

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061219\
 Data File : VU032649.D
 Acq On : 12 Jun 2019 14:10
 Operator : JC/SP
 Sample : K3286-08
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JW8

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	1.396	89	95	108	rVB	91998	95547	9.32%	1.295%
2	1.675	176	182	196	rVB	70592	85604	8.35%	1.160%
3	2.267	357	366	376	rBV	148702	222154	21.66%	3.010%
4	2.563	455	458	461	rBV2	415	328	0.03%	0.004%
5	2.698	490	500	511	rVB3	6833	11851	1.16%	0.161%
6	2.833	538	542	547	rBV3	467	464	0.05%	0.006%
7	2.888	557	559	564	rBV3	245	177	0.02%	0.002%
8	2.929	569	572	575	rBV3	196	94	0.01%	0.001%
9	3.080	616	619	623	rBV	220	198	0.02%	0.003%
10	3.174	643	648	650	rBV2	616	565	0.06%	0.008%
11	3.412	709	722	737	rBV6	4160	9872	0.96%	0.134%
12	3.511	751	753	756	rVB2	307	162	0.02%	0.002%
13	3.543	756	763	767	rBV2	307	323	0.03%	0.004%
14	3.624	784	788	790	rBV2	213	154	0.02%	0.002%
15	3.759	827	830	833	rBV2	109	75	0.01%	0.001%
16	3.810	844	846	850	rVB	238	142	0.01%	0.002%
17	3.839	851	855	857	rBV	184	122	0.01%	0.002%
18	3.913	875	878	881	rVB	173	95	0.01%	0.001%
19	3.965	888	894	896	rBV2	193	188	0.02%	0.003%
20	4.042	916	918	921	rBV	187	128	0.01%	0.002%
21	4.064	923	925	933	rVB	358	286	0.03%	0.004%
22	4.167	946	957	982	rBV2	58508	150579	14.68%	2.040%
23	4.576	1077	1084	1086	rBV2	280	365	0.04%	0.005%
24	4.640	1089	1104	1127	rVV	105508	250155	24.39%	3.389%
25	4.810	1155	1157	1160	rBV4	338	169	0.02%	0.002%
26	4.826	1160	1162	1166	rVB	136	82	0.01%	0.001%
27	4.884	1177	1180	1188	rVB3	357	457	0.04%	0.006%
28	4.942	1193	1198	1203	rBV	265	262	0.03%	0.004%
29	4.965	1203	1205	1208	rVB	169	91	0.01%	0.001%
30	4.984	1208	1211	1217	rVB2	372	246	0.02%	0.003%
31	5.010	1217	1219	1221	rBV	141	76	0.01%	0.001%
32	5.048	1228	1231	1232	rBV	138	84	0.01%	0.001%
33	5.061	1232	1235	1238	rVB2	178	112	0.01%	0.002%
34	5.084	1238	1242	1243	rBV2	178	116	0.01%	0.002%

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 Title : VOC Analysis

35	5.113	1249	1251	1254	rBV	123	74	0.01%	0.001%
36	5.151	1254	1263	1267	rBV2	309	403	0.04%	0.005%
37	5.232	1285	1288	1291	rBV	143	89	0.01%	0.001%
38	5.334	1298	1320	1342	rBV2	215558	629467	61.37%	8.529%
39	5.707	1433	1436	1438	rBV2	243	194	0.02%	0.003%
40	5.823	1449	1472	1473	rBV3	9139	25009	2.44%	0.339%
41	5.881	1481	1490	1514	rVB	194239	377916	36.85%	5.121%
42	6.325	1616	1628	1647	rVB	142128	281419	27.44%	3.813%
43	6.698	1733	1744	1781	rBV	570637	1025613	100.00%	13.897%
44	7.222	1897	1907	1932	rBV	82725	148518	14.48%	2.012%
45	7.415	1957	1967	1991	rBV	106552	184182	17.96%	2.496%
46	7.559	2000	2012	2031	rBV	293996	520802	50.78%	7.057%
47	7.846	2092	2101	2123	rBV2	65166	113723	11.09%	1.541%
48	8.151	2184	2196	2212	rBV	58150	98352	9.59%	1.333%
49	8.305	2235	2244	2266	rVV	199759	337336	32.89%	4.571%
50	8.411	2267	2277	2302	rVB	364255	579816	56.53%	7.856%
51	8.855	2412	2415	2416	rBV	369	196	0.02%	0.003%
52	8.900	2418	2429	2464	rVV	268241	429953	41.92%	5.826%
53	9.083	2475	2486	2516	rBV	285415	478310	46.64%	6.481%
54	9.350	2567	2569	2572	rBV2	183	91	0.01%	0.001%
55	9.399	2580	2584	2587	rBV	281	250	0.02%	0.003%
56	9.415	2587	2589	2591	rVB2	278	80	0.01%	0.001%
57	9.611	2637	2650	2661	rBV5	2497	5135	0.50%	0.070%
58	9.694	2674	2676	2682	rVB2	271	147	0.01%	0.002%
59	9.765	2686	2698	2714	rBV3	9147	16742	1.63%	0.227%
60	9.855	2724	2726	2729	rVB	305	151	0.01%	0.002%
61	9.881	2729	2734	2739	rBV2	327	437	0.04%	0.006%
62	9.932	2747	2750	2753	rBV2	257	191	0.02%	0.003%
63	10.128	2809	2811	2814	rBV2	148	111	0.01%	0.002%
64	10.273	2854	2856	2862	rVB2	318	190	0.02%	0.003%
65	10.302	2862	2865	2867	rBV	210	149	0.01%	0.002%
66	10.315	2867	2869	2871	rBV2	143	84	0.01%	0.001%
67	10.386	2889	2891	2892	rBV	151	73	0.01%	0.001%
68	10.427	2892	2904	2921	rVV	205954	331232	32.30%	4.488%
69	10.546	2937	2941	2944	rVB	195	132	0.01%	0.002%
70	10.572	2945	2949	2952	rVB2	263	231	0.02%	0.003%
71	10.601	2952	2958	2966	rBV3	1019	1885	0.18%	0.026%

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72	10.646	2969	2972	2977	rVB2	356	298	0.03%	0.004%
73	10.672	2977	2980	2984	rBV	310	238	0.02%	0.003%
74	10.694	2984	2987	2989	rBV2	210	153	0.01%	0.002%
75	10.771	3002	3011	3016	rBV3	557	689	0.07%	0.009%
76	10.794	3016	3018	3024	rBV2	294	238	0.02%	0.003%
77	10.935	3058	3062	3069	rVB3	345	416	0.04%	0.006%
78	10.980	3073	3076	3079	rVB2	295	183	0.02%	0.002%
79	11.025	3086	3090	3092	rBV2	225	184	0.02%	0.002%
80	11.144	3125	3127	3130	rBV2	168	109	0.01%	0.001%
81	11.186	3138	3140	3143	rBV	140	115	0.01%	0.002%
82	11.366	3193	3196	3199	rBV	246	174	0.02%	0.002%
83	11.440	3214	3219	3220	rBV	266	243	0.02%	0.003%
84	11.479	3220	3231	3251	rBV	294280	473405	46.16%	6.414%
85	11.759	3316	3318	3319	rBV	344	150	0.01%	0.002%
86	11.778	3322	3324	3329	rVV3	439	382	0.04%	0.005%
87	11.810	3332	3334	3336	rBV	258	111	0.01%	0.002%
88	11.855	3336	3348	3373	rBV	290196	480721	46.87%	6.514%
89	12.132	3431	3434	3439	rVB3	331	274	0.03%	0.004%
90	12.196	3452	3454	3456	rBV	237	100	0.01%	0.001%
91	12.688	3604	3607	3609	rBV	250	190	0.02%	0.003%
92	13.025	3710	3712	3715	rVB	279	150	0.01%	0.002%
93	13.328	3804	3806	3809	rBV	357	162	0.02%	0.002%
94	13.582	3883	3885	3889	rVB2	353	236	0.02%	0.003%
95	13.604	3890	3892	3894	rBV	316	152	0.01%	0.002%
96	13.691	3917	3919	3925	rVB2	511	457	0.04%	0.006%
97	13.717	3925	3927	3929	rBV	280	124	0.01%	0.002%
98	13.877	3972	3977	3979	rBV	312	246	0.02%	0.003%
99	14.173	4066	4069	4071	rBV2	356	211	0.02%	0.003%
100	14.360	4124	4127	4129	rBV	341	238	0.02%	0.003%

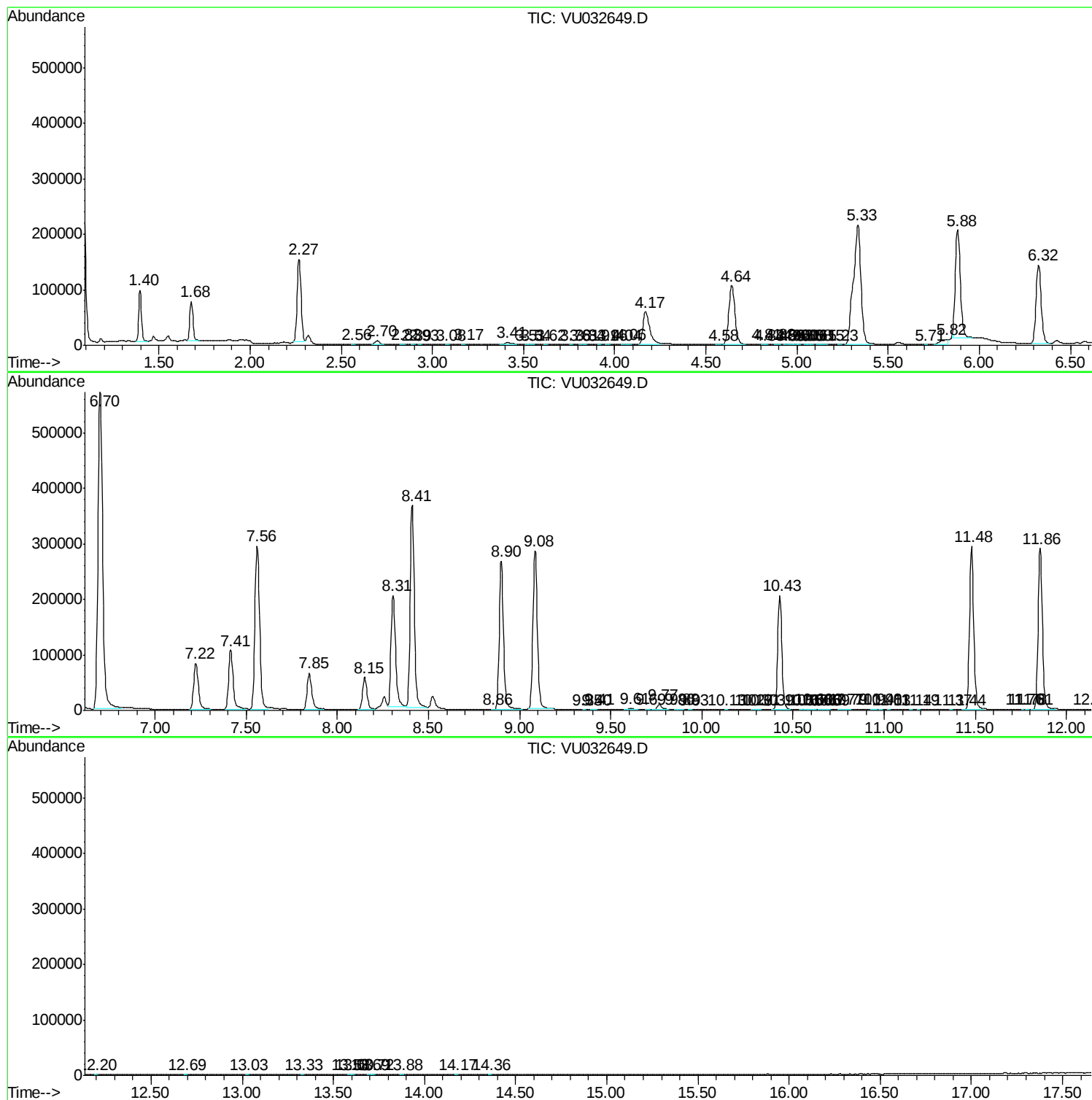
Sum of corrected areas: 7380355

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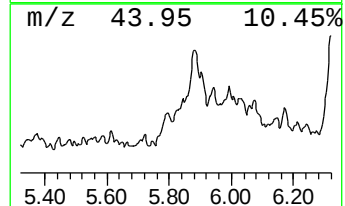
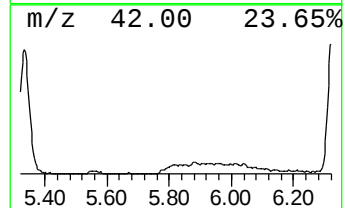
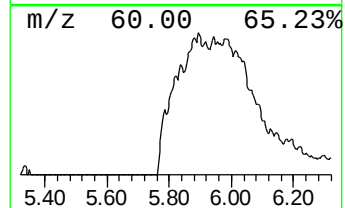
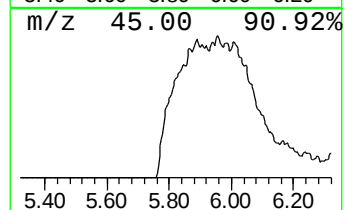
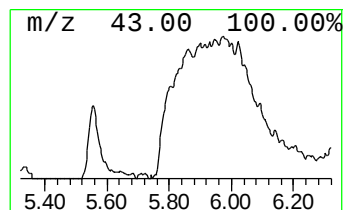
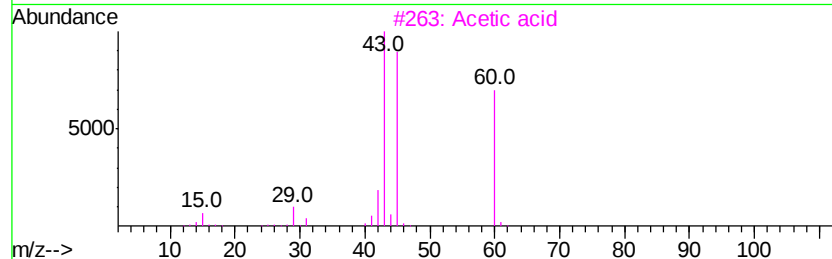
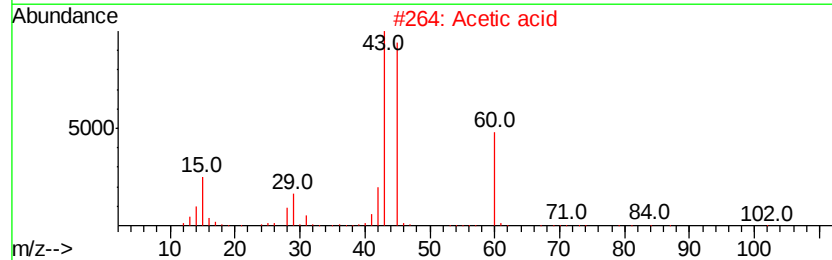
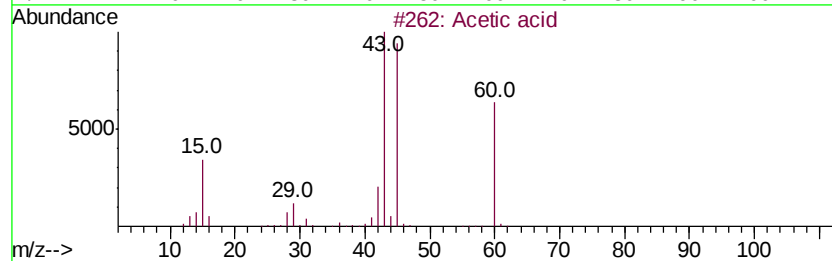
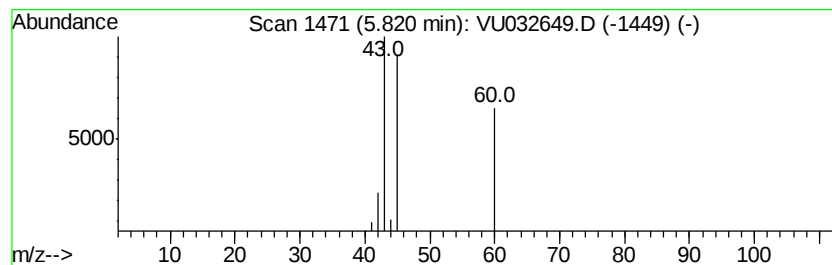
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Acetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.82	3.31 ug/L	25009	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid	60	C2H4O2	000064-19-7	90
2		Acetic acid	60	C2H4O2	000064-19-7	86
3		Acetic acid	60	C2H4O2	000064-19-7	83
4		Acetic acid	60	C2H4O2	000064-19-7	64
5		Acetic acid	60	C2H4O2	000064-19-7	9



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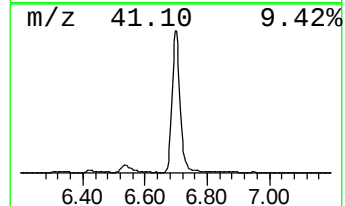
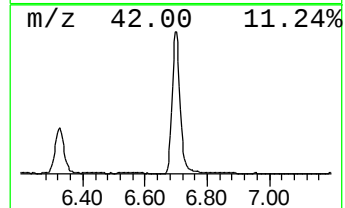
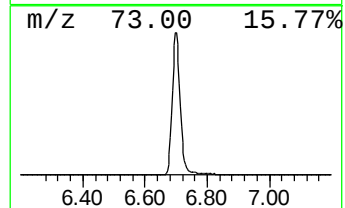
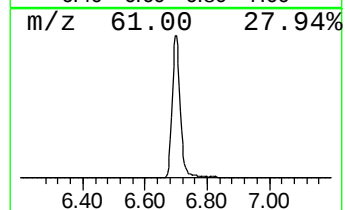
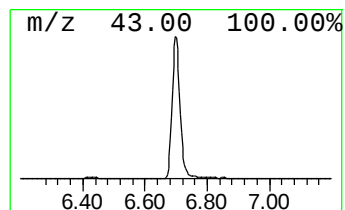
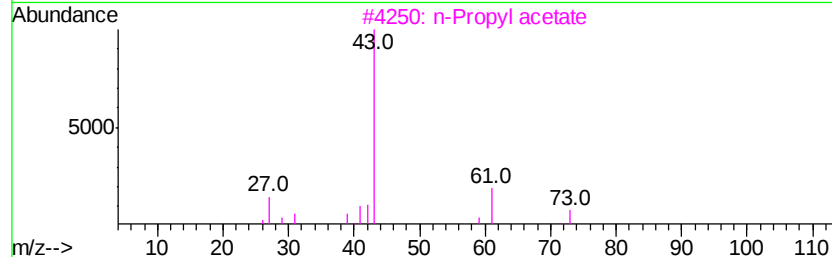
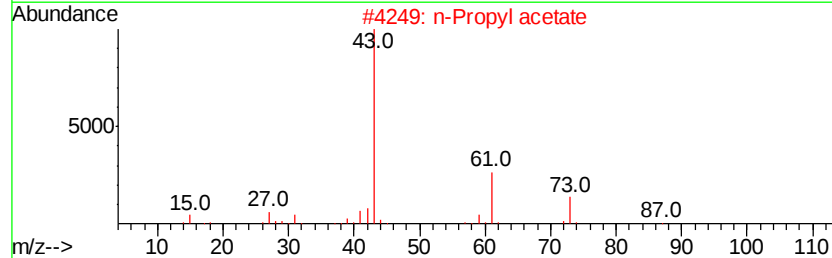
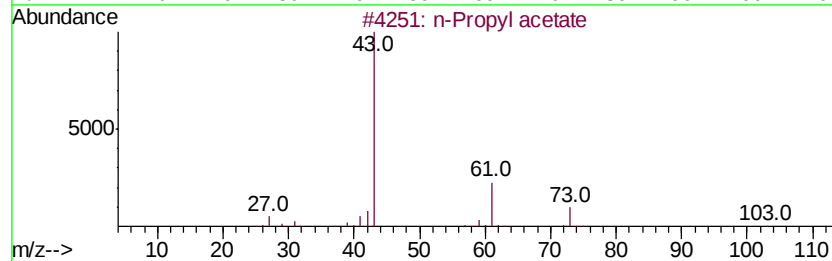
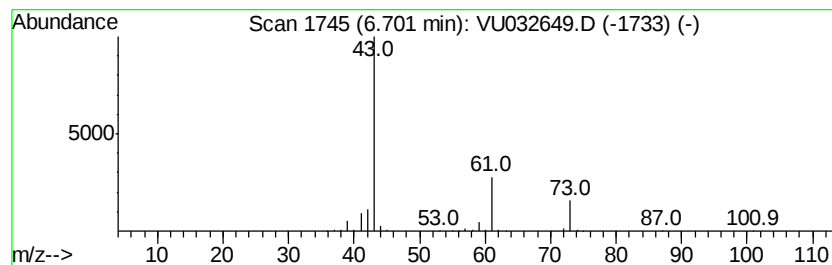
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Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	135.69 ug/L	1025610	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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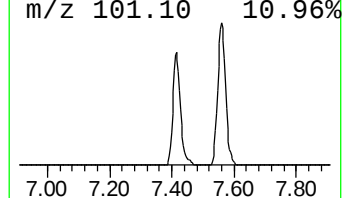
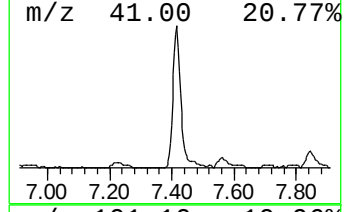
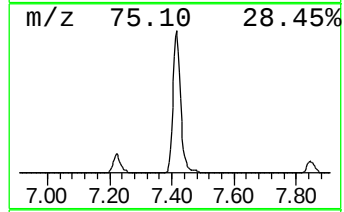
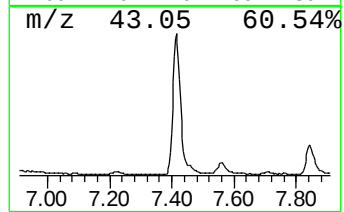
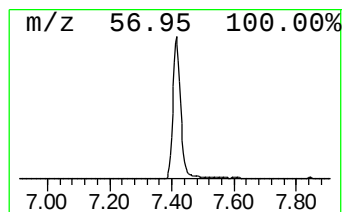
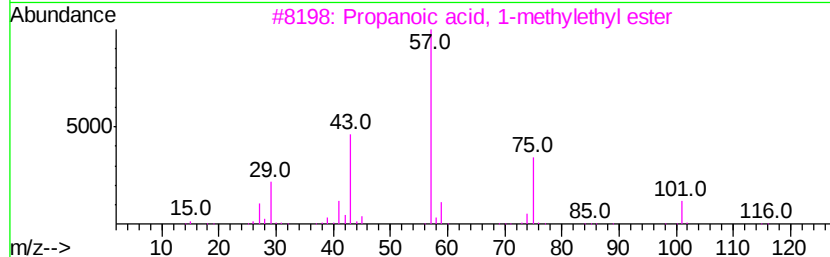
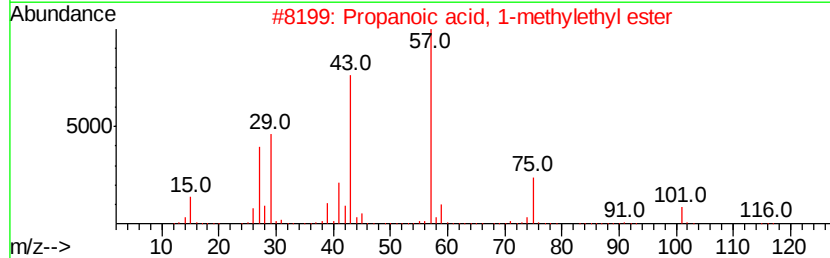
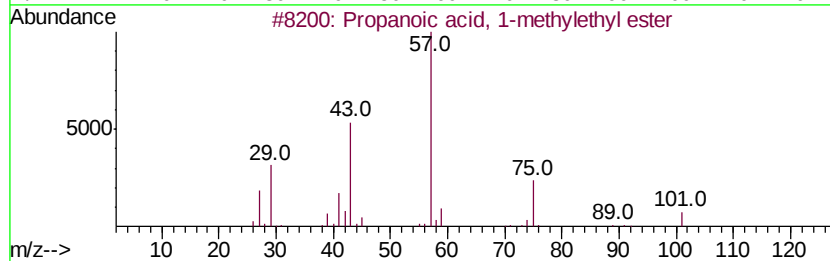
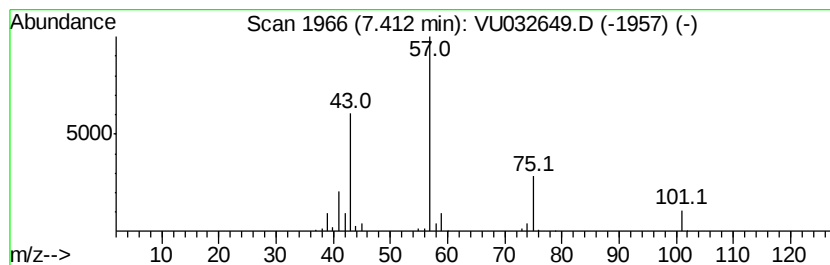
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	24.37 ug/L	184182	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	78
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45
5		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45



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Sample : K3286-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW8

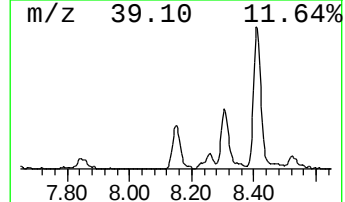
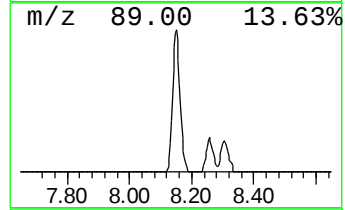
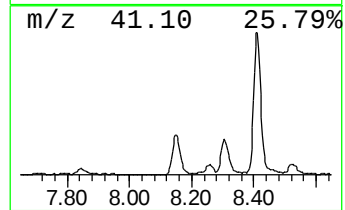
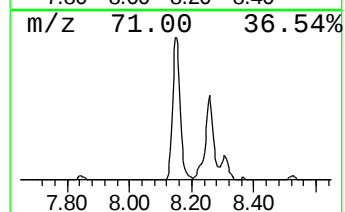
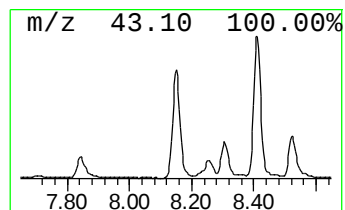
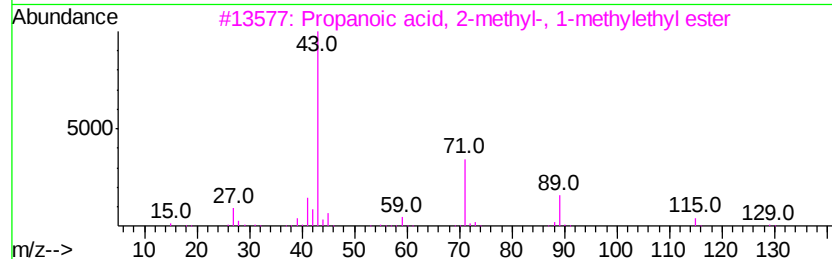
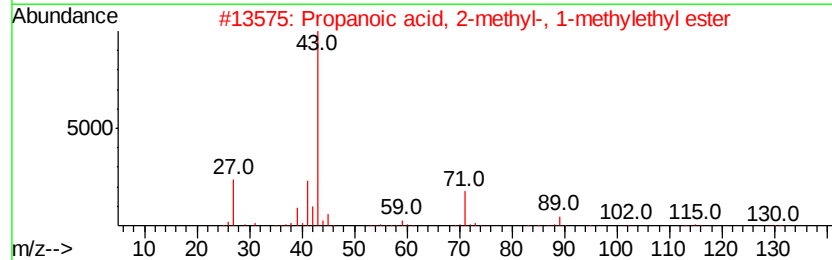
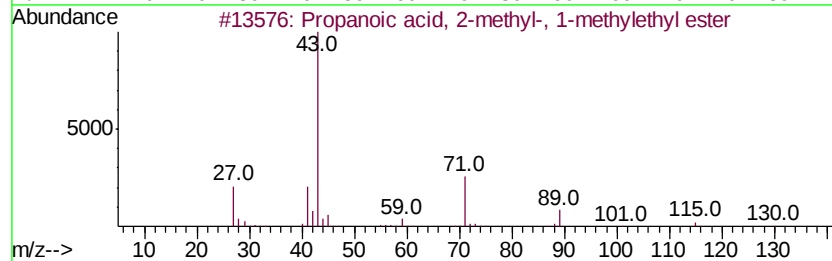
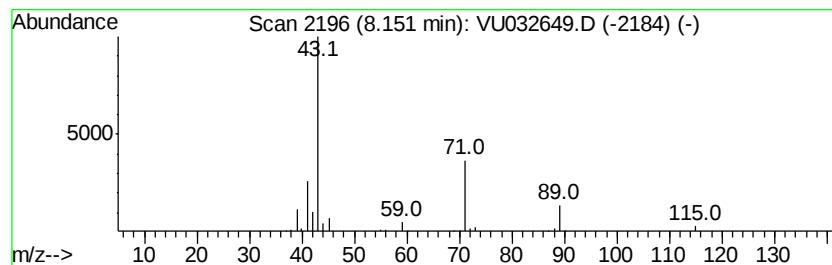
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	10.28 ug/L	98352	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		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
5		N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032649.D
Acq On : 12 Jun 2019 14:10
Operator : JC/SP
Sample : K3286-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW8

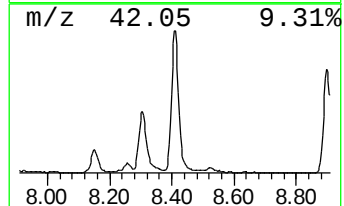
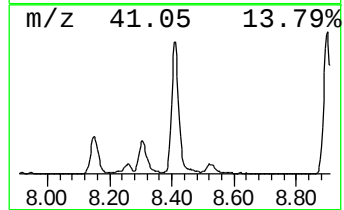
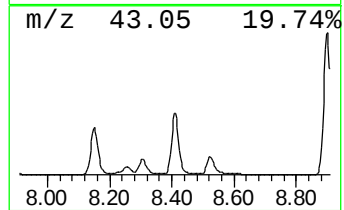
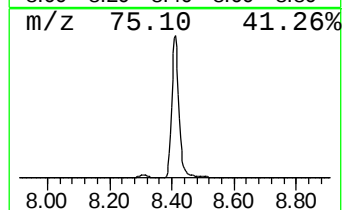
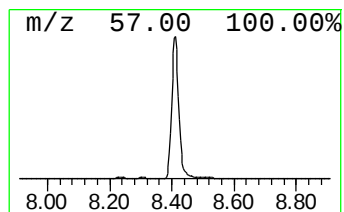
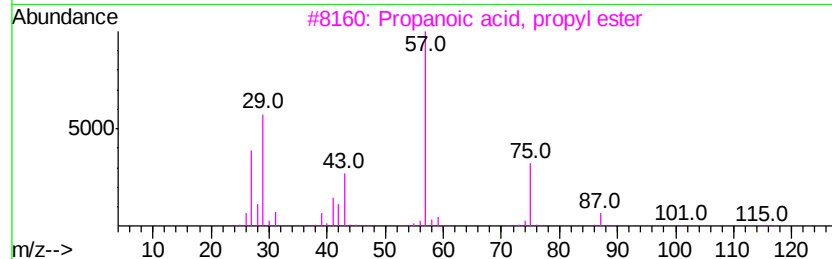
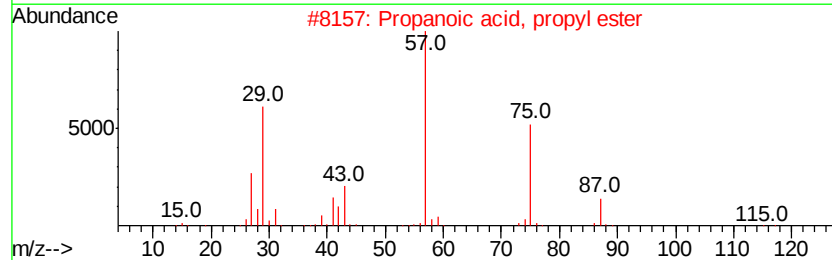
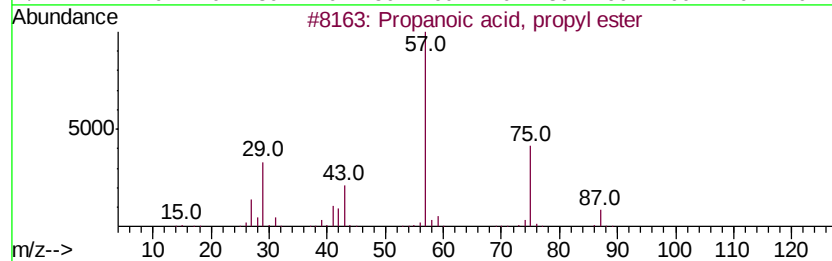
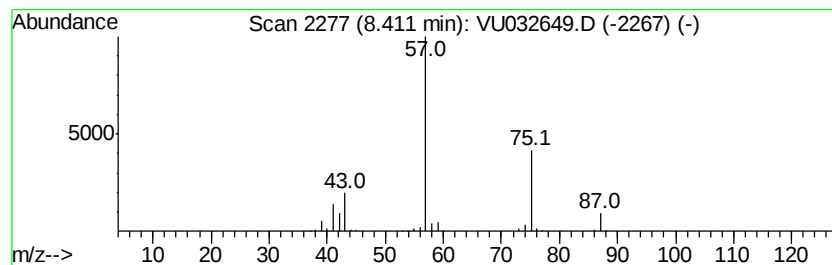
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	60.61 ug/L	579816	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	39



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032649.D
Acq On : 12 Jun 2019 14:10
Operator : JC/SP
Sample : K3286-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

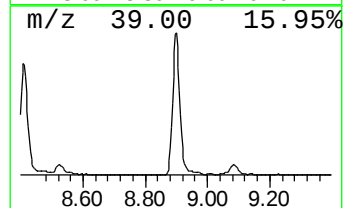
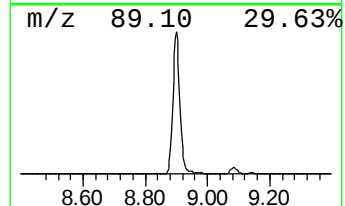
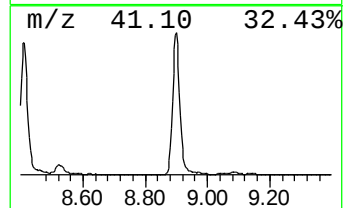
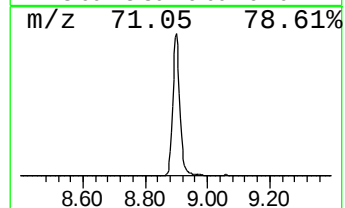
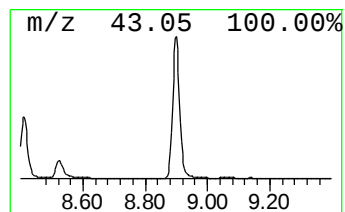
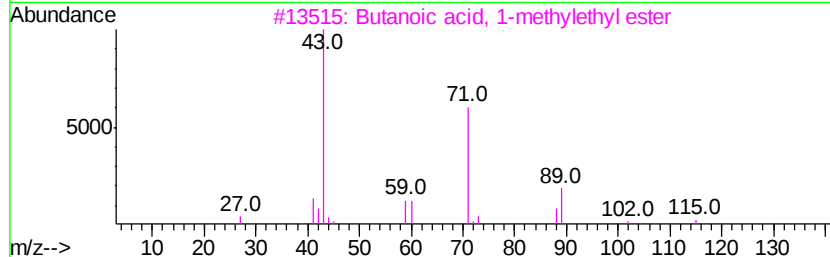
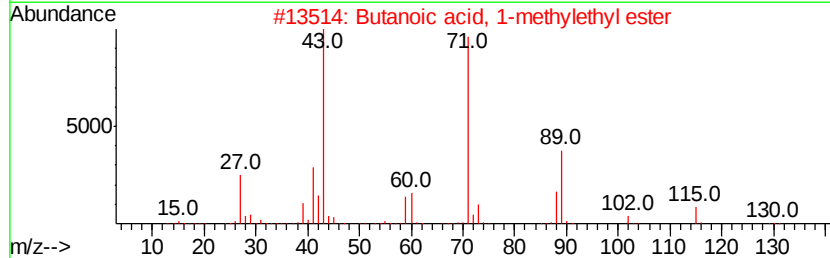
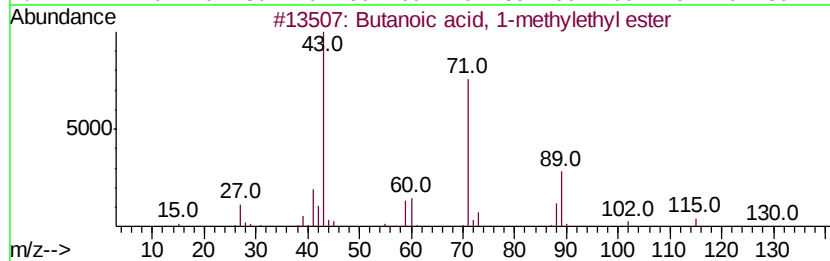
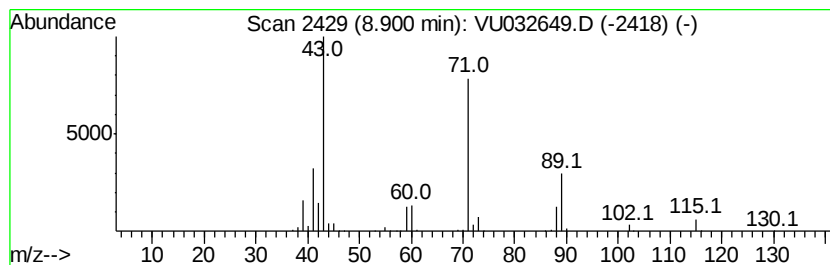
Instrument :
MSVOA_U
ClientSampleId :
C0JW8

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	44.95 ug/L	429953	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	91
3		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83
4		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061219\
Data File : VU032649.D
Acq On : 12 Jun 2019 14:10
Operator : JC/SP
Sample : K3286-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW8

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
Acetic acid	5.82	3.3	ug/L	25009	1	5.88	377916	50.0
n-Propyl acetate	6.70	135.7	ug/L	1025610	1	5.88	377916	50.0
Propanoic acid, 1...	7.41	24.4	ug/L	184182	1	5.88	377916	50.0
Propanoic acid, 2...	8.15	10.3	ug/L	98352	2	9.08	478310	50.0
Propanoic acid, p...	8.41	60.6	ug/L	579816	2	9.08	478310	50.0
Butanoic acid, 1-...	8.90	45.0	ug/L	429953	2	9.08	478310	50.0