

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061319\
 Data File : VU032689.D
 Acq On : 13 Jun 2019 13:13
 Operator : JC/SP
 Sample : K3286-16
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JQ1

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	34	rBV2	4229	4451	0.43%	0.062%
2	1.396	88	95	108	rBV	71283	70754	6.84%	0.978%
3	1.675	175	182	195	rVB	58244	69841	6.75%	0.965%
4	2.267	357	366	376	rBV	116335	176087	17.02%	2.433%
5	2.318	377	382	395	rVB2	10082	15885	1.54%	0.219%
6	2.431	414	417	421	rBV3	358	349	0.03%	0.005%
7	2.627	467	478	481	rBV2	730	978	0.09%	0.014%
8	2.698	490	500	510	rVB	8176	13474	1.30%	0.186%
9	2.736	510	512	516	rBV2	252	182	0.02%	0.003%
10	2.830	533	541	544	rBV	334	503	0.05%	0.007%
11	2.875	551	555	559	rBV2	241	199	0.02%	0.003%
12	2.923	565	570	572	rBV2	267	245	0.02%	0.003%
13	2.968	580	584	587	rBV	296	255	0.02%	0.004%
14	3.064	610	614	619	rBV2	147	174	0.02%	0.002%
15	3.254	669	673	675	rBV	228	168	0.02%	0.002%
16	3.273	676	679	685	rVB2	219	183	0.02%	0.003%
17	3.315	690	692	697	rBV2	224	201	0.02%	0.003%
18	3.418	717	724	727	rBV3	982	1200	0.12%	0.017%
19	3.466	736	739	744	rVB3	210	176	0.02%	0.002%
20	3.579	771	774	780	rVB2	256	259	0.03%	0.004%
21	3.752	822	828	829	rBV2	244	176	0.02%	0.002%
22	4.010	902	908	910	rBV2	152	172	0.02%	0.002%
23	4.051	917	921	924	rBV2	201	188	0.02%	0.003%
24	4.116	934	941	945	rBV2	157	196	0.02%	0.003%
25	4.170	945	958	998	rBV	61925	164750	15.92%	2.276%
26	4.566	1077	1081	1083	rBV2	268	171	0.02%	0.002%
27	4.643	1089	1105	1126	rBV	98158	229332	22.16%	3.169%
28	4.794	1150	1152	1156	rVB3	301	177	0.02%	0.002%
29	4.948	1197	1200	1203	rBV2	217	175	0.02%	0.002%
30	5.254	1290	1295	1298	rBV	195	173	0.02%	0.002%
31	5.334	1298	1320	1345	rBV2	185815	559195	54.04%	7.727%
32	5.489	1366	1368	1371	rVB3	333	159	0.02%	0.002%
33	5.553	1379	1388	1406	rBV3	3301	7926	0.77%	0.110%
34	5.704	1431	1435	1439	rBV2	342	311	0.03%	0.004%

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 Title : VOC Analysis

35	5.800	1461	1465	1467	rBV2	314	205	0.02%	0.003%
36	5.881	1468	1490	1516	rBV	215248	452254	43.70%	6.249%
37	6.183	1574	1584	1599	rVB6	10619	22089	2.13%	0.305%
38	6.325	1615	1628	1648	rBV2	130353	260428	25.17%	3.598%
39	6.424	1653	1659	1672	rVB2	4588	8789	0.85%	0.121%
40	6.530	1687	1692	1699	rBV3	1614	2762	0.27%	0.038%
41	6.575	1702	1706	1715	rVV	3062	4872	0.47%	0.067%
42	6.698	1732	1744	1779	rBV	572042	1034847	100.00%	14.299%
43	7.080	1861	1863	1867	rBV3	349	223	0.02%	0.003%
44	7.225	1896	1908	1930	rVV	73044	132972	12.85%	1.837%
45	7.415	1956	1967	1994	rBV	101168	179787	17.37%	2.484%
46	7.559	2000	2012	2032	rBV	248825	439154	42.44%	6.068%
47	7.701	2053	2056	2059	rBV3	765	655	0.06%	0.009%
48	7.845	2091	2101	2116	rBV2	57840	99934	9.66%	1.381%
49	8.151	2184	2196	2211	rBV	53082	89139	8.61%	1.232%
50	8.228	2211	2220	2223	rBV3	13560	19747	1.91%	0.273%
51	8.305	2235	2244	2266	rVV	208827	349806	33.80%	4.833%
52	8.411	2267	2277	2302	rVV	371509	591975	57.20%	8.179%
53	8.524	2304	2312	2333	rVB	21087	39624	3.83%	0.547%
54	8.633	2343	2346	2357	rVB4	604	706	0.07%	0.010%
55	8.900	2418	2429	2457	rBV	240403	386326	37.33%	5.338%
56	9.083	2474	2486	2518	rBV	308050	514572	49.72%	7.110%
57	9.296	2550	2552	2555	rBV3	219	168	0.02%	0.002%
58	9.347	2564	2568	2571	rBV2	306	330	0.03%	0.005%
59	9.389	2577	2581	2583	rBV3	210	192	0.02%	0.003%
60	9.443	2594	2598	2602	rBV2	350	276	0.03%	0.004%
61	9.521	2616	2622	2624	rBV2	313	291	0.03%	0.004%
62	9.611	2643	2650	2668	rVV3	2122	3922	0.38%	0.054%
63	9.768	2690	2699	2713	rBV	8473	14904	1.44%	0.206%
64	9.919	2743	2746	2749	rVB2	241	182	0.02%	0.003%
65	9.961	2752	2759	2762	rBV2	338	344	0.03%	0.005%
66	10.003	2770	2772	2777	rVB	469	297	0.03%	0.004%
67	10.048	2783	2786	2792	rVB2	306	327	0.03%	0.005%
68	10.080	2792	2796	2800	rBV3	233	199	0.02%	0.003%
69	10.154	2815	2819	2823	rBV2	284	260	0.03%	0.004%
70	10.324	2869	2872	2875	rVV2	242	162	0.02%	0.002%
71	10.357	2878	2882	2885	rVV2	277	229	0.02%	0.003%

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72	10.427	2891	2904	2929	rVV	203256	326751	31.57%	4.515%
73	10.514	2929	2931	2934	rVB	364	233	0.02%	0.003%
74	10.672	2975	2980	2982	rBV	194	187	0.02%	0.003%
75	11.334	3182	3186	3192	rBV2	234	289	0.03%	0.004%
76	11.392	3199	3204	3207	rBV	235	238	0.02%	0.003%
77	11.479	3219	3231	3252	rBV	305372	491692	47.51%	6.794%
78	11.800	3327	3331	3334	rBV2	214	182	0.02%	0.003%
79	11.855	3334	3348	3371	rBV	263399	440185	42.54%	6.082%
80	12.260	3471	3474	3478	rVB2	197	160	0.02%	0.002%
81	12.302	3483	3487	3491	rBV	231	191	0.02%	0.003%
82	12.340	3497	3499	3503	rVB	238	160	0.02%	0.002%
83	12.466	3534	3538	3542	rBV2	220	187	0.02%	0.003%
84	12.819	3644	3648	3652	rBV	234	236	0.02%	0.003%
85	12.926	3677	3681	3683	rBV2	245	206	0.02%	0.003%
86	13.000	3699	3704	3708	rBV	252	290	0.03%	0.004%
87	13.077	3724	3728	3732	rBV2	311	253	0.02%	0.003%
88	13.498	3854	3859	3864	rBV2	196	269	0.03%	0.004%
89	13.578	3881	3884	3887	rVB2	263	182	0.02%	0.003%
90	13.720	3919	3928	3930	rBV2	313	383	0.04%	0.005%
91	14.028	4021	4024	4027	rVV2	289	181	0.02%	0.003%
92	14.125	4050	4054	4059	rVB2	276	247	0.02%	0.003%
93	14.356	4121	4126	4131	rBV2	307	463	0.04%	0.006%
94	14.543	4180	4184	4189	rBV3	407	513	0.05%	0.007%
95	14.588	4195	4198	4202	rBV3	318	219	0.02%	0.003%
96	15.437	4459	4462	4466	rBV2	392	226	0.02%	0.003%
97	16.141	4678	4681	4686	rBV	512	478	0.05%	0.007%
98	16.302	4728	4731	4736	rBV4	433	441	0.04%	0.006%
99	16.324	4736	4738	4740	rBV2	415	202	0.02%	0.003%
100	16.575	4814	4816	4819	rBV3	578	443	0.04%	0.006%

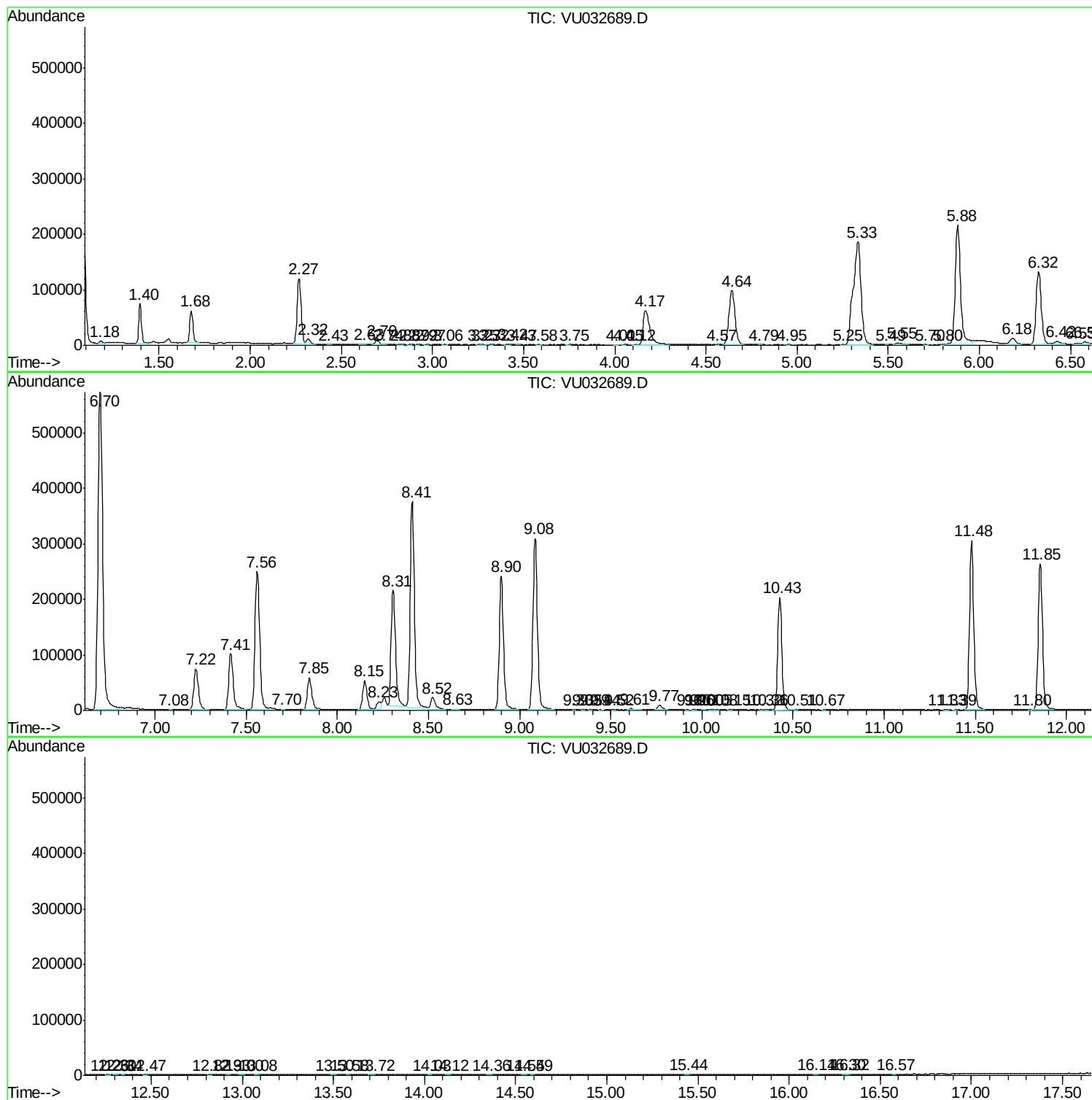
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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



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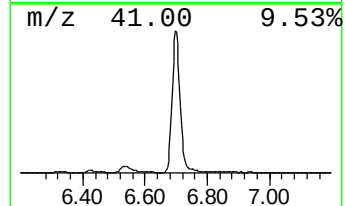
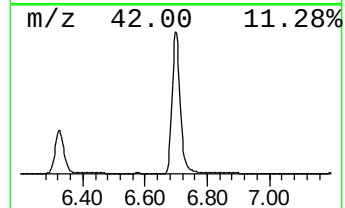
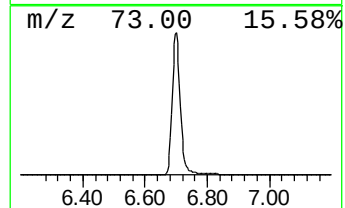
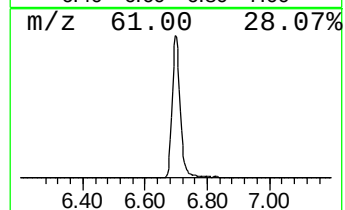
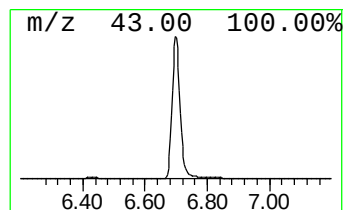
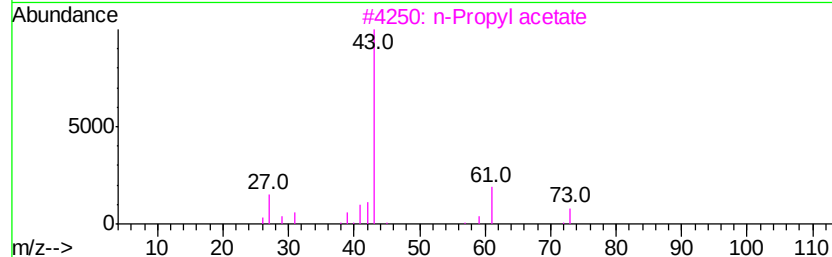
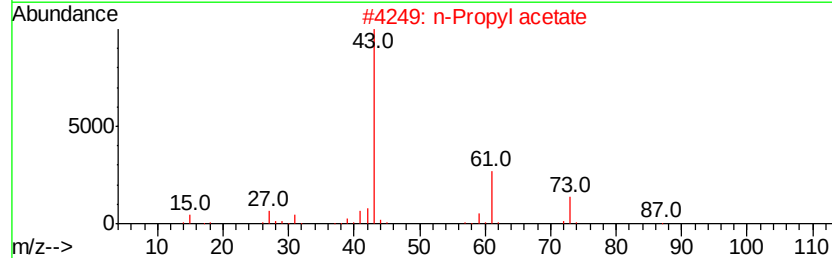
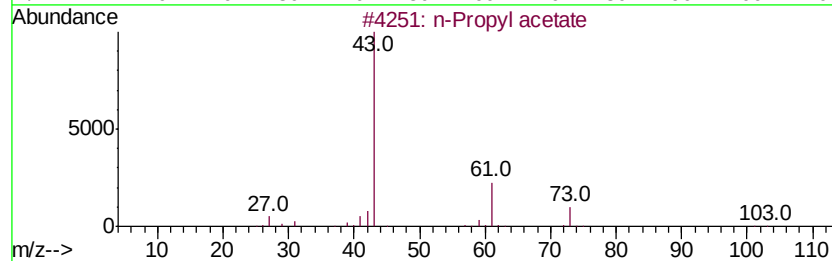
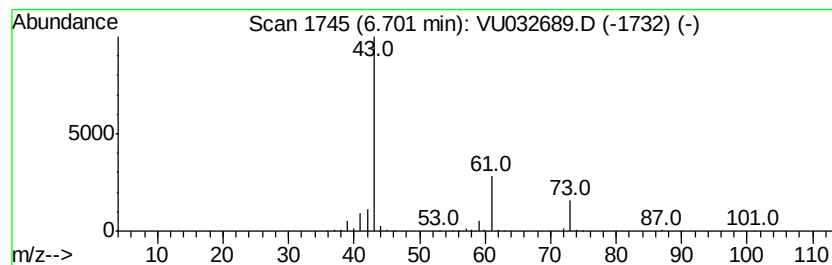
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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	114.41 ug/L	1034850	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	33



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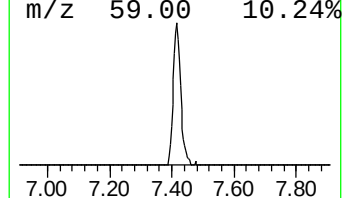
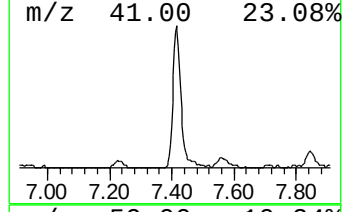
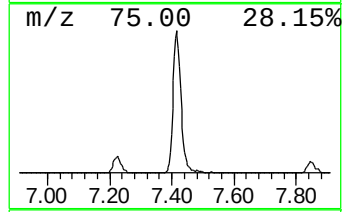
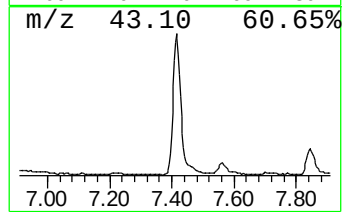
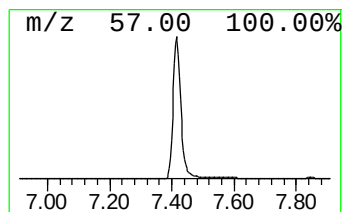
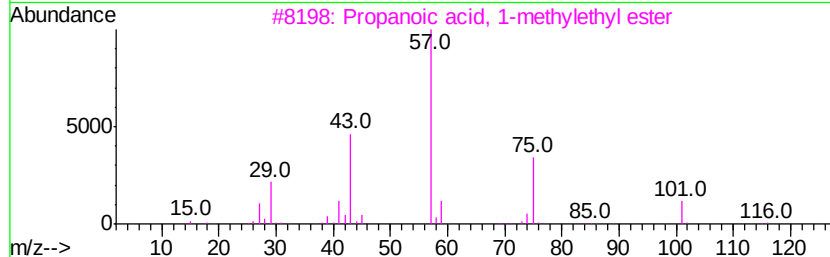
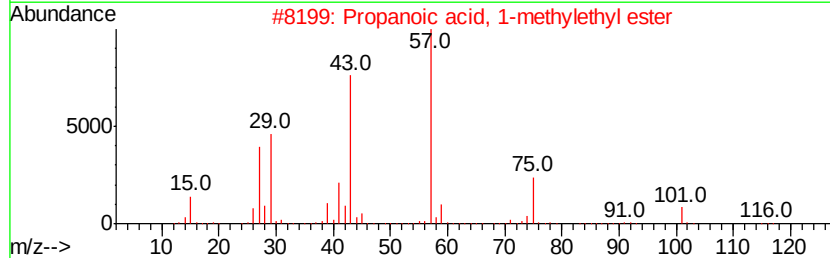
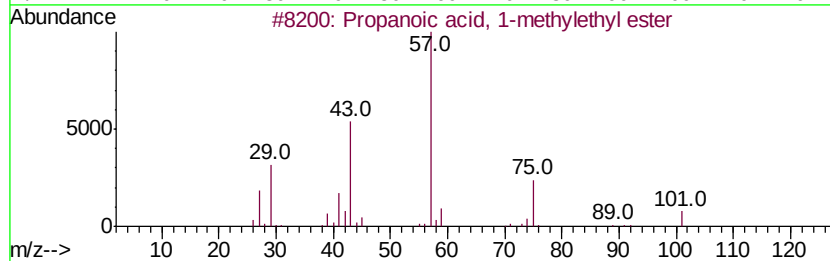
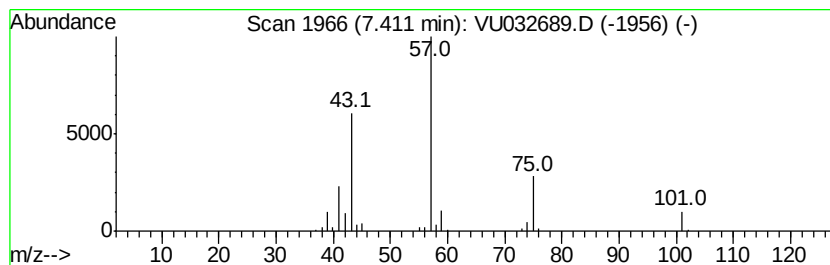
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
7.41	19.88 ug/L	179787	1,4-Difluorobenzene	5.88		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	64	
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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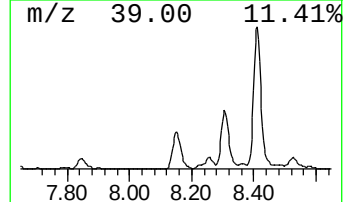
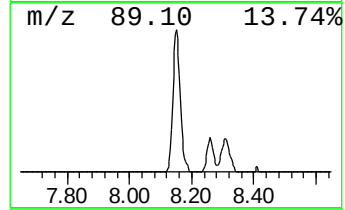
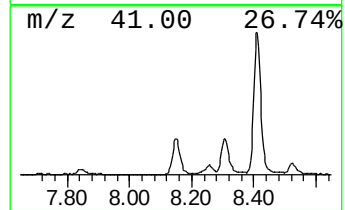
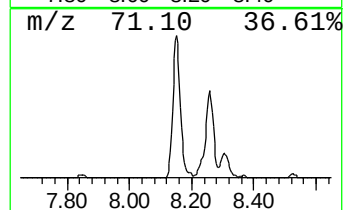
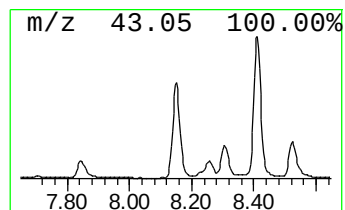
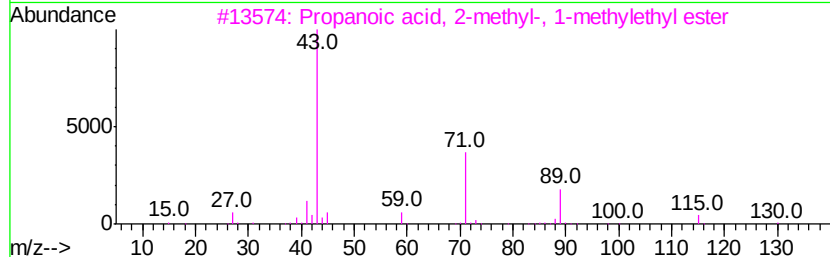
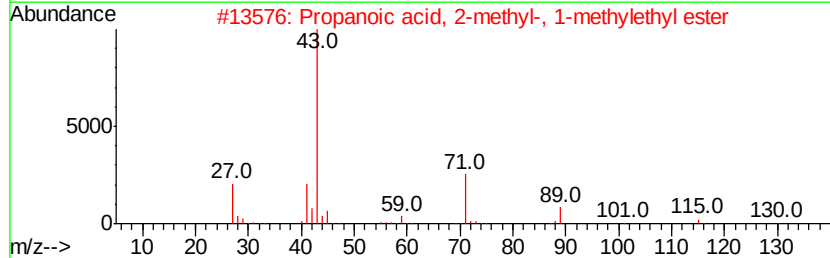
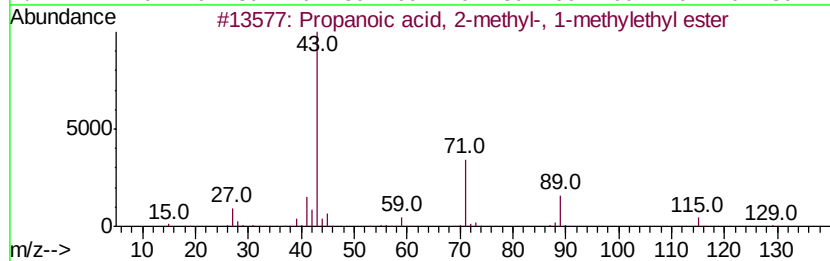
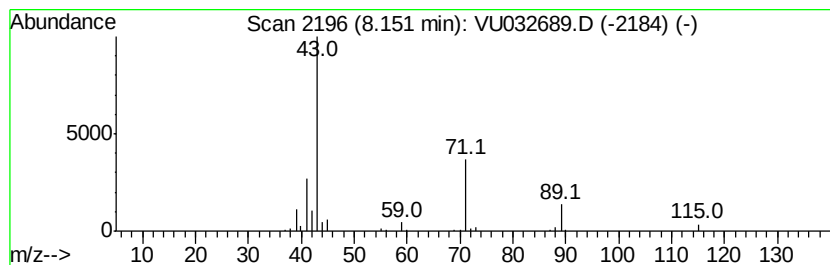
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Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.15	8.66 ug/L	89139	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	78	
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78	
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72	
4	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72	
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061319\
Data File : VU032689.D
Acq On : 13 Jun 2019 13:13
Operator : JC/SP
Sample : K3286-16
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JQ1

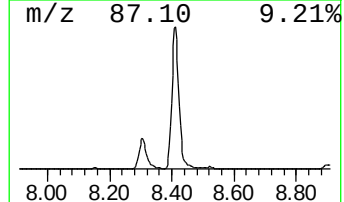
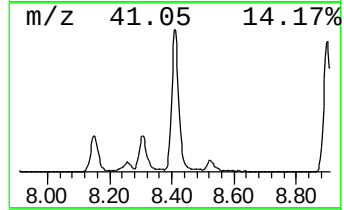
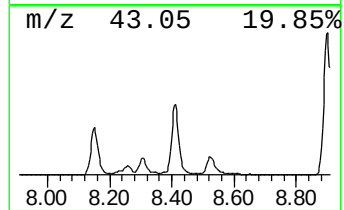
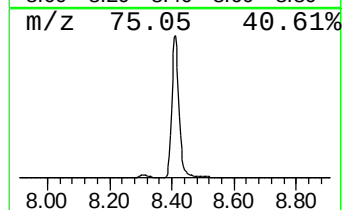
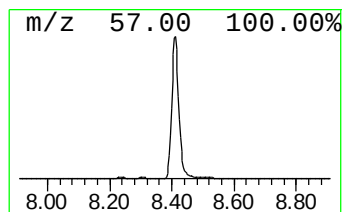
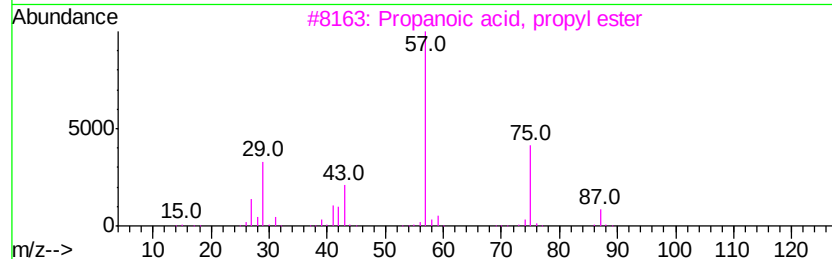
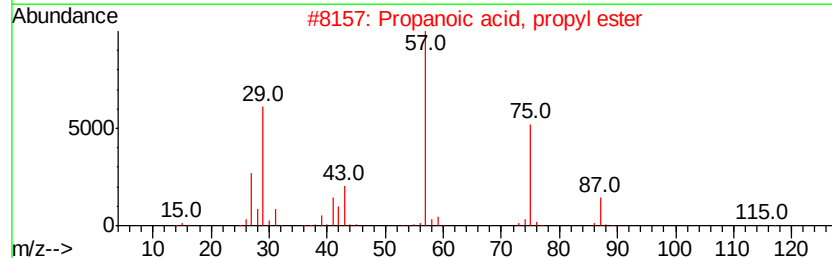
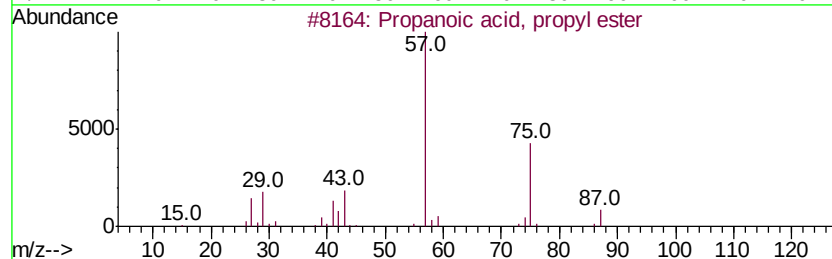
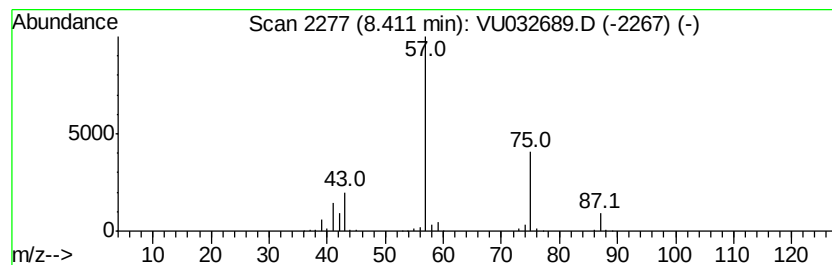
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Quant Title : VOC Analysis

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	57.52 ug/L	591975	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	83
5		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061319\
Data File : VU032689.D
Acq On : 13 Jun 2019 13:13
Operator : JC/SP
Sample : K3286-16
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JQ1

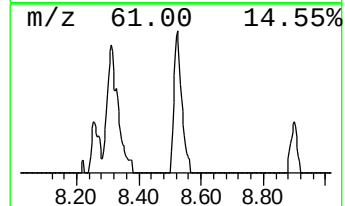
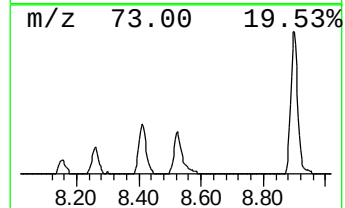
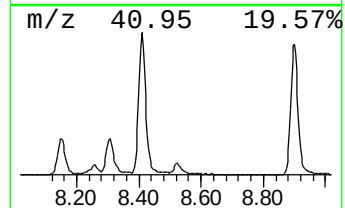
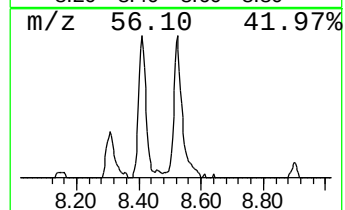
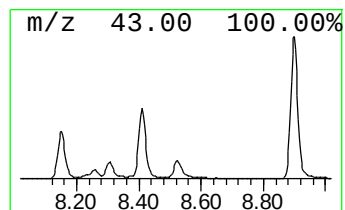
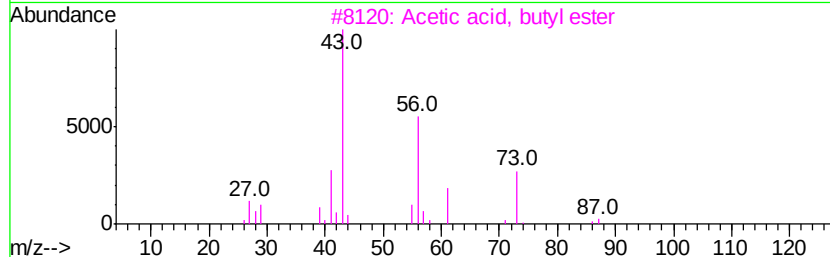
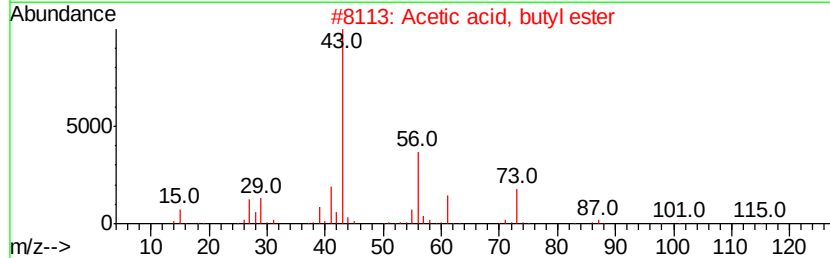
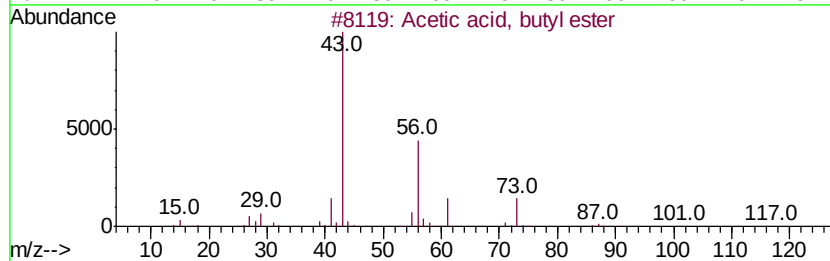
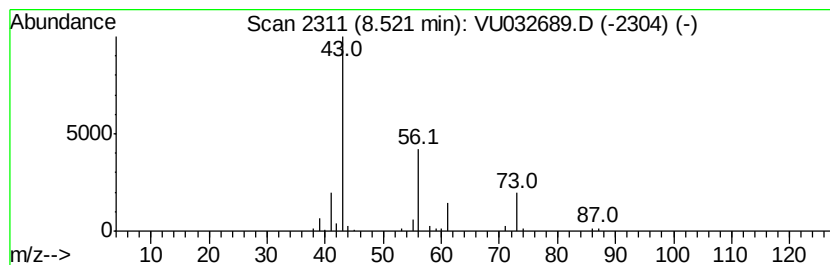
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	3.85 ug/L	39624	Chlorobenzene-d5	9.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	40
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	39
5			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061319\
Data File : VU032689.D
Acq On : 13 Jun 2019 13:13
Operator : JC/SP
Sample : K3286-16
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JQ1

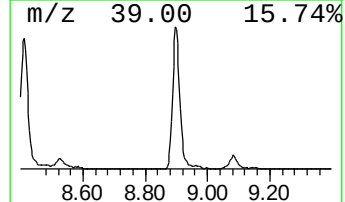
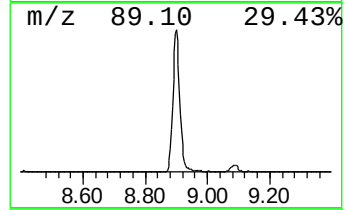
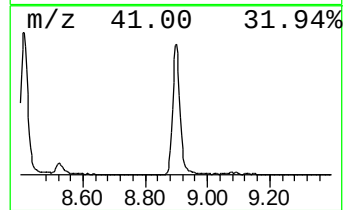
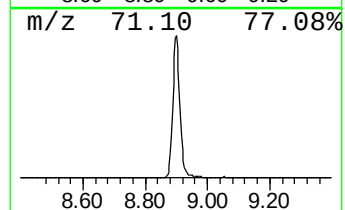
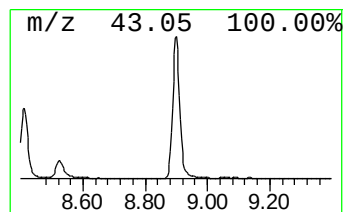
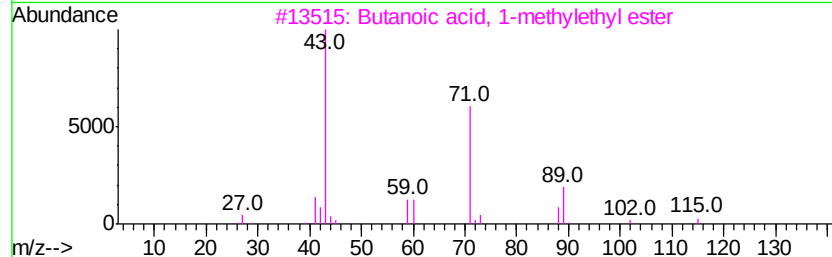
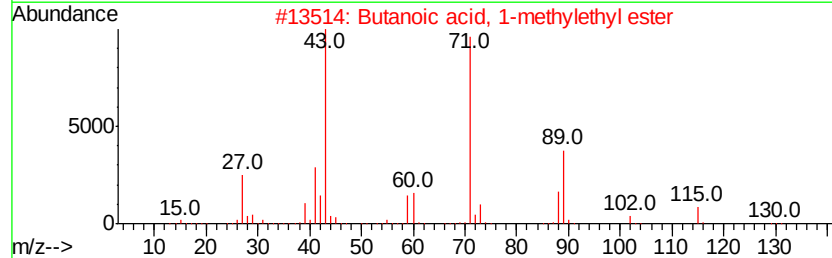
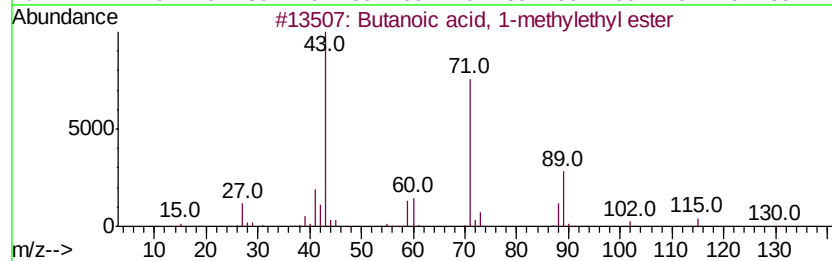
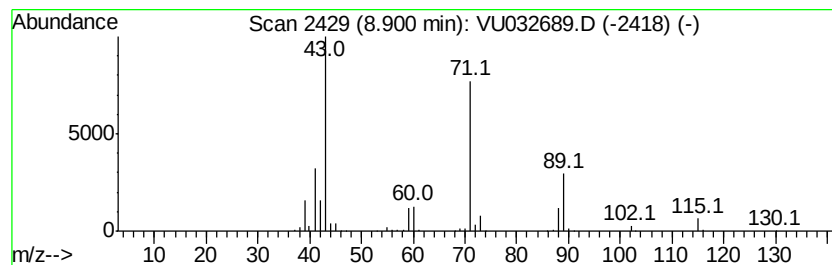
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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	37.54 ug/L	386326	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	91
3		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83
4		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



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Data File : VU032689.D
Acq On : 13 Jun 2019 13:13
Operator : JC/SP
Sample : K3286-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JQ1

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	114.4	ug/L	1034850	1	5.88	452254	50.0
Propanoic acid, 1...	7.41	19.9	ug/L	179787	1	5.88	452254	50.0
Propanoic acid, 2...	8.15	8.7	ug/L	89139	2	9.08	514572	50.0
Propanoic acid, p...	8.41	57.5	ug/L	591975	2	9.08	514572	50.0
Acetic acid, buty...	8.52	3.9	ug/L	39624	2	9.08	514572	50.0
Butanoic acid, 1-...	8.90	37.5	ug/L	386326	2	9.08	514572	50.0