

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
 Data File : VU032821.D
 Acq On : 18 Jun 2019 14:00
 Operator : JC/SP
 Sample : K3363-22
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JS9

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	rBV	6384	6479	0.49%	0.065%
2	1.396	88	95	107	rBV	112214	113802	8.65%	1.136%
3	1.675	174	182	200	rVB	93041	116089	8.82%	1.159%
4	2.267	355	366	377	rBV	175074	265054	20.15%	2.645%
5	2.466	426	428	432	rVB3	521	274	0.02%	0.003%
6	2.547	449	453	455	rBV2	481	267	0.02%	0.003%
7	2.592	464	467	468	rBV	681	411	0.03%	0.004%
8	2.617	468	475	488	rVB3	2440	4601	0.35%	0.046%
9	2.695	489	499	510	rVB2	7551	12696	0.97%	0.127%
10	2.817	532	537	539	rBV3	740	574	0.04%	0.006%
11	3.305	682	689	694	rBV2	442	640	0.05%	0.006%
12	3.331	694	697	701	rVV2	313	307	0.02%	0.003%
13	3.350	701	703	706	rVV2	359	249	0.02%	0.002%
14	3.521	751	756	759	rBV3	335	361	0.03%	0.004%
15	3.614	781	785	790	rBV3	436	425	0.03%	0.004%
16	3.640	790	793	795	rBV	389	257	0.02%	0.003%
17	3.723	817	819	823	rVB	438	295	0.02%	0.003%
18	3.749	823	827	830	rBV2	361	269	0.02%	0.003%
19	3.810	842	846	849	rBV3	302	260	0.02%	0.003%
20	3.881	862	868	872	rBV	533	465	0.04%	0.005%
21	3.907	872	876	881	rVB	527	416	0.03%	0.004%
22	4.016	908	910	916	rVB2	355	347	0.03%	0.003%
23	4.048	916	920	923	rBV	381	337	0.03%	0.003%
24	4.167	945	957	991	rBV	87717	237778	18.07%	2.373%
25	4.521	1063	1067	1070	rBV3	451	378	0.03%	0.004%
26	4.640	1087	1104	1127	rBV	149132	346924	26.37%	3.462%
27	4.756	1137	1140	1146	rVB2	398	276	0.02%	0.003%
28	4.871	1172	1176	1178	rBV2	468	408	0.03%	0.004%
29	4.936	1192	1196	1198	rBV2	352	287	0.02%	0.003%
30	5.225	1282	1286	1289	rBV2	318	284	0.02%	0.003%
31	5.244	1289	1292	1295	rVV	366	303	0.02%	0.003%
32	5.331	1296	1319	1343	rVV2	288437	862919	65.59%	8.612%
33	5.418	1343	1346	1350	rVB3	833	634	0.05%	0.006%
34	5.495	1364	1370	1374	rVB3	388	460	0.03%	0.005%

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

35	5.550	1374	1387	1405	rBV3	5819	12712	0.97%	0.127%
36	5.640	1412	1415	1420	rVB2	319	260	0.02%	0.003%
37	5.720	1435	1440	1442	rBV3	519	493	0.04%	0.005%
38	5.881	1475	1490	1509	rBV	252711	496696	37.75%	4.957%
39	6.003	1519	1528	1530	rBV5	1344	1935	0.15%	0.019%
40	6.325	1614	1628	1647	rBV	199375	397936	30.25%	3.971%
41	6.421	1650	1658	1665	rBV2	6289	10329	0.79%	0.103%
42	6.530	1685	1692	1698	rBV3	2473	4349	0.33%	0.043%
43	6.575	1701	1706	1713	rVV2	4028	6074	0.46%	0.061%
44	6.698	1731	1744	1776	rBV	739994	1315609	100.00%	13.129%
45	7.003	1837	1839	1843	rVB	422	282	0.02%	0.003%
46	7.042	1847	1851	1852	rBV2	377	252	0.02%	0.003%
47	7.138	1876	1881	1883	rBV2	571	474	0.04%	0.005%
48	7.154	1883	1886	1892	rVB4	555	442	0.03%	0.004%
49	7.222	1894	1907	1929	rVV2	104875	188880	14.36%	1.885%
50	7.328	1936	1940	1942	rBV3	345	274	0.02%	0.003%
51	7.360	1946	1950	1951	rBV3	487	330	0.03%	0.003%
52	7.415	1955	1967	1994	rVB	141660	243375	18.50%	2.429%
53	7.559	1998	2012	2028	rBV	382526	663227	50.41%	6.619%
54	7.698	2048	2055	2065	rBV7	1572	2790	0.21%	0.028%
55	7.772	2075	2078	2083	rVB4	1081	808	0.06%	0.008%
56	7.842	2089	2100	2117	rBV2	86921	150446	11.44%	1.501%
57	7.981	2139	2143	2147	rVB2	862	780	0.06%	0.008%
58	8.006	2147	2151	2154	rBV3	539	487	0.04%	0.005%
59	8.022	2154	2156	2161	rVV4	638	480	0.04%	0.005%
60	8.061	2166	2168	2176	rVB2	516	425	0.03%	0.004%
61	8.148	2184	2195	2210	rBV	75988	125515	9.54%	1.253%
62	8.228	2211	2220	2222	rBV2	8365	10611	0.81%	0.106%
63	8.257	2223	2229	2235	rVV2	27763	41971	3.19%	0.419%
64	8.305	2235	2244	2265	rVV	298680	504805	38.37%	5.038%
65	8.411	2266	2277	2297	rVB	524884	819917	62.32%	8.183%
66	8.521	2303	2311	2332	rVB	34227	58373	4.44%	0.583%
67	8.897	2414	2428	2452	rBV	365390	582165	44.25%	5.810%
68	9.083	2466	2486	2504	rBV	379808	630327	47.91%	6.291%
69	9.228	2528	2531	2538	rVB3	344	303	0.02%	0.003%
70	9.415	2587	2589	2592	rVV3	429	257	0.02%	0.003%
71	9.598	2638	2646	2657	rBV3	5219	9083	0.69%	0.091%

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72	9.697	2674	2677	2679	rBV3	417	298	0.02%	0.003%
73	9.714	2679	2682	2686	rVV3	390	302	0.02%	0.003%
74	9.762	2686	2697	2711	rVV2	17611	28088	2.13%	0.280%
75	9.813	2711	2713	2717	rVB2	622	341	0.03%	0.003%
76	9.871	2726	2731	2733	rBV3	532	424	0.03%	0.004%
77	9.958	2754	2758	2762	rBV3	345	371	0.03%	0.004%
78	10.099	2798	2802	2809	rBV5	493	654	0.05%	0.007%
79	10.148	2813	2817	2818	rBV2	345	278	0.02%	0.003%
80	10.305	2862	2866	2874	rBV4	400	576	0.04%	0.006%
81	10.424	2887	2903	2924	rBV	295281	476833	36.24%	4.759%
82	10.572	2946	2949	2954	rBV3	358	263	0.02%	0.003%
83	10.768	3006	3010	3013	rBV3	517	439	0.03%	0.004%
84	10.794	3015	3018	3024	rVB2	420	339	0.03%	0.003%
85	10.829	3024	3029	3030	rBV	335	238	0.02%	0.002%
86	11.029	3086	3091	3093	rBV2	350	301	0.02%	0.003%
87	11.058	3097	3100	3103	rBV2	261	234	0.02%	0.002%
88	11.128	3116	3122	3127	rBV3	400	539	0.04%	0.005%
89	11.160	3127	3132	3136	rVB3	381	441	0.03%	0.004%
90	11.479	3219	3231	3251	rBV	384520	606961	46.14%	6.057%
91	11.758	3315	3318	3321	rBV3	402	274	0.02%	0.003%
92	11.855	3335	3348	3366	rBV	391809	640508	48.69%	6.392%
93	12.257	3469	3473	3477	rBV2	315	374	0.03%	0.004%
94	12.604	3577	3581	3582	rBV2	371	263	0.02%	0.003%
95	12.897	3669	3672	3676	rBV	340	258	0.02%	0.003%
96	13.003	3701	3705	3709	rBV3	487	498	0.04%	0.005%
97	13.154	3750	3752	3756	rVB2	442	289	0.02%	0.003%
98	13.475	3850	3852	3857	rVV2	329	300	0.02%	0.003%
99	13.893	3979	3982	3987	rBV3	457	343	0.03%	0.003%
100	14.598	4199	4201	4204	rBV2	503	272	0.02%	0.003%

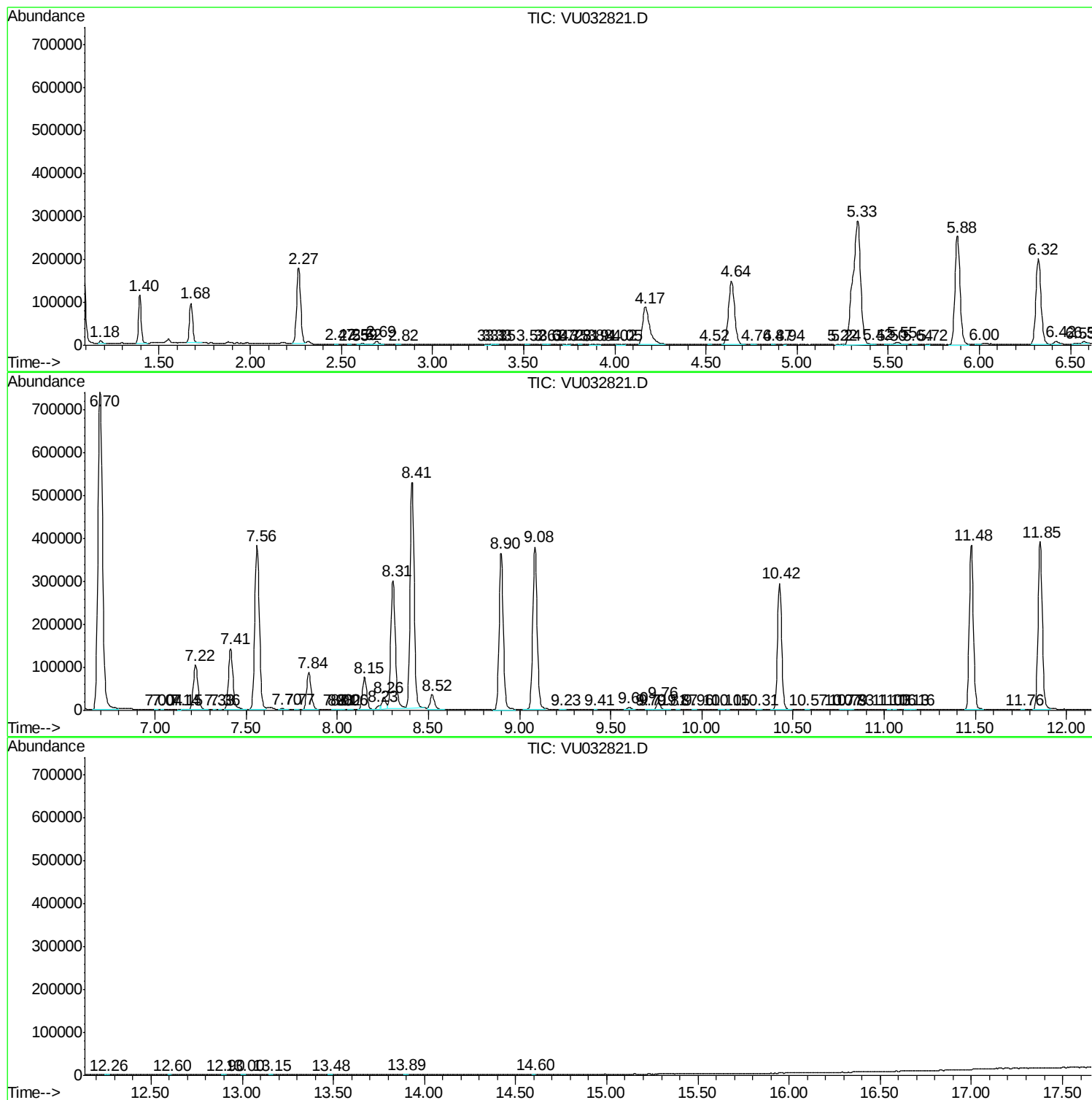
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TIC Library : C:\DATABASE\NIST11.L
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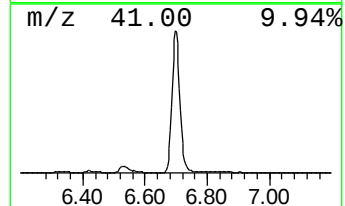
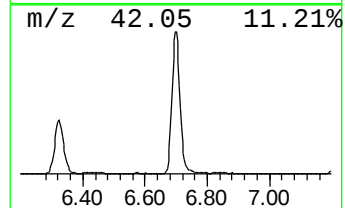
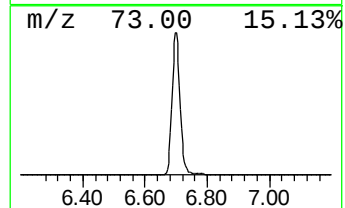
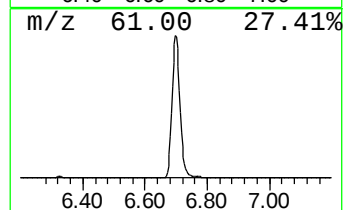
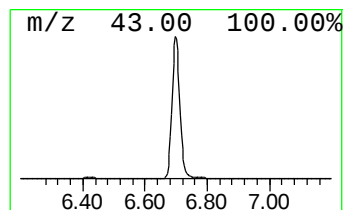
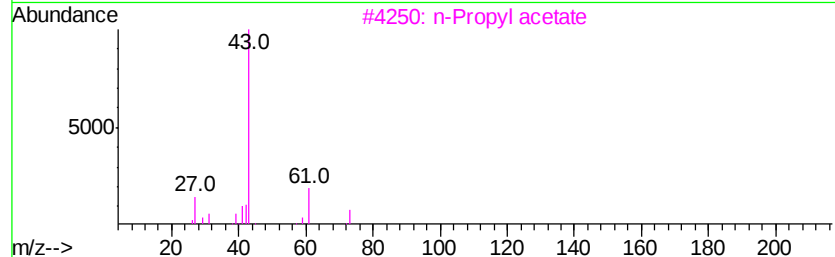
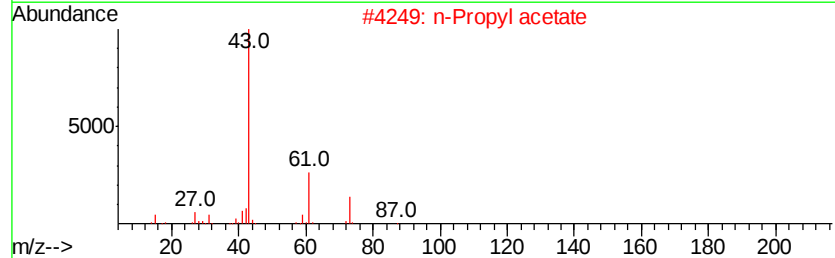
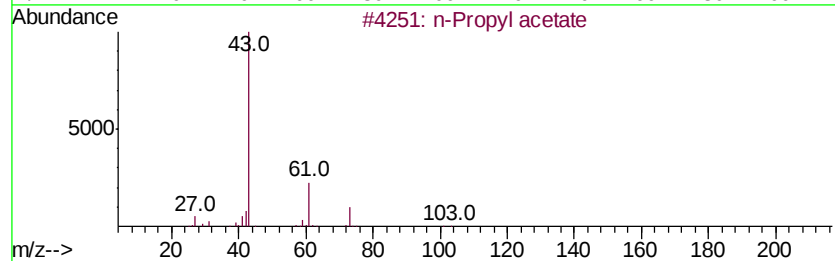
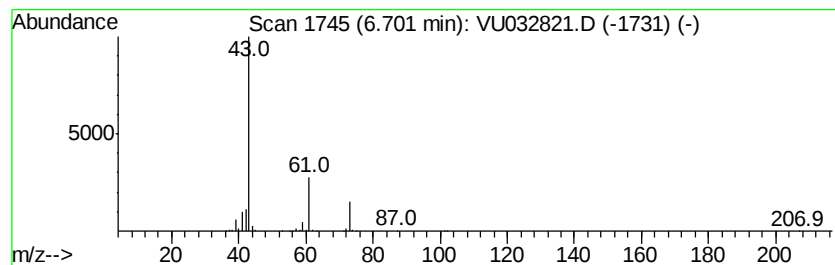
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	132.44 ug/L	1315610	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	9



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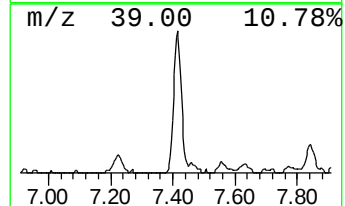
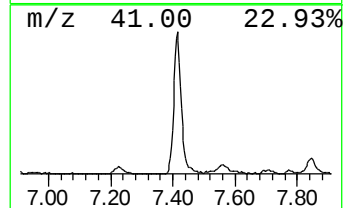
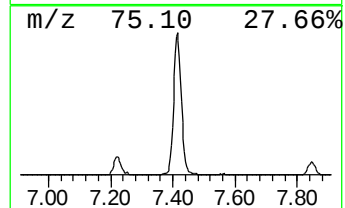
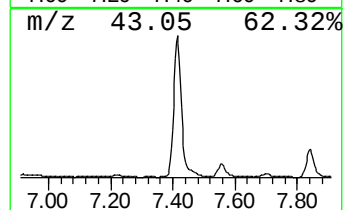
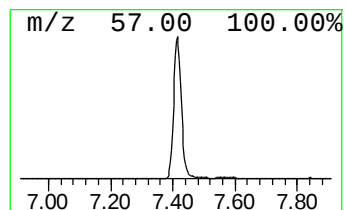
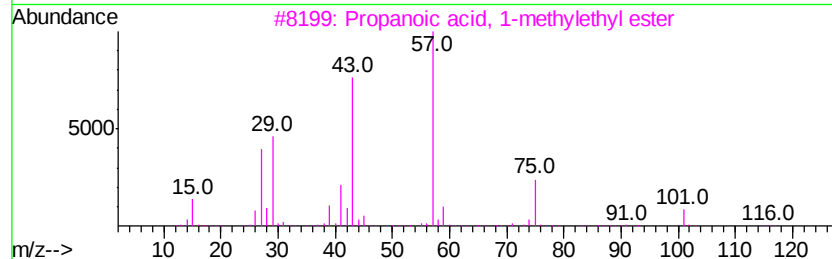
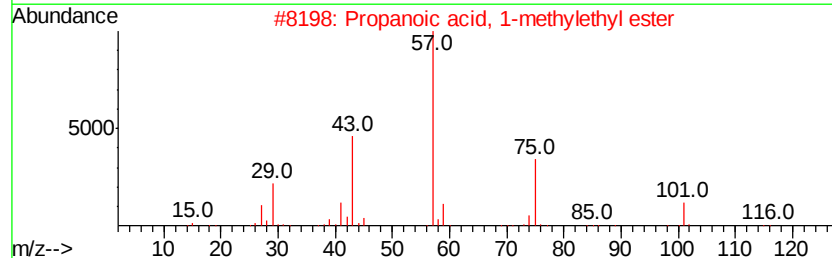
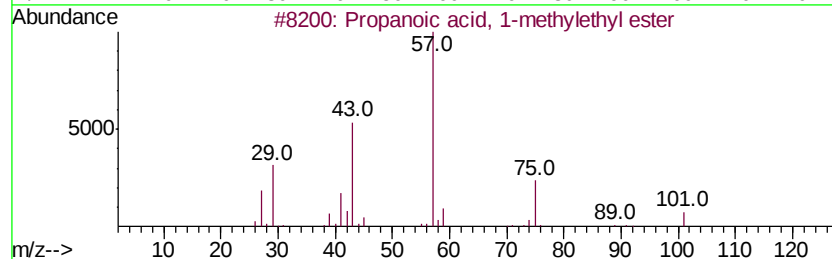
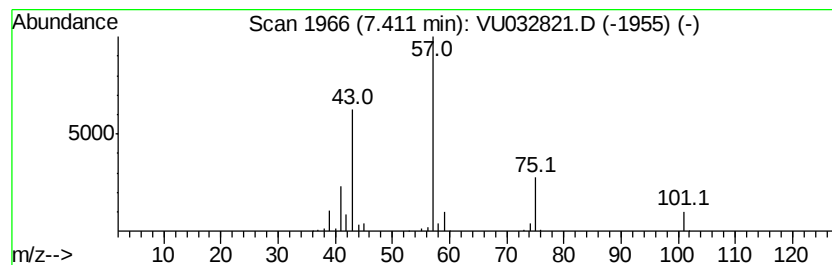
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Quant Title : VOC Analysis

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	24.50 ug/L	243375	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	83
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45
5		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	42



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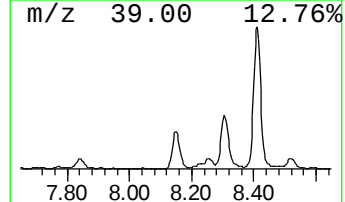
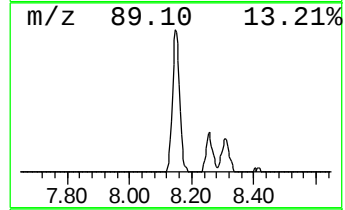
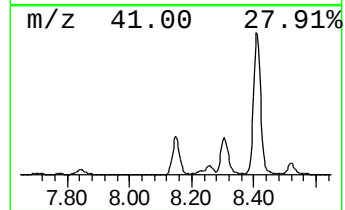
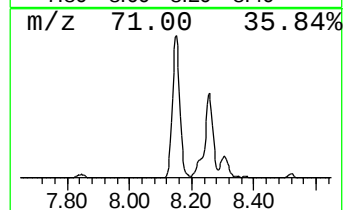
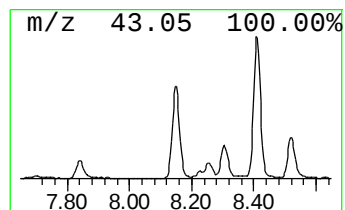
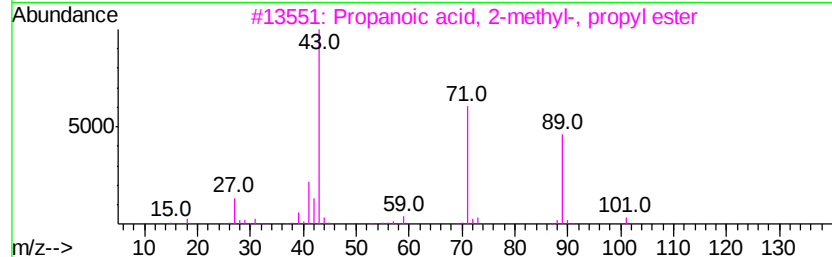
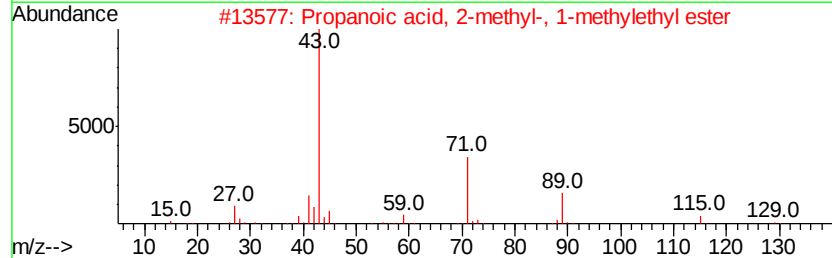
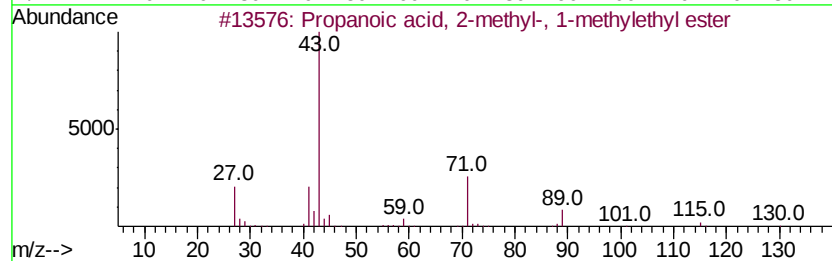
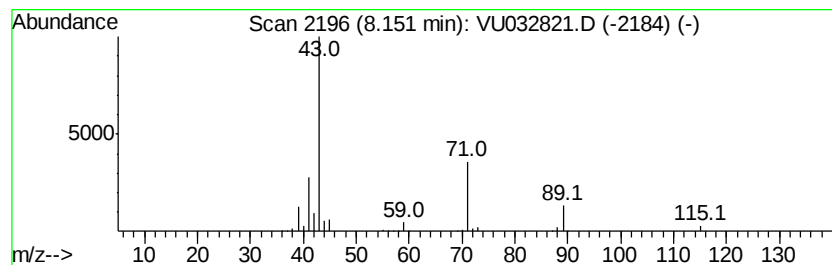
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Quant Title : VOC Analysis

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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	9.96 ug/L	125515	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-, propyl...	130	C7H14O2	000644-49-5	64
4		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032821.D
Acq On : 18 Jun 2019 14:00
Operator : JC/SP
Sample : K3363-22
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JS9

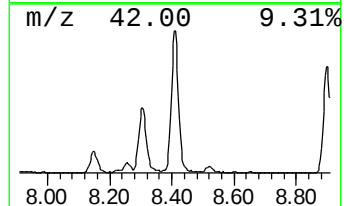
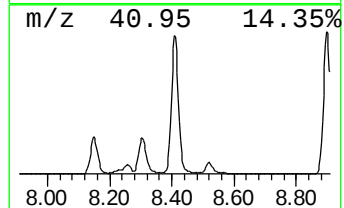
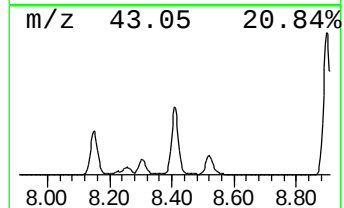
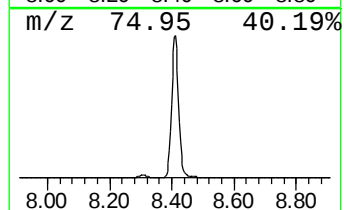
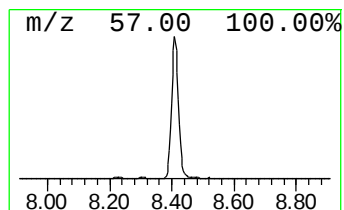
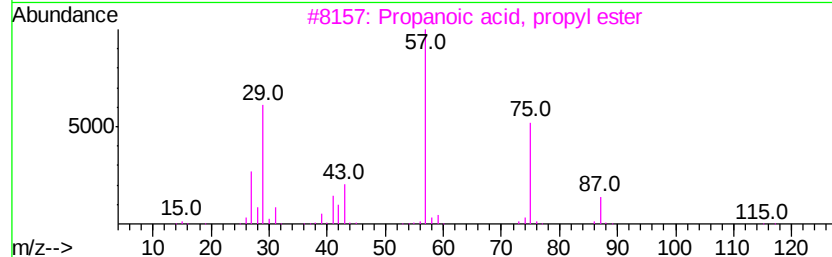
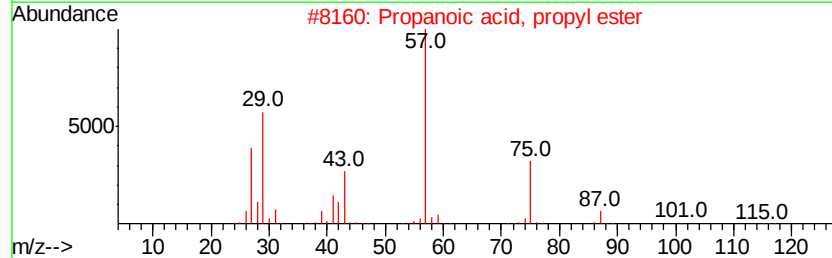
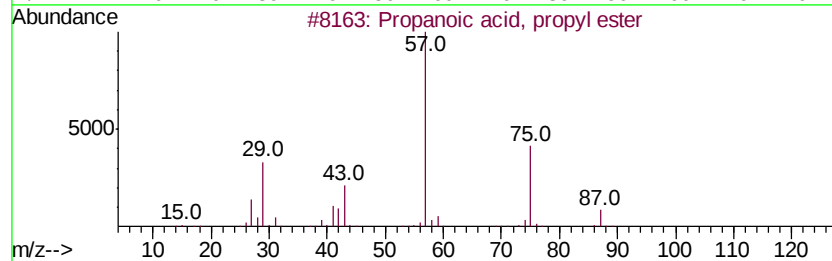
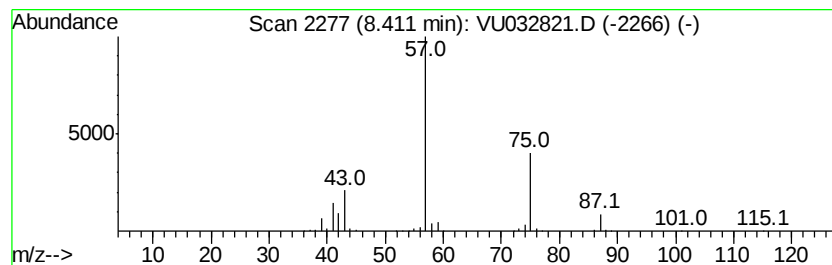
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Quant Title : VOC Analysis

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	65.04 ug/L	819917	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:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032821.D
Acq On : 18 Jun 2019 14:00
Operator : JC/SP
Sample : K3363-22
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JS9

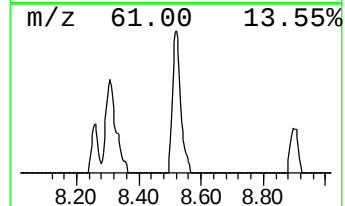
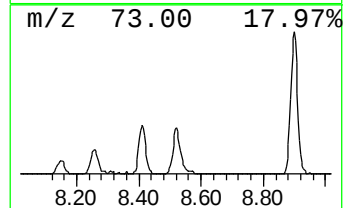
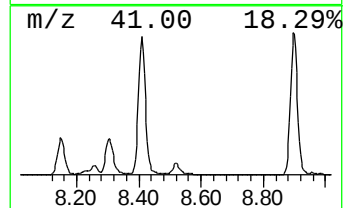
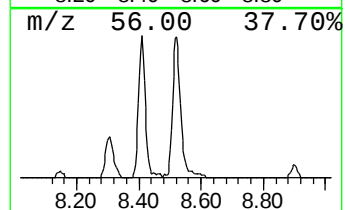
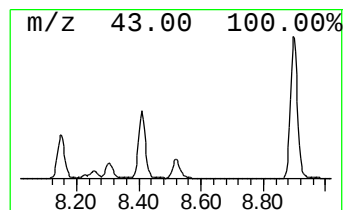
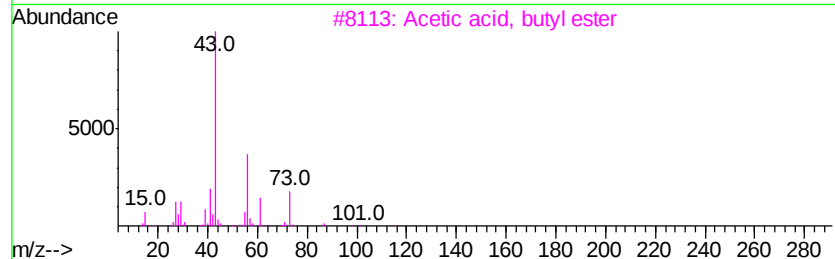
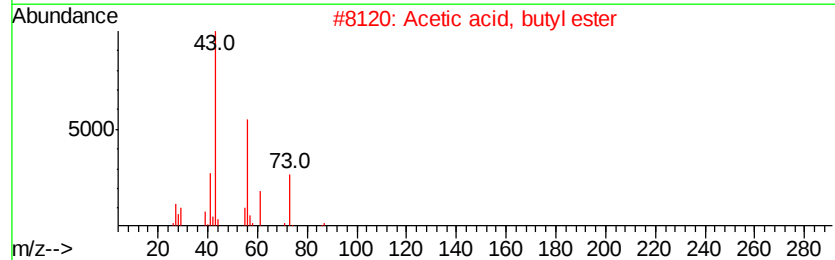
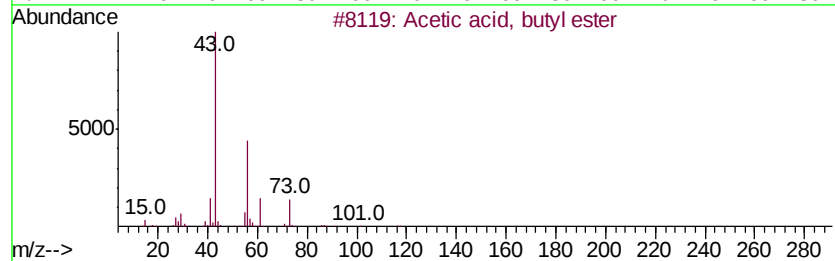
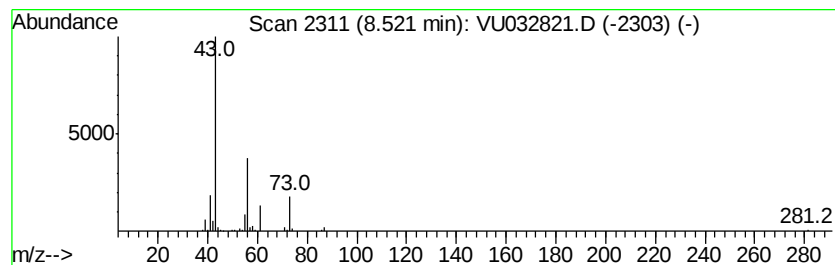
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Quant Title : VOC Analysis

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	4.63 ug/L	58373	Chlorobenzene-d5	9.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	78
2	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	64
3	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	64
4	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	45
5	Acetic acid, hexyl ester			144	C8H16O2	000142-92-7	33



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032821.D
Acq On : 18 Jun 2019 14:00
Operator : JC/SP
Sample : K3363-22
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JS9

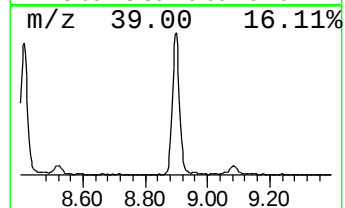
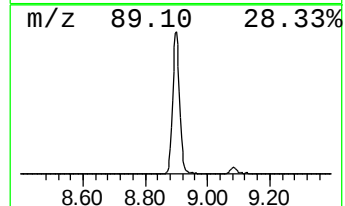
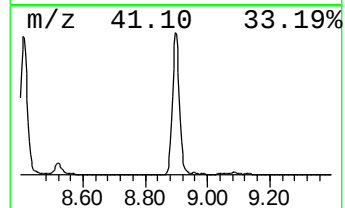
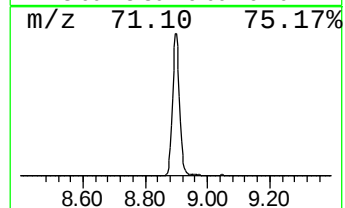
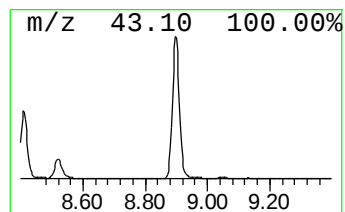
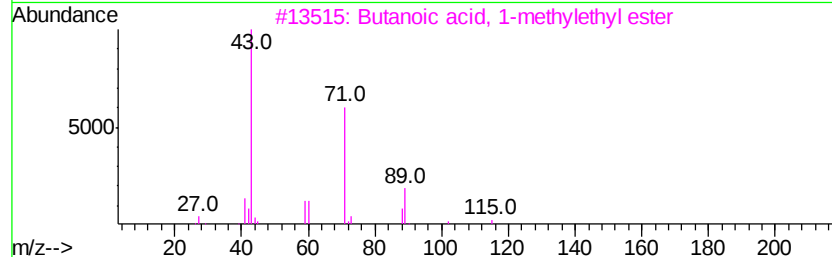
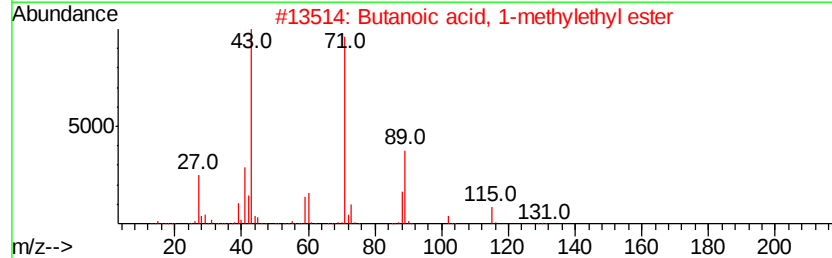
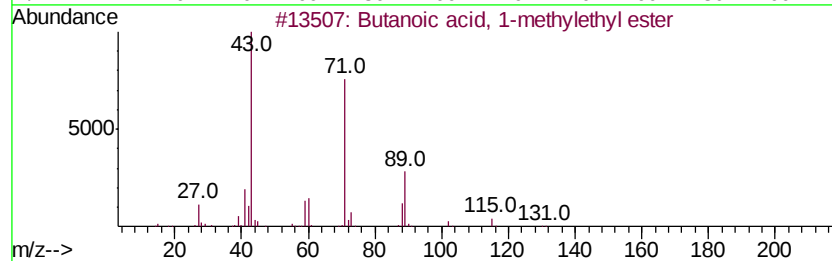
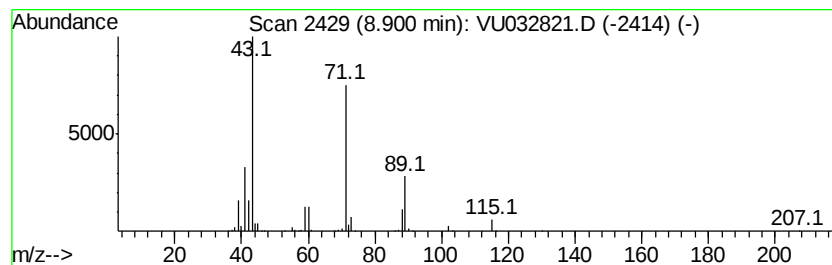
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	46.18 ug/L	582165	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	83
4		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032821.D
Acq On : 18 Jun 2019 14:00
Operator : JC/SP
Sample : K3363-22
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JS9

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	132.4	ug/L	1315610	1	5.88	496696	50.0
Propanoic acid, 1...	7.41	24.5	ug/L	243375	1	5.88	496696	50.0
Propanoic acid, 2...	8.15	10.0	ug/L	125515	2	9.08	630327	50.0
Propanoic acid, p...	8.41	65.0	ug/L	819917	2	9.08	630327	50.0
Acetic acid, buty...	8.52	4.6	ug/L	58373	2	9.08	630327	50.0
Butanoic acid, 1-...	8.90	46.2	ug/L	582165	2	9.08	630327	50.0