

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061219\
 Data File : VU032644.D
 Acq On : 12 Jun 2019 12:16
 Operator : JC/SP
 Sample : K3286-03
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JS5

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\SOMULM060619WMA.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	35	rBV	4682	4454	0.40%	0.056%
2	1.396	88	95	104	rBV	89731	94766	8.60%	1.187%
3	1.675	174	182	195	rBV	72297	90843	8.24%	1.138%
4	2.267	355	366	377	rBV	155863	234270	21.25%	2.935%
5	2.454	419	424	428	rVB3	330	333	0.03%	0.004%
6	2.624	469	477	481	rBV3	504	860	0.08%	0.011%
7	2.695	490	499	514	rVB2	6219	10490	0.95%	0.131%
8	2.830	535	541	543	rBV2	364	397	0.04%	0.005%
9	3.064	611	614	617	rVB	272	169	0.02%	0.002%
10	3.277	676	680	686	rVB2	165	199	0.02%	0.002%
11	3.315	686	692	696	rBV2	221	304	0.03%	0.004%
12	3.418	718	724	729	rBV4	703	991	0.09%	0.012%
13	3.617	783	786	790	rBV2	191	180	0.02%	0.002%
14	3.669	798	802	805	rBV2	190	178	0.02%	0.002%
15	3.752	824	828	834	rVV2	218	222	0.02%	0.003%
16	4.026	907	913	917	rBV2	150	175	0.02%	0.002%
17	4.051	917	921	927	rVB2	164	179	0.02%	0.002%
18	4.170	945	958	982	rBV2	60205	155925	14.15%	1.954%
19	4.640	1082	1104	1133	rBV	108301	255405	23.17%	3.200%
20	4.887	1177	1181	1183	rBV2	331	277	0.03%	0.003%
21	5.055	1228	1233	1237	rVB	282	243	0.02%	0.003%
22	5.334	1297	1320	1350	rBV2	218188	640806	58.14%	8.029%
23	5.553	1377	1388	1400	rBV3	3909	8398	0.76%	0.105%
24	5.630	1410	1412	1420	rVB2	376	361	0.03%	0.005%
25	5.678	1420	1427	1430	rBV	251	297	0.03%	0.004%
26	5.881	1459	1490	1510	rBV	209282	471101	42.74%	5.903%
27	6.183	1574	1584	1596	rVB3	17663	34176	3.10%	0.428%
28	6.325	1615	1628	1650	rBV	145815	287596	26.09%	3.603%
29	6.424	1652	1659	1671	rVB2	5018	9039	0.82%	0.113%
30	6.579	1701	1707	1713	rBV	3384	5167	0.47%	0.065%
31	6.698	1733	1744	1777	rBV	613984	1102268	100.00%	13.811%
32	7.151	1883	1885	1889	rVB3	372	215	0.02%	0.003%
33	7.222	1896	1907	1928	rBV	86469	152340	13.82%	1.909%
34	7.415	1954	1967	1998	rBV	109123	193095	17.52%	2.419%

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35	7.559	2000	2012	2040	rBV	304929	539592	48.95%	6.761%
36	7.707	2054	2058	2065	rVB4	863	1156	0.10%	0.014%
37	7.765	2074	2076	2079	rVB2	471	284	0.03%	0.004%
38	7.791	2079	2084	2087	rBV2	564	613	0.06%	0.008%
39	7.810	2087	2090	2091	rVV	531	334	0.03%	0.004%
40	7.846	2091	2101	2127	rVB2	67813	120836	10.96%	1.514%
41	7.974	2138	2141	2148	rVB4	517	480	0.04%	0.006%
42	8.151	2184	2196	2211	rBV	60510	99671	9.04%	1.249%
43	8.257	2214	2229	2235	rVV2	24950	46139	4.19%	0.578%
44	8.305	2235	2244	2266	rVV	216098	385656	34.99%	4.832%
45	8.408	2266	2276	2302	rVV	421030	684216	62.07%	8.573%
46	8.521	2304	2311	2333	rVB	27354	48102	4.36%	0.603%
47	8.617	2338	2341	2343	rBV2	452	307	0.03%	0.004%
48	8.669	2355	2357	2363	rVV2	346	232	0.02%	0.003%
49	8.698	2364	2366	2370	rVB2	530	337	0.03%	0.004%
50	8.813	2396	2402	2407	rBV3	326	430	0.04%	0.005%
51	8.900	2417	2429	2454	rBV	275180	441030	40.01%	5.526%
52	9.083	2474	2486	2514	rBV	298397	495819	44.98%	6.212%
53	9.254	2537	2539	2542	rBV	288	172	0.02%	0.002%
54	9.379	2576	2578	2581	rVB	338	185	0.02%	0.002%
55	9.402	2581	2585	2587	rBV2	210	196	0.02%	0.002%
56	9.444	2595	2598	2601	rBV2	313	260	0.02%	0.003%
57	9.518	2618	2621	2625	rBV3	381	311	0.03%	0.004%
58	9.563	2630	2635	2640	rVB3	401	433	0.04%	0.005%
59	9.611	2640	2650	2659	rBV5	2879	5665	0.51%	0.071%
60	9.669	2665	2668	2672	rVB3	378	295	0.03%	0.004%
61	9.765	2690	2698	2716	rBV2	11545	19811	1.80%	0.248%
62	9.858	2725	2727	2739	rVB3	505	590	0.05%	0.007%
63	9.916	2739	2745	2748	rBV3	186	191	0.02%	0.002%
64	9.961	2754	2759	2761	rBV2	254	246	0.02%	0.003%
65	10.193	2828	2831	2833	rVV2	274	180	0.02%	0.002%
66	10.209	2833	2836	2839	rVV3	326	250	0.02%	0.003%
67	10.241	2844	2846	2850	rBV	233	203	0.02%	0.003%
68	10.427	2892	2904	2930	rBV	207919	335567	30.44%	4.204%
69	10.604	2951	2959	2968	rVB2	1094	1814	0.16%	0.023%
70	10.839	3029	3032	3037	rBV2	327	190	0.02%	0.002%
71	10.997	3077	3081	3087	rVB2	243	305	0.03%	0.004%

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72	11.025	3087	3090	3093	rBV2	260	222	0.02%	0.003%
73	11.257	3159	3162	3164	rBV	278	198	0.02%	0.002%
74	11.312	3175	3179	3184	rBV2	348	248	0.02%	0.003%
75	11.373	3193	3198	3203	rVB2	197	231	0.02%	0.003%
76	11.479	3219	3231	3252	rBV	306143	492244	44.66%	6.168%
77	11.607	3269	3271	3275	rVB3	299	182	0.02%	0.002%
78	11.726	3305	3308	3311	rBV2	285	206	0.02%	0.003%
79	11.855	3336	3348	3369	rBV	297728	492268	44.66%	6.168%
80	12.138	3432	3436	3440	rBV2	334	325	0.03%	0.004%
81	12.161	3440	3443	3447	rVB2	314	217	0.02%	0.003%
82	12.270	3474	3477	3482	rVB2	325	257	0.02%	0.003%
83	12.476	3536	3541	3543	rBV2	572	535	0.05%	0.007%
84	12.604	3578	3581	3586	rVB2	226	168	0.02%	0.002%
85	12.630	3586	3589	3600	rVB2	281	272	0.02%	0.003%
86	12.759	3627	3629	3634	rVB2	231	197	0.02%	0.002%
87	12.787	3634	3638	3641	rBV	236	184	0.02%	0.002%
88	12.939	3681	3685	3689	rBV3	297	356	0.03%	0.004%
89	13.041	3715	3717	3724	rVB3	298	266	0.02%	0.003%
90	13.254	3778	3783	3785	rBV2	269	287	0.03%	0.004%
91	13.646	3903	3905	3909	rVB	443	254	0.02%	0.003%
92	13.675	3909	3914	3917	rBV2	305	311	0.03%	0.004%
93	13.996	4011	4014	4016	rBV	276	186	0.02%	0.002%
94	14.199	4074	4077	4080	rBV2	310	252	0.02%	0.003%
95	14.273	4093	4100	4109	rBV4	959	1784	0.16%	0.022%
96	14.440	4150	4152	4155	rBV3	259	180	0.02%	0.002%
97	14.858	4279	4282	4288	rVB3	278	263	0.02%	0.003%
98	14.967	4312	4316	4321	rBV3	335	407	0.04%	0.005%
99	15.373	4439	4442	4447	rBV2	286	269	0.02%	0.003%
100	15.803	4572	4576	4580	rBV3	501	563	0.05%	0.007%

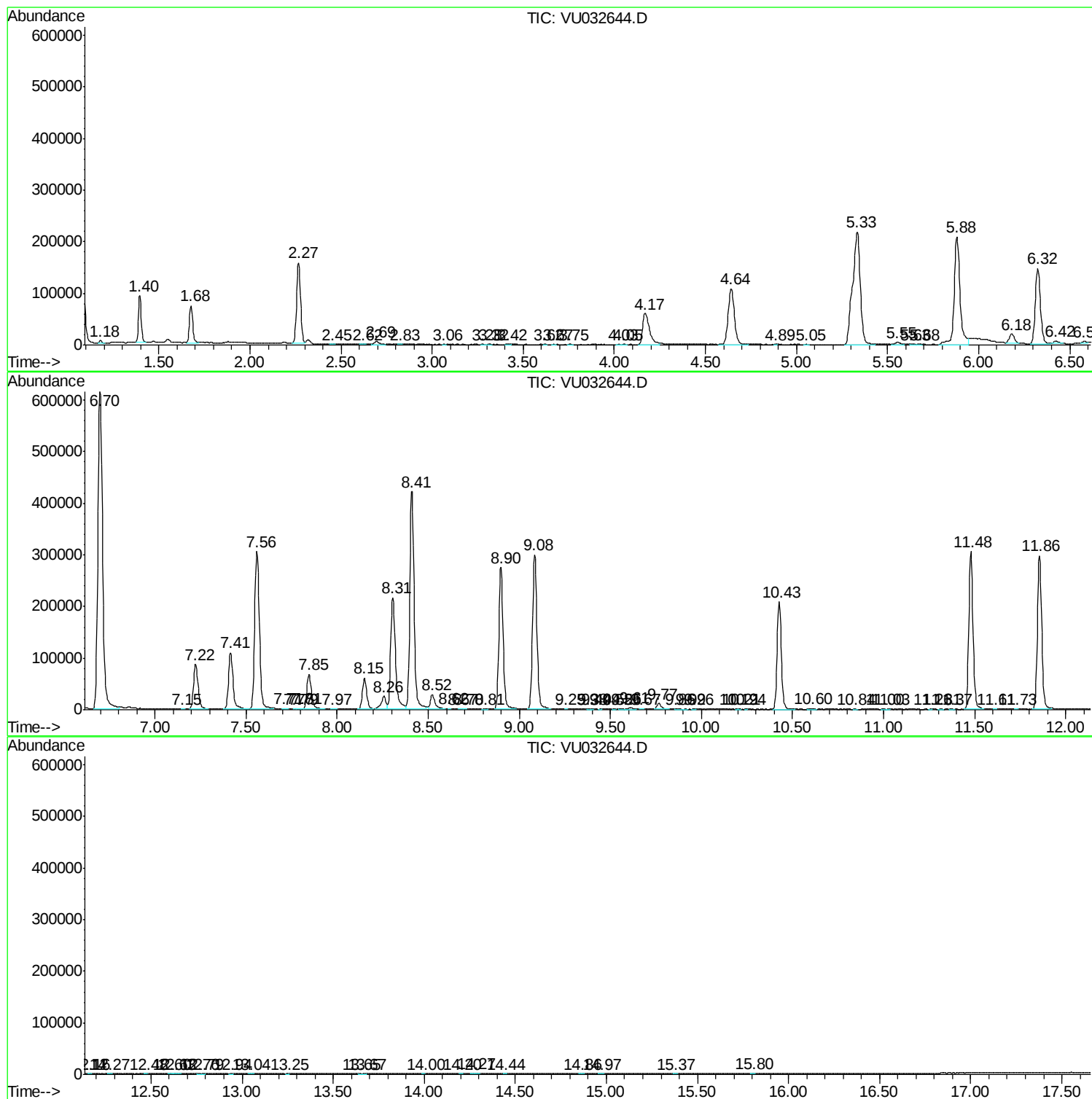
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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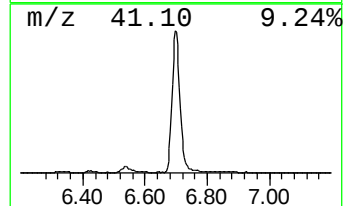
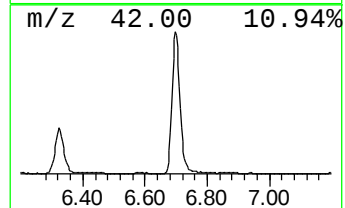
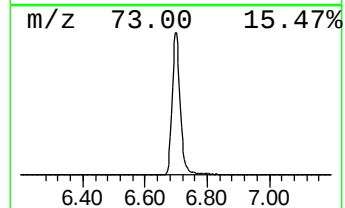
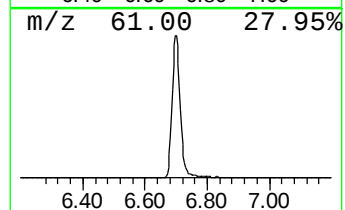
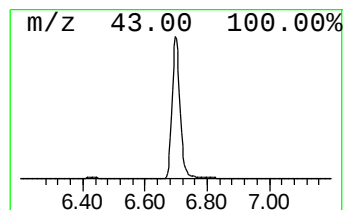
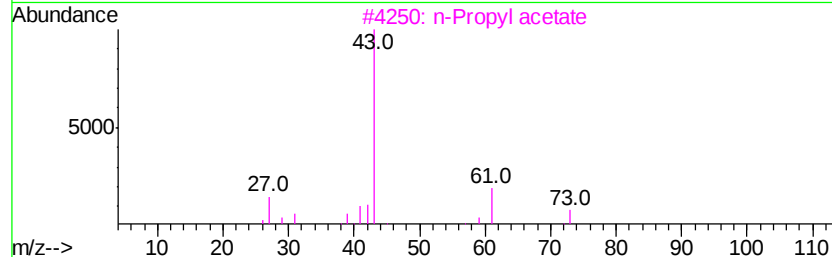
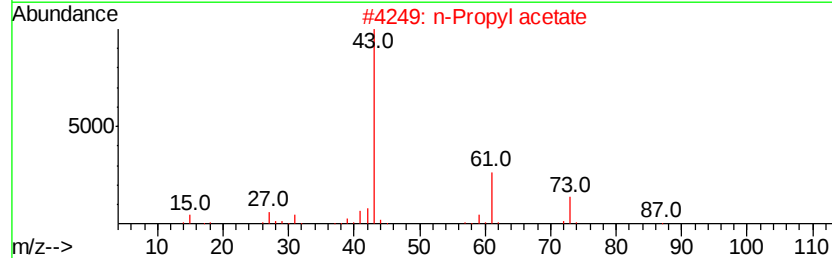
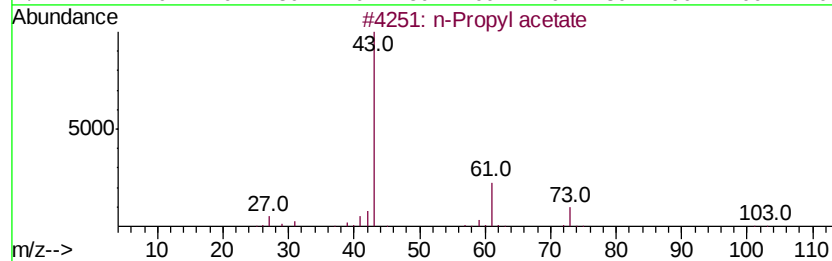
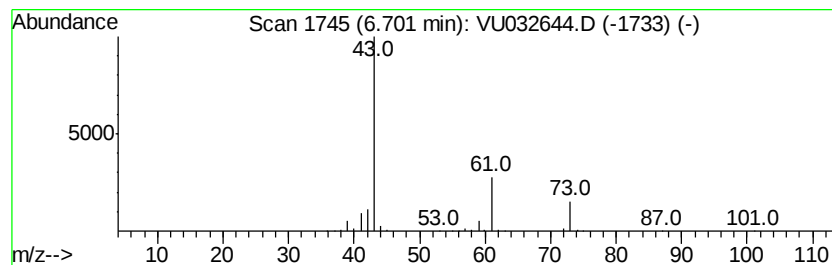
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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	116.99 ug/L	1102270	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	9
5		Isobutyl acetate	116	C6H12O2	000110-19-0	9



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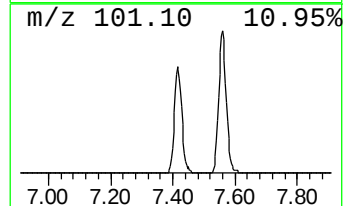
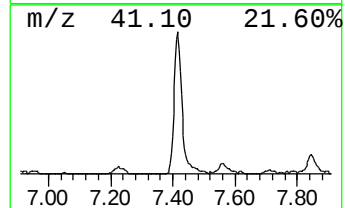
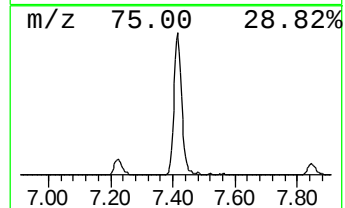
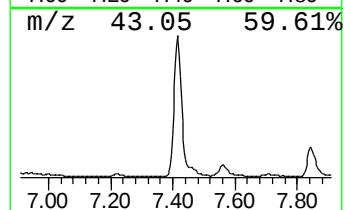
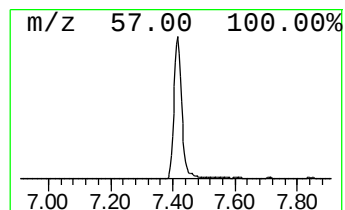
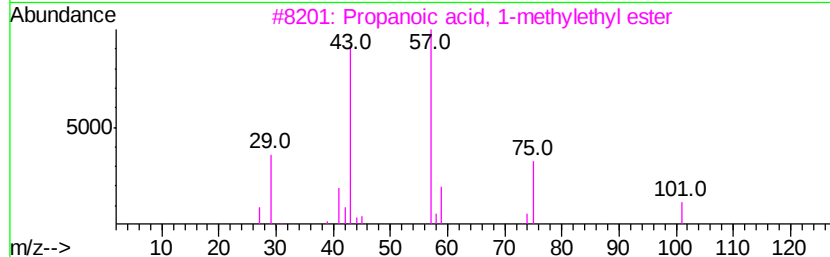
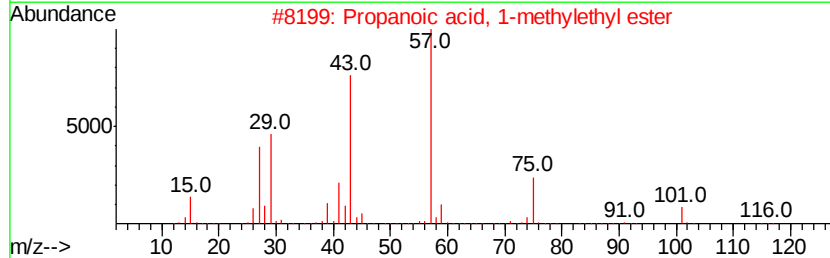
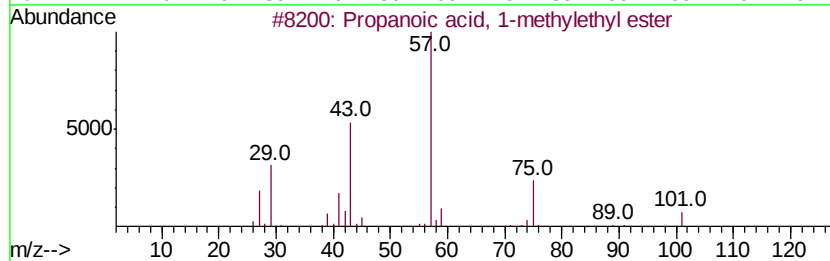
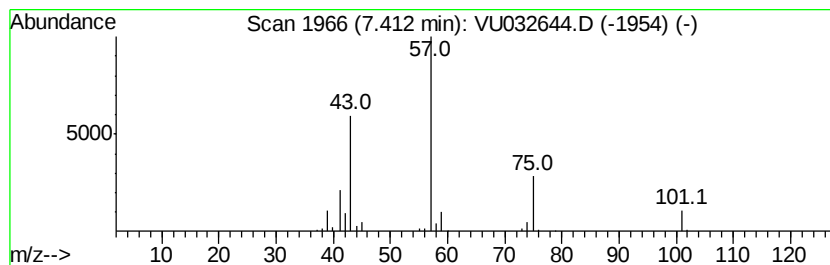
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	20.49 ug/L	193095	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	59
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53
5		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



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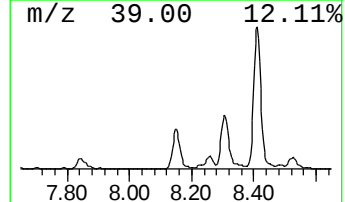
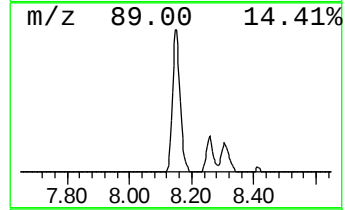
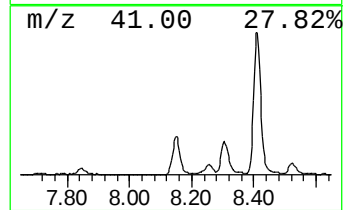
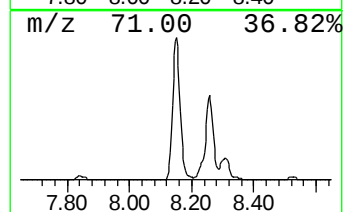
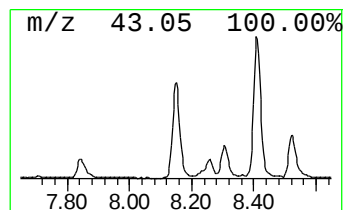
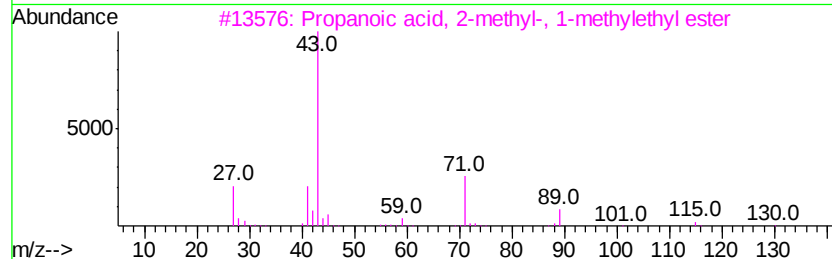
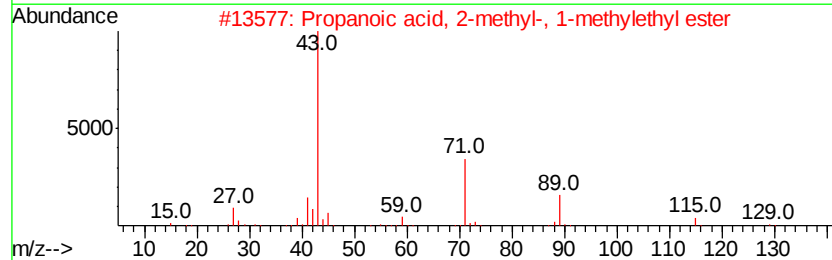
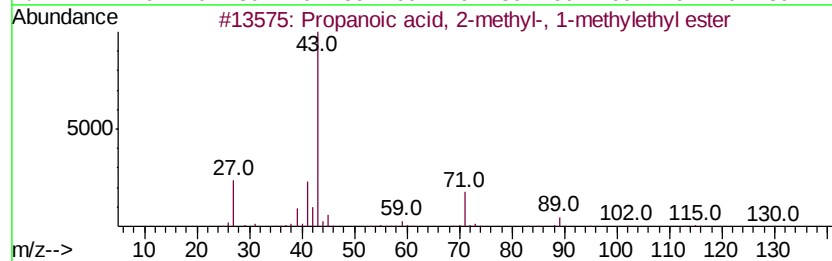
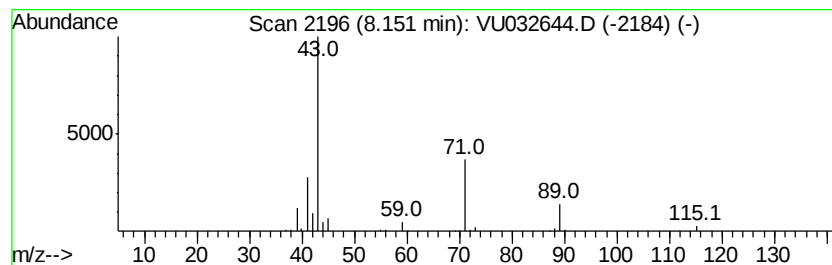
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Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	10.05 ug/L	99671	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			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032644.D
Acq On : 12 Jun 2019 12:16
Operator : JC/SP
Sample : K3286-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JS5

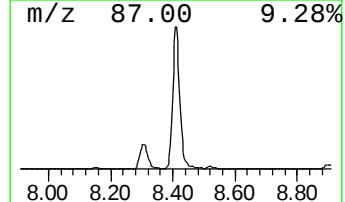
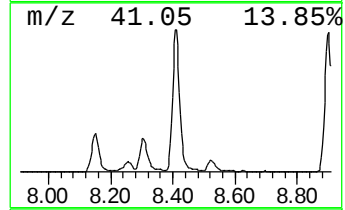
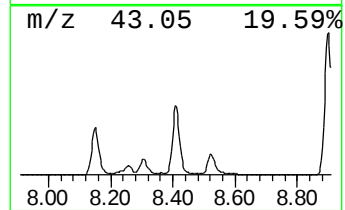
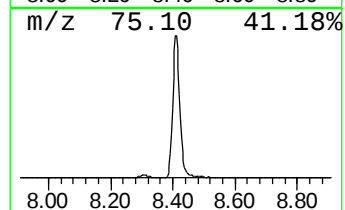
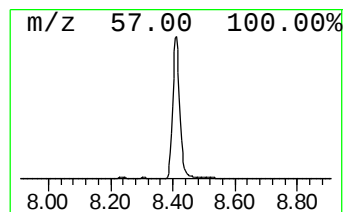
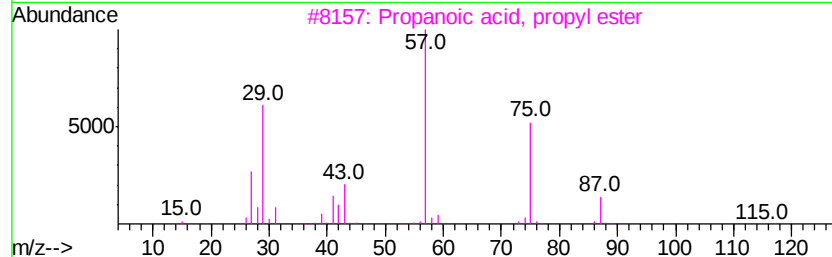
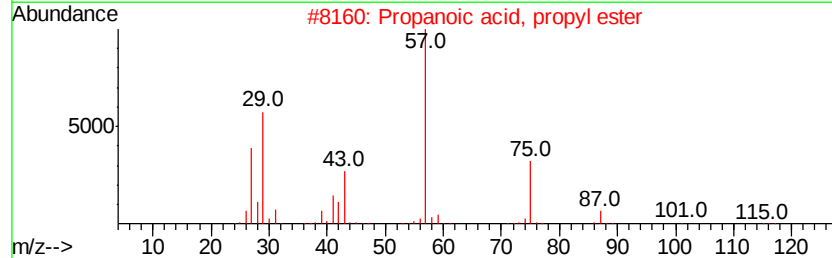
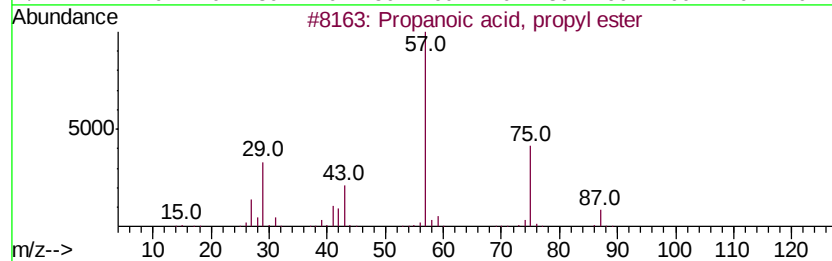
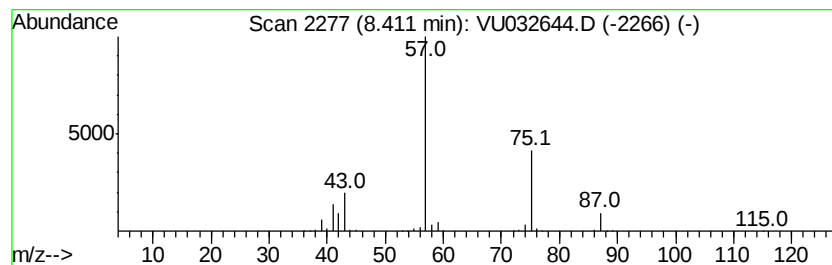
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Quant Title : VOC Analysis

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	69.00 ug/L	684216	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	39



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032644.D
Acq On : 12 Jun 2019 12:16
Operator : JC/SP
Sample : K3286-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JS5

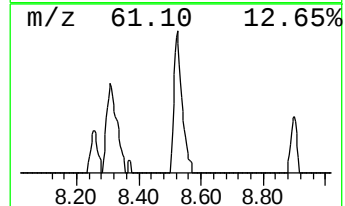
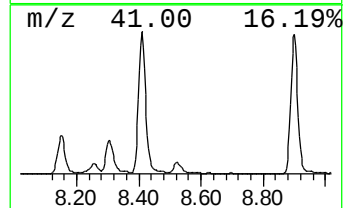
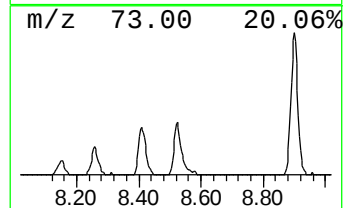
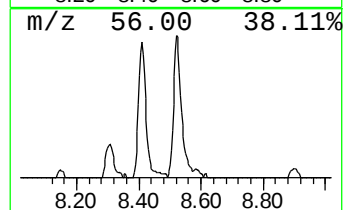
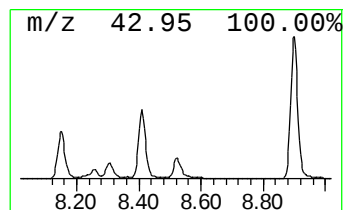
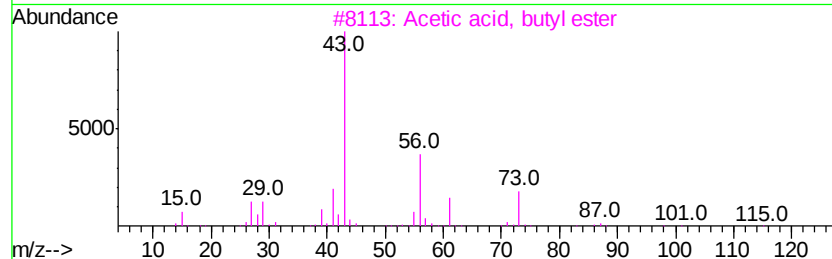
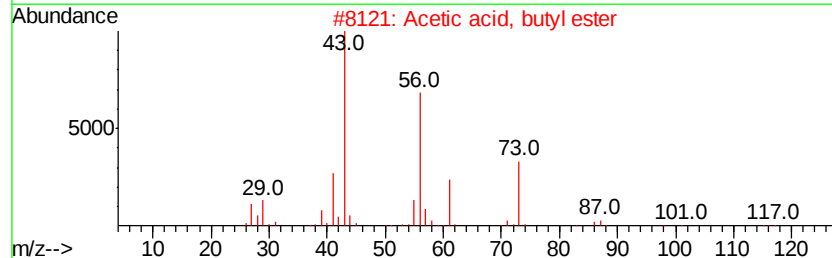
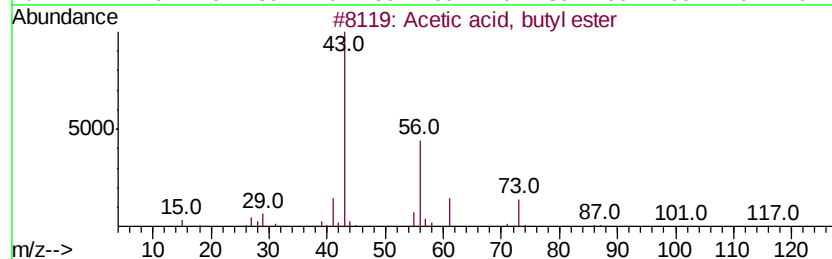
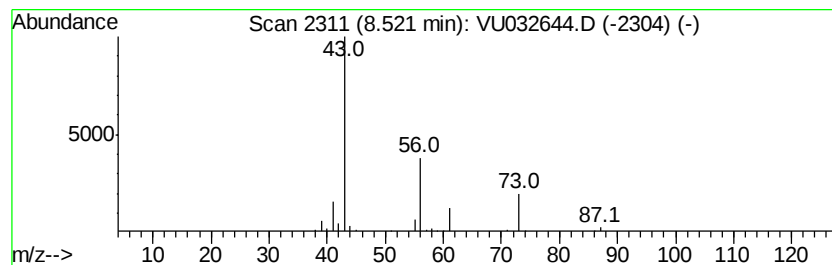
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Quant Title : VOC Analysis

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	4.85 ug/L	48102	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
3		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
4		Isobutyl acetate	116	C6H12O2	000110-19-0	56
5		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032644.D
Acq On : 12 Jun 2019 12:16
Operator : JC/SP
Sample : K3286-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

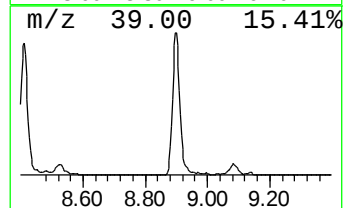
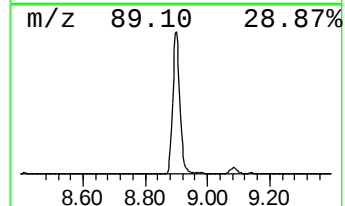
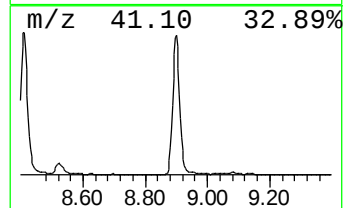
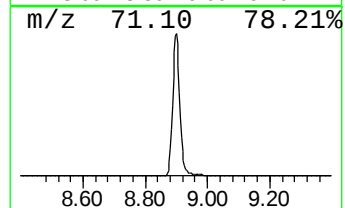
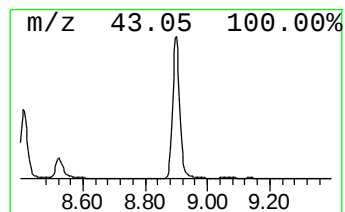
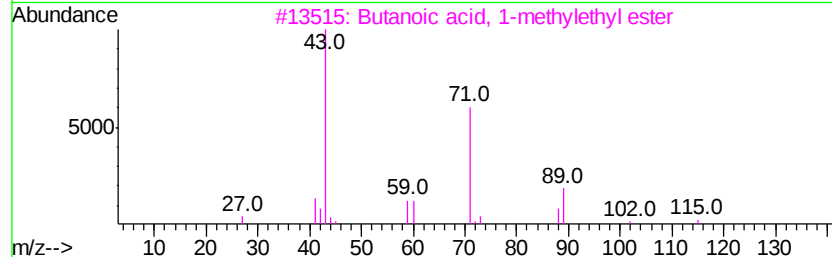
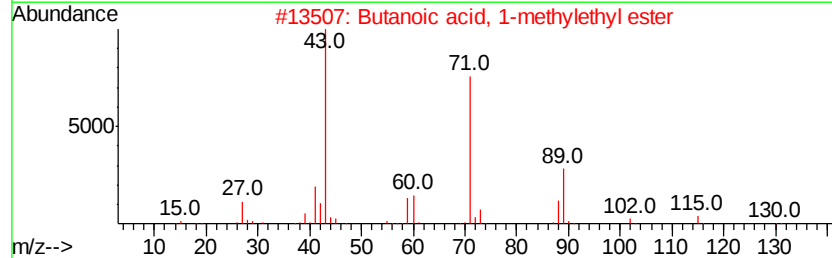
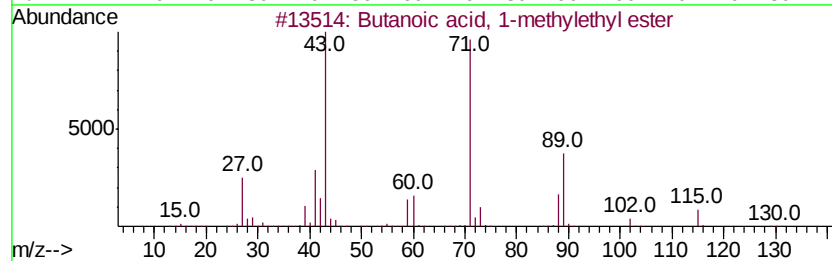
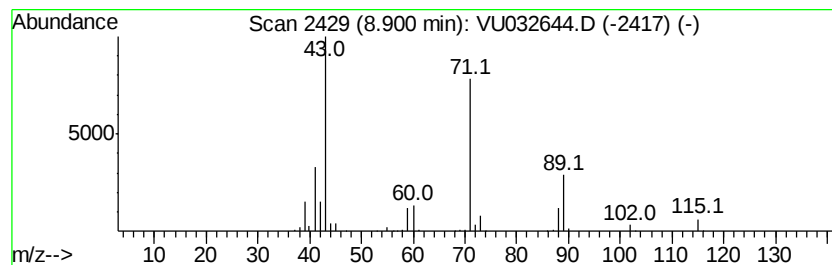
Instrument :
MSVOA_U
ClientSampleId :
C0JS5

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.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	44.47 ug/L	441030	Chlorobenzene-d5	9.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64	
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64	



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061219\
Data File : VU032644.D
Acq On : 12 Jun 2019 12:16
Operator : JC/SP
Sample : K3286-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JS5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.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	117.0	ug/L	1102270	1	5.88	471101	50.0
Propanoic acid, 1...	7.41	20.5	ug/L	193095	1	5.88	471101	50.0
Propanoic acid, 2...	8.15	10.1	ug/L	99671	2	9.08	495819	50.0
Propanoic acid, p...	8.41	69.0	ug/L	684216	2	9.08	495819	50.0
Acetic acid, buty...	8.52	4.8	ug/L	48102	2	9.08	495819	50.0
Butanoic acid, 1-...	8.90	44.5	ug/L	441030	2	9.08	495819	50.0