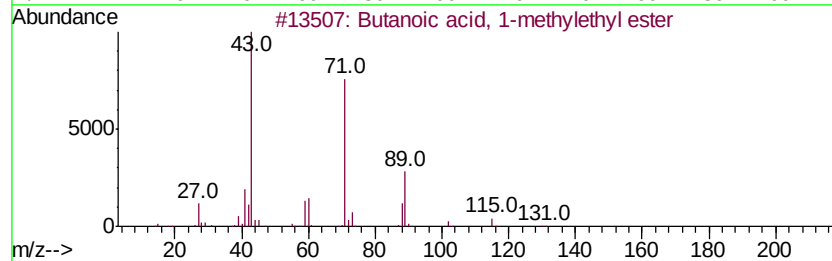
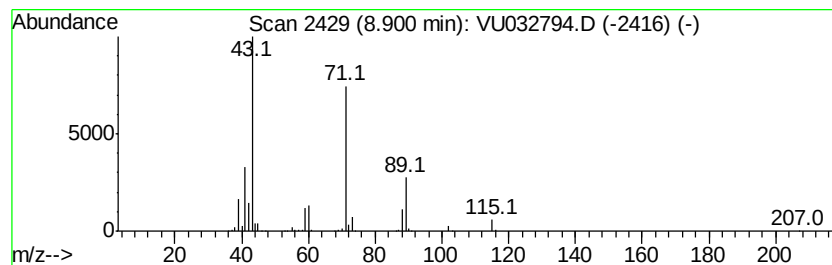
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	43.08 ug/L	609857	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	90
4		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	64
5		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061719\
Data File : VU032794.D
Acq On : 17 Jun 2019 19:44
Operator : JC/SP
Sample : K3324-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR5

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	124.0	ug/L	1364070	1	5.88	549939	50.0
Propanoic acid, 1...	7.41	22.4	ug/L	246231	1	5.88	549939	50.0
Propanoic acid, 2...	8.15	9.7	ug/L	137422	2	9.08	707812	50.0
Propanoic acid, p...	8.41	59.5	ug/L	842896	2	9.08	707812	50.0
Acetic acid, buty...	8.52	4.2	ug/L	59513	2	9.08	707812	50.0
Butanoic acid, 1-...	8.90	43.1	ug/L	609857	2	9.08	707812	50.0