

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061719\
 Data File : VU032793.D
 Acq On : 17 Jun 2019 19:21
 Operator : JC/SP
 Sample : K3324-08
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JR4

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	33	rBV2	7545	6930	0.49%	0.066%
2	1.392	88	94	105	rVB	97091	102101	7.15%	0.971%
3	1.675	175	182	197	rVB	85407	104302	7.31%	0.991%
4	2.267	356	366	377	rVB	170943	254133	17.81%	2.416%
5	2.428	412	416	418	rBV2	519	464	0.03%	0.004%
6	2.553	453	455	458	rBV3	464	281	0.02%	0.003%
7	2.617	469	475	480	rBV3	1153	1305	0.09%	0.012%
8	2.695	491	499	513	rVB2	5599	9764	0.68%	0.093%
9	2.813	531	536	537	rBV3	430	283	0.02%	0.003%
10	2.894	557	561	568	rVB3	431	554	0.04%	0.005%
11	2.929	568	572	576	rBV2	352	330	0.02%	0.003%
12	3.084	614	620	623	rBV2	657	495	0.03%	0.005%
13	3.206	654	658	661	rBV	499	351	0.02%	0.003%
14	3.350	700	703	708	rVB3	338	303	0.02%	0.003%
15	3.511	749	753	758	rBV2	398	406	0.03%	0.004%
16	3.669	798	802	806	rBV3	346	300	0.02%	0.003%
17	3.711	813	815	821	rVB3	382	320	0.02%	0.003%
18	3.894	866	872	877	rVV4	420	462	0.03%	0.004%
19	3.948	885	889	898	rVB3	351	371	0.03%	0.004%
20	3.990	898	902	907	rBV2	439	437	0.03%	0.004%
21	4.167	944	957	992	rBV	86187	227006	15.91%	2.158%
22	4.463	1047	1049	1054	rVB4	395	293	0.02%	0.003%
23	4.489	1054	1057	1064	rVB4	439	374	0.03%	0.004%
24	4.640	1085	1104	1127	rBV	143168	334182	23.42%	3.177%
25	5.199	1274	1278	1281	rBV	421	294	0.02%	0.003%
26	5.331	1296	1319	1345	rBV2	271489	815795	57.17%	7.754%
27	5.546	1377	1386	1402	rVV3	5770	12998	0.91%	0.124%
28	5.733	1439	1444	1449	rBV3	413	397	0.03%	0.004%
29	5.794	1460	1463	1466	rBV2	406	379	0.03%	0.004%
30	5.878	1475	1489	1512	rBV	280491	554659	38.87%	5.272%
31	6.325	1613	1628	1648	rBV	191743	382849	26.83%	3.639%
32	6.418	1650	1657	1674	rVB3	6823	14461	1.01%	0.137%
33	6.530	1684	1692	1698	rBV	2749	4483	0.31%	0.043%
34	6.575	1699	1706	1715	rBV	4891	8558	0.60%	0.081%

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 Title : VOC Analysis

35	6.698	1731	1744	1779	rBV	809266	1427047	100.00%	13.565%
36	7.077	1859	1862	1865	rBV4	423	365	0.03%	0.003%
37	7.138	1878	1881	1883	rBV2	400	278	0.02%	0.003%
38	7.222	1892	1907	1923	rBV	110750	197021	13.81%	1.873%
39	7.366	1949	1952	1954	rBV3	658	366	0.03%	0.003%
40	7.415	1954	1967	1992	rVB	150199	256897	18.00%	2.442%
41	7.559	1999	2012	2030	rBV	370031	646781	45.32%	6.148%
42	7.694	2050	2054	2058	rBV4	1399	1653	0.12%	0.016%
43	7.842	2089	2100	2121	rBV2	92867	162119	11.36%	1.541%
44	8.003	2148	2150	2154	rVB5	390	259	0.02%	0.002%
45	8.103	2178	2181	2184	rBV3	452	301	0.02%	0.003%
46	8.148	2184	2195	2210	rVV	86904	144786	10.15%	1.376%
47	8.228	2211	2220	2221	rVV3	9292	11338	0.79%	0.108%
48	8.257	2223	2229	2235	rVV2	33314	51440	3.60%	0.489%
49	8.305	2235	2244	2265	rVV	310995	530156	37.15%	5.039%
50	8.408	2265	2276	2300	rVV	603517	952530	66.75%	9.054%
51	8.517	2303	2310	2324	rVB	40751	65485	4.59%	0.622%
52	8.807	2397	2400	2405	rBV4	498	599	0.04%	0.006%
53	8.897	2416	2428	2461	rBV	414224	658156	46.12%	6.256%
54	9.083	2468	2486	2510	rBV	425750	706519	49.51%	6.716%
55	9.247	2534	2537	2541	rVB2	577	442	0.03%	0.004%
56	9.331	2561	2563	2570	rBV5	355	426	0.03%	0.004%
57	9.369	2570	2575	2579	rBV3	278	289	0.02%	0.003%
58	9.488	2608	2612	2617	rVB	456	476	0.03%	0.005%
59	9.511	2617	2619	2622	rBV2	441	337	0.02%	0.003%
60	9.598	2637	2646	2659	rBV	5854	10431	0.73%	0.099%
61	9.678	2665	2671	2675	rVB4	585	688	0.05%	0.007%
62	9.710	2677	2681	2685	rBV2	537	594	0.04%	0.006%
63	9.762	2687	2697	2713	rVV	23046	37542	2.63%	0.357%
64	9.858	2724	2727	2731	rBV3	385	288	0.02%	0.003%
65	10.099	2799	2802	2805	rBV	426	322	0.02%	0.003%
66	10.160	2817	2821	2826	rVB	606	643	0.05%	0.006%
67	10.199	2827	2833	2834	rBV2	377	284	0.02%	0.003%
68	10.254	2846	2850	2853	rBV4	642	460	0.03%	0.004%
69	10.302	2862	2865	2870	rVB3	532	347	0.02%	0.003%
70	10.424	2889	2903	2923	rVV	288030	464003	32.51%	4.410%
71	10.495	2923	2925	2929	rVB4	672	449	0.03%	0.004%

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72	10.591	2952	2955	2959	rBV4	592	528	0.04%	0.005%
73	10.643	2967	2971	2974	rBV2	369	287	0.02%	0.003%
74	10.701	2986	2989	2992	rVB	538	309	0.02%	0.003%
75	10.765	3006	3009	3013	rVV3	688	629	0.04%	0.006%
76	10.894	3046	3049	3051	rVV	481	354	0.02%	0.003%
77	11.112	3112	3117	3121	rVB5	706	758	0.05%	0.007%
78	11.141	3121	3126	3127	rBV3	376	375	0.03%	0.004%
79	11.221	3149	3151	3155	rVB3	337	265	0.02%	0.003%
80	11.286	3169	3171	3180	rVB4	320	318	0.02%	0.003%
81	11.331	3183	3185	3189	rBV2	393	369	0.03%	0.004%
82	11.479	3219	3231	3254	rBV	435076	693317	48.58%	6.590%
83	11.691	3295	3297	3300	rBV3	551	387	0.03%	0.004%
84	11.742	3310	3313	3316	rBV3	448	344	0.02%	0.003%
85	11.855	3335	3348	3373	rBV	385584	643029	45.06%	6.112%
86	12.135	3432	3435	3439	rVB3	686	426	0.03%	0.004%
87	12.263	3468	3475	3476	rBV3	699	710	0.05%	0.007%
88	12.311	3485	3490	3494	rBV3	377	495	0.03%	0.005%
89	12.472	3537	3540	3542	rBV3	476	319	0.02%	0.003%
90	12.649	3593	3595	3600	rBV3	359	366	0.03%	0.003%
91	13.218	3768	3772	3777	rBV3	397	383	0.03%	0.004%
92	13.276	3788	3790	3793	rVB2	506	275	0.02%	0.003%
93	13.434	3836	3839	3845	rBV4	490	557	0.04%	0.005%
94	13.813	3954	3957	3962	rBV2	283	270	0.02%	0.003%
95	14.118	4047	4052	4057	rBV3	539	581	0.04%	0.006%
96	14.372	4128	4131	4134	rVB3	515	356	0.02%	0.003%
97	14.418	4141	4145	4149	rBV4	624	595	0.04%	0.006%
98	14.485	4164	4166	4169	rVB2	512	265	0.02%	0.003%
99	14.578	4192	4195	4197	rBV3	478	364	0.03%	0.003%
100	14.713	4234	4237	4241	rVB3	682	455	0.03%	0.004%

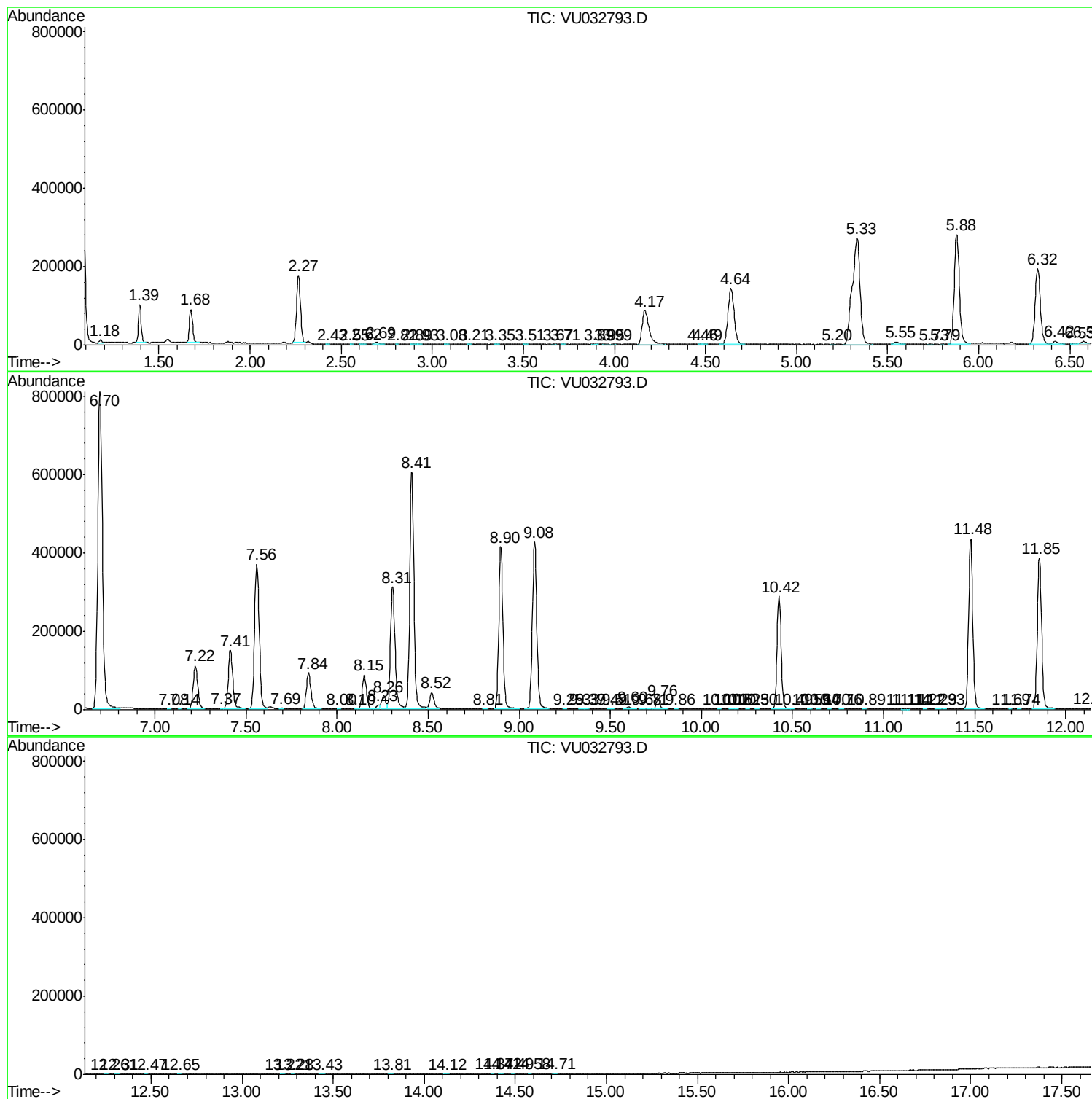
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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



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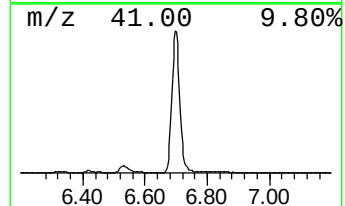
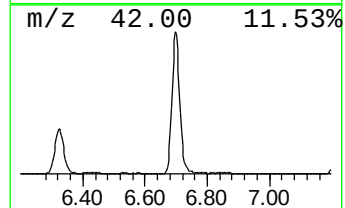
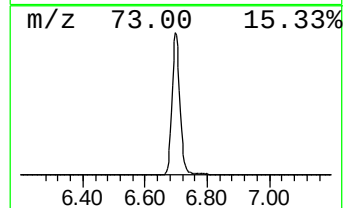
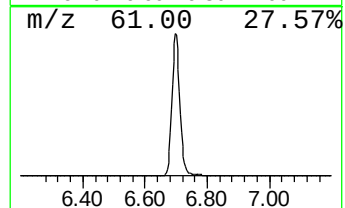
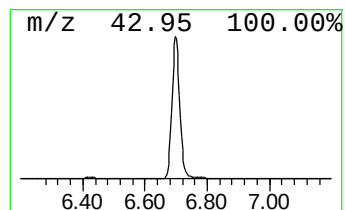
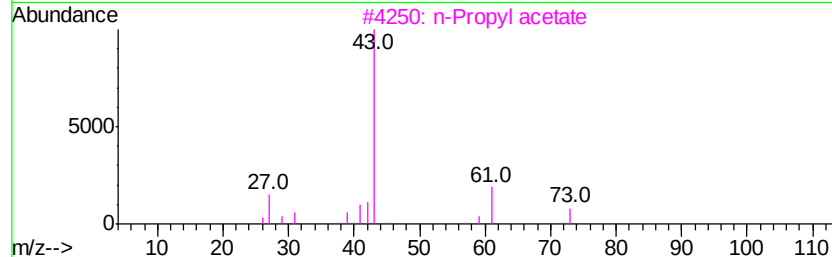
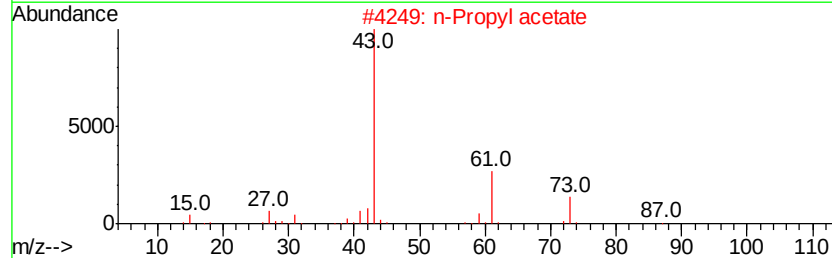
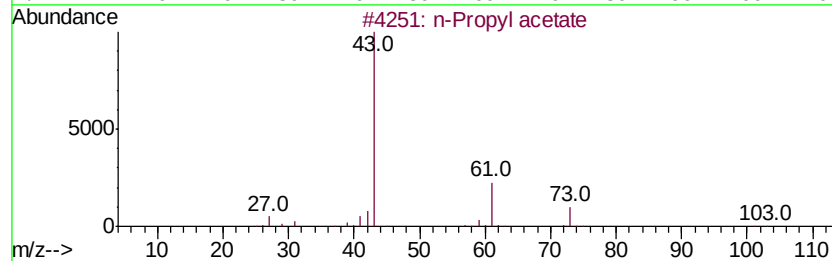
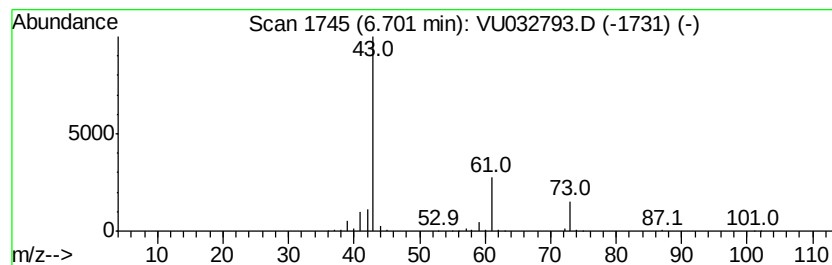
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	128.64 ug/L	1427050	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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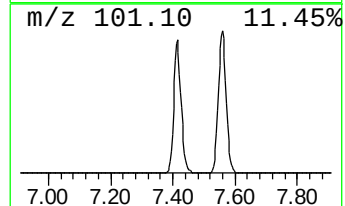
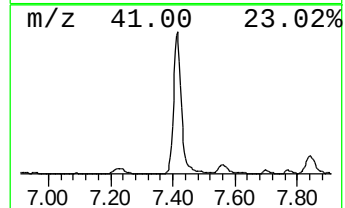
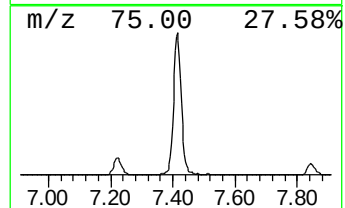
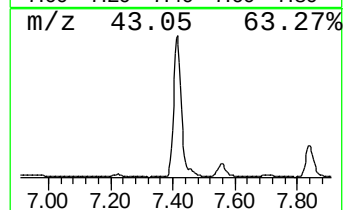
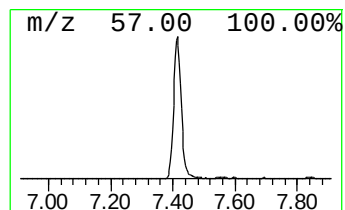
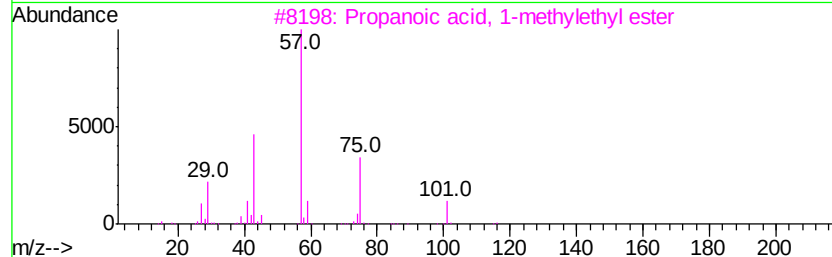
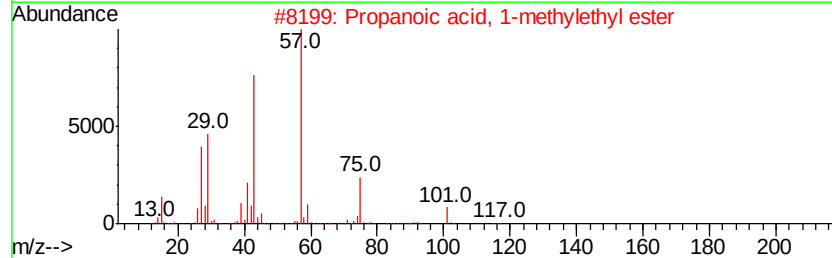
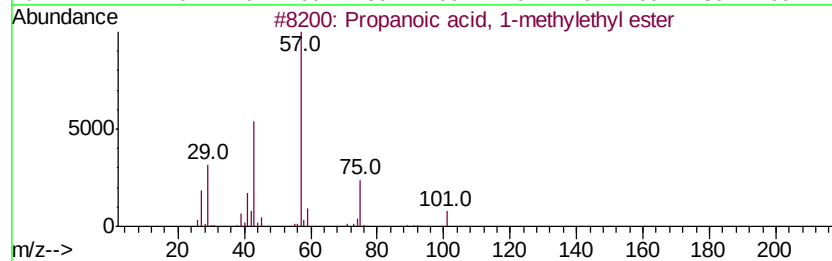
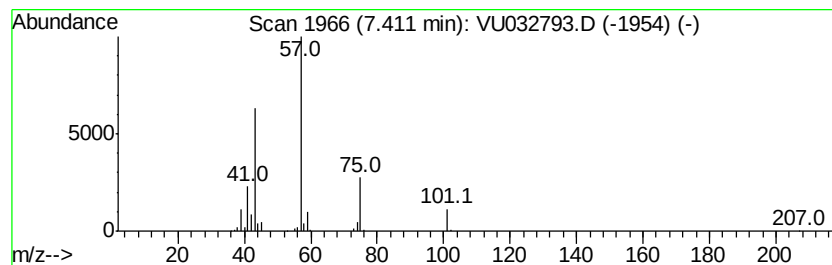
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	23.16 ug/L	256897	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	59
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40



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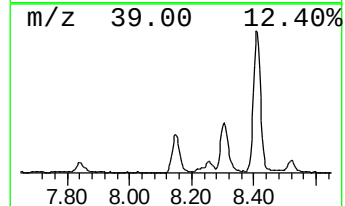
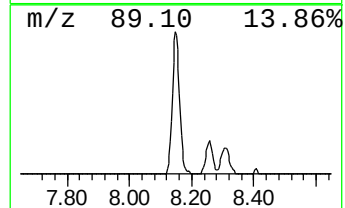
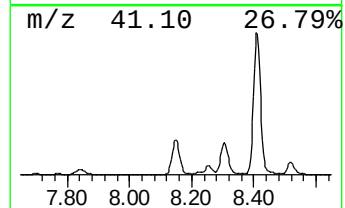
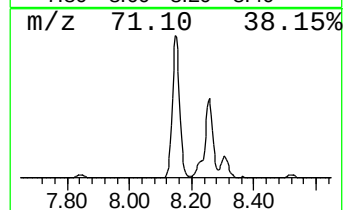
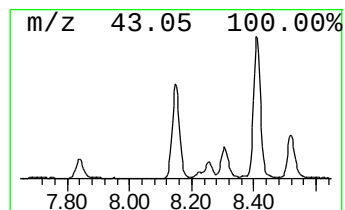
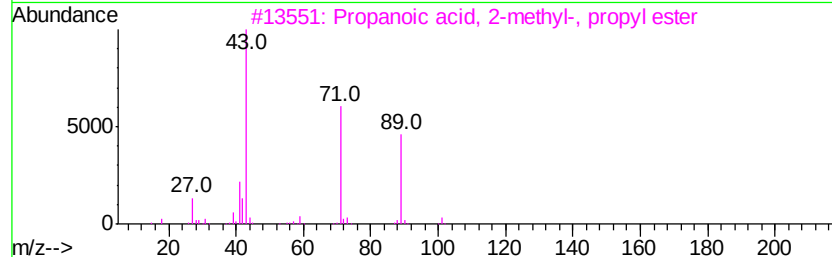
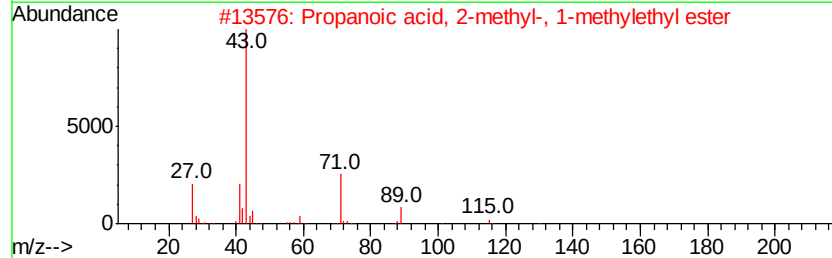
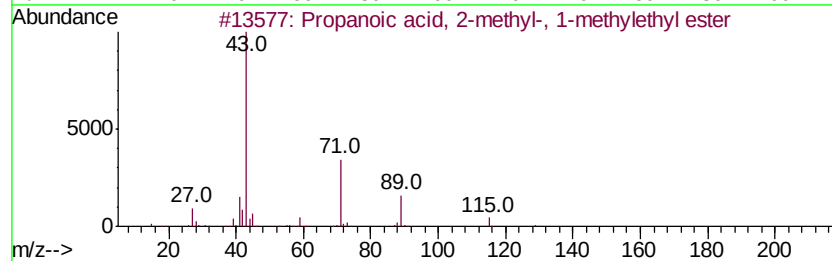
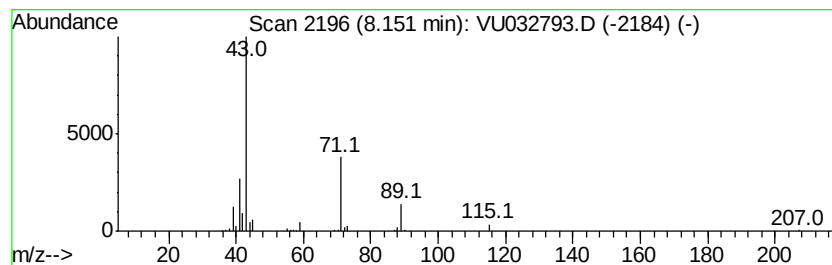
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Quant Title : VOC Analysis

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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	10.25 ug/L	144786	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-, propy...	130	C7H14O2	000644-49-5	78
4		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
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Acq On : 17 Jun 2019 19:21
Operator : JC/SP
Sample : K3324-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JR4

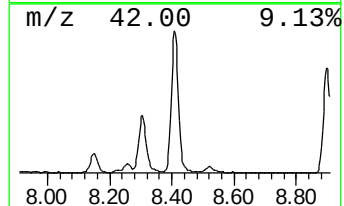
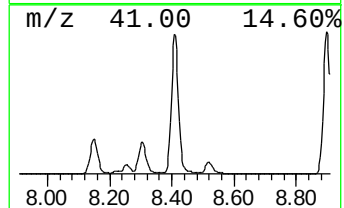
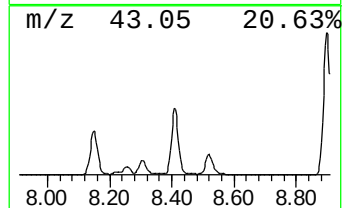
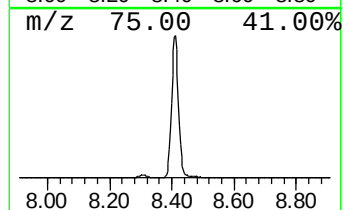
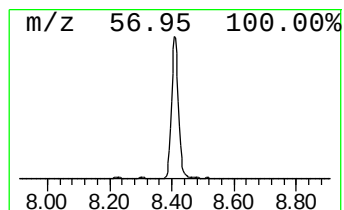
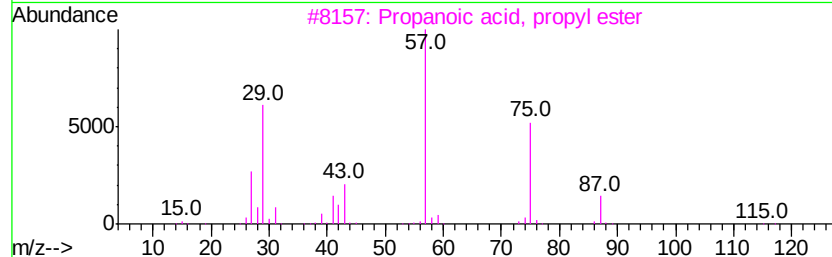
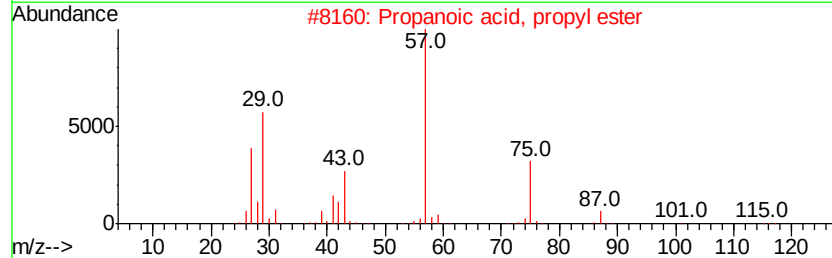
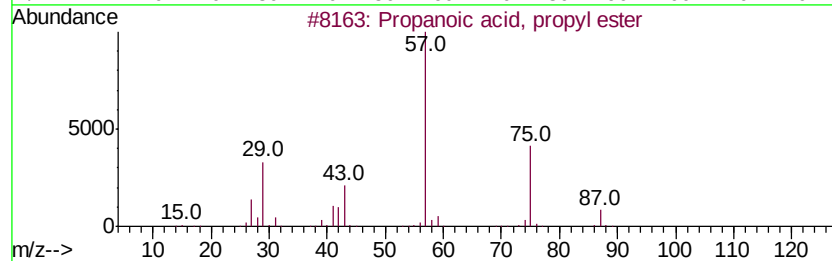
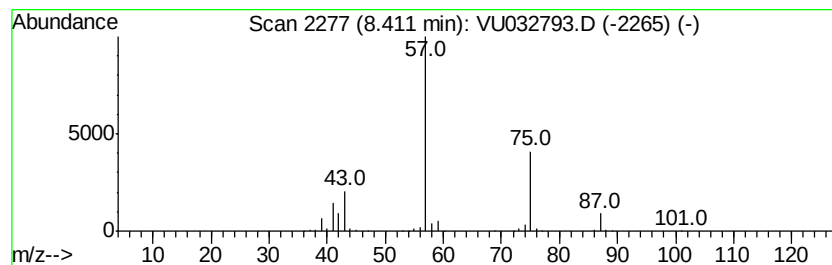
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Quant Title : VOC Analysis

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	67.41 ug/L	952530	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\VU061719\
Data File : VU032793.D
Acq On : 17 Jun 2019 19:21
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Sample : K3324-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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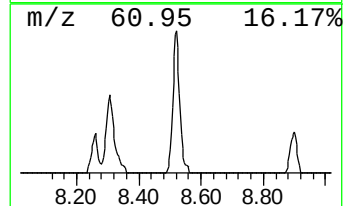
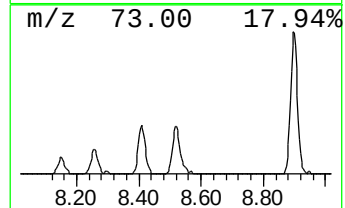
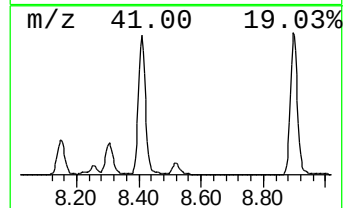
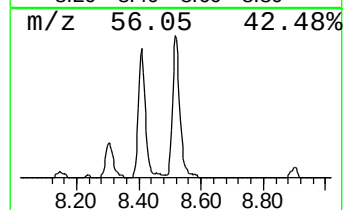
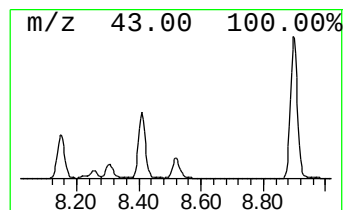
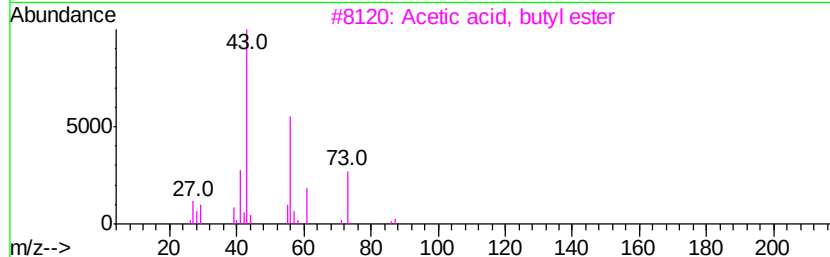
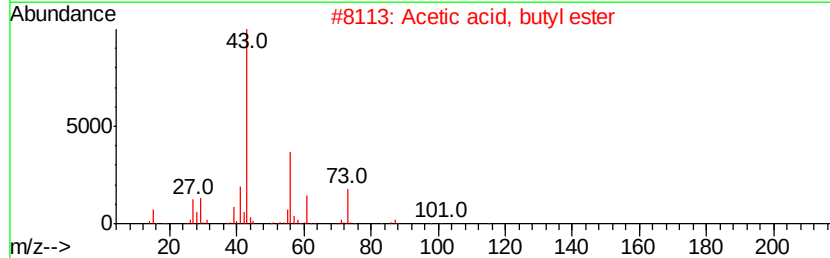
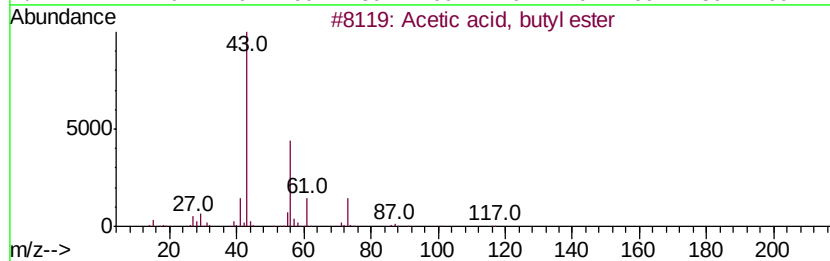
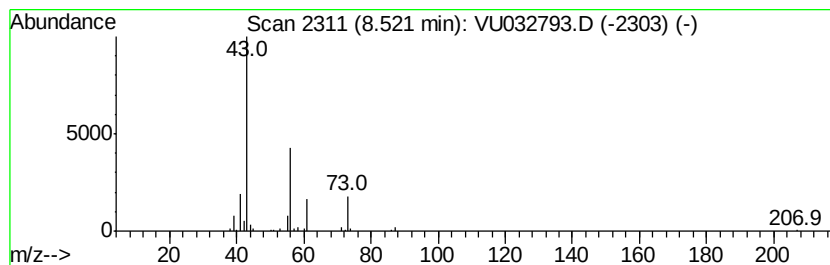
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	4.63 ug/L	65485	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	72
4		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
5		1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	17



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061719\
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Acq On : 17 Jun 2019 19:21
Operator : JC/SP
Sample : K3324-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 24 Sample Multiplier: 1

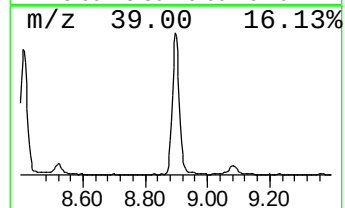
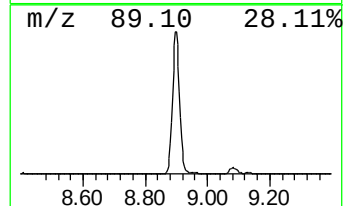
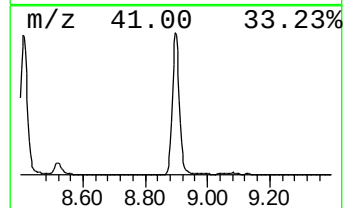
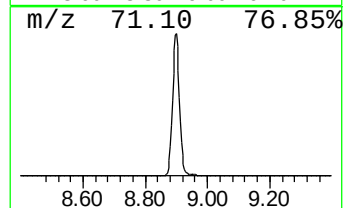
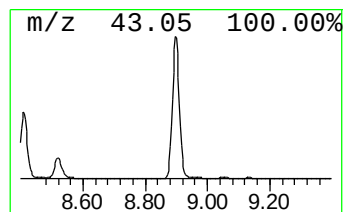
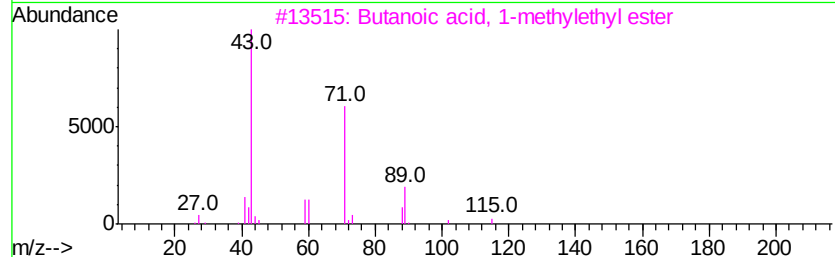
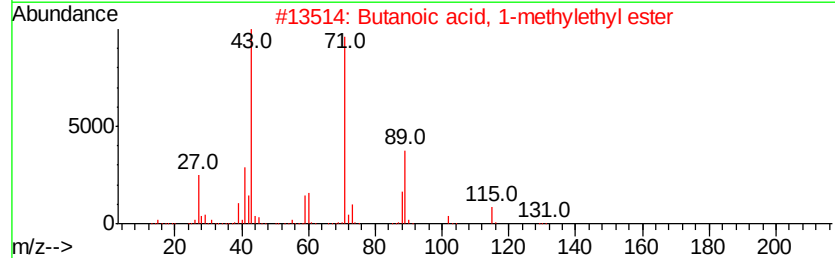
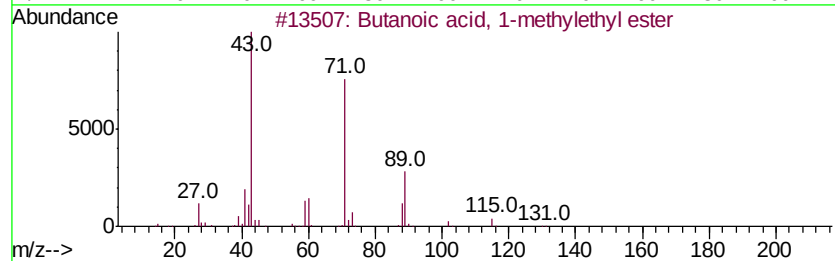
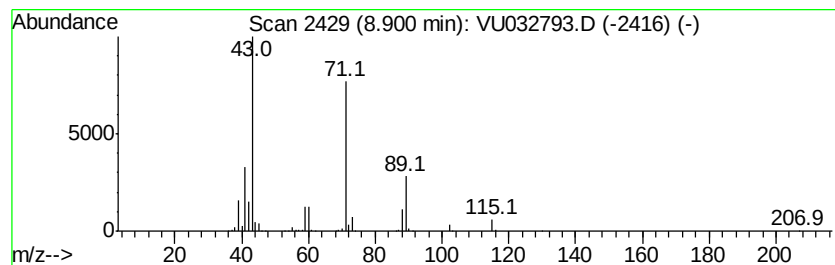
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.90	46.58 ug/L	658156	Chlorobenzene-d5	9.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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-, 1-met...	130	C7H14O2	000617-50-5	78	
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72	



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Operator : JC/SP
Sample : K3324-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR4

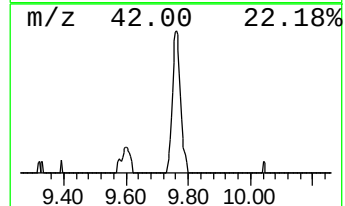
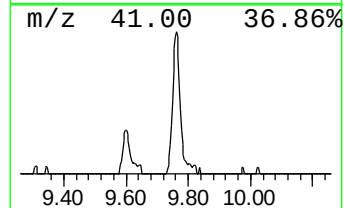
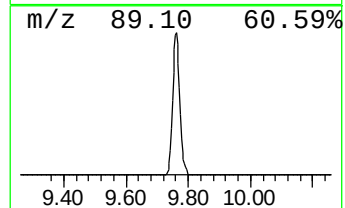
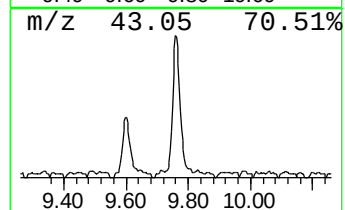
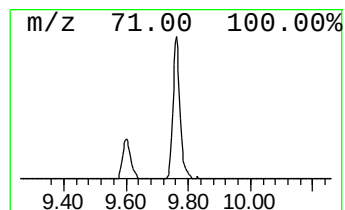
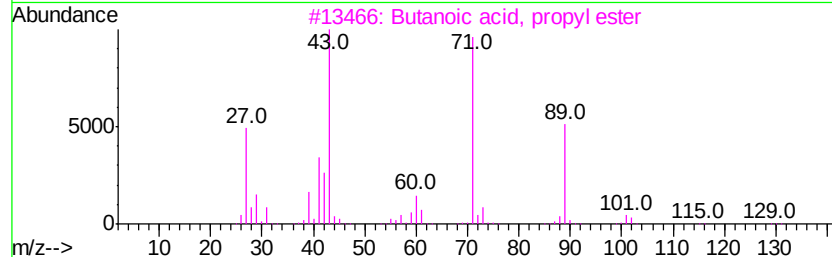
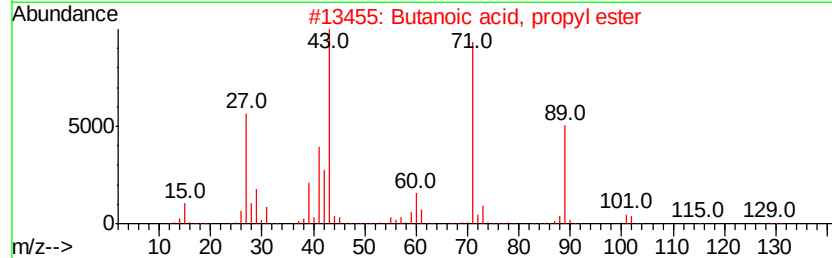
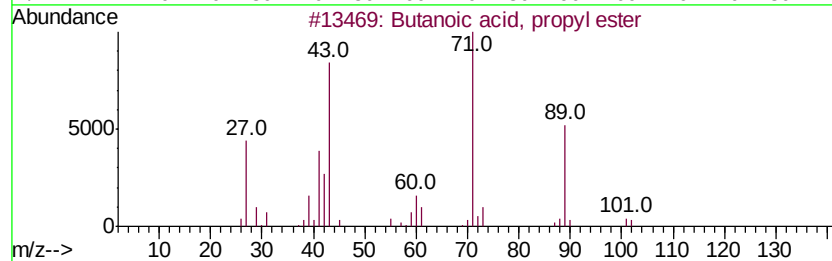
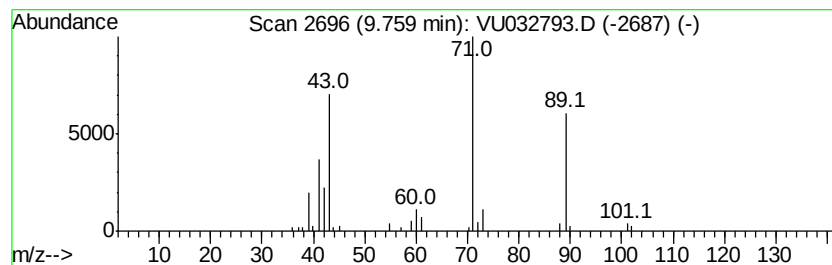
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	2.66 ug/L	37542	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
2		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	83
3		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	83
4		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
5		Malic Acid	134	C4H6O5	006915-15-7	72



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR4

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	128.6	ug/L	1427050	1	5.88	554659	50.0
Propanoic acid, 1...	7.41	23.2	ug/L	256897	1	5.88	554659	50.0
Propanoic acid, 2...	8.15	10.3	ug/L	144786	2	9.08	706519	50.0
Propanoic acid, p...	8.41	67.4	ug/L	952530	2	9.08	706519	50.0
Acetic acid, buty...	8.52	4.6	ug/L	65485	2	9.08	706519	50.0
Butanoic acid, 1-...	8.90	46.6	ug/L	658156	2	9.08	706519	50.0
Butanoic acid, pr...	9.76	2.7	ug/L	37542	2	9.08	706519	50.0