

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061219\
 Data File : VU032647.D
 Acq On : 12 Jun 2019 13:25
 Operator : JC/SP
 Sample : K3286-06
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JW4

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	24	28	33	rBV3	4903	4402	0.48%	0.061%
2	1.395	88	95	107	rBV	96127	96177	10.47%	1.331%
3	1.675	175	182	195	rBV	68852	85828	9.34%	1.188%
4	2.267	356	366	377	rBV	149428	226387	24.64%	3.133%
5	2.318	377	382	395	rVB3	8637	14028	1.53%	0.194%
6	2.508	437	441	444	rBV2	323	208	0.02%	0.003%
7	2.540	449	451	457	rVB3	412	346	0.04%	0.005%
8	2.630	473	479	485	rVB2	524	598	0.07%	0.008%
9	2.698	491	500	510	rVB2	4372	6951	0.76%	0.096%
10	2.836	536	543	546	rBV3	330	447	0.05%	0.006%
11	2.897	558	562	565	rBV2	254	224	0.02%	0.003%
12	2.919	566	569	573	rVV	302	238	0.03%	0.003%
13	3.000	589	594	595	rBV	211	205	0.02%	0.003%
14	3.450	730	734	743	rVB2	272	420	0.05%	0.006%
15	3.582	772	775	780	rVB2	305	290	0.03%	0.004%
16	3.681	801	806	810	rVB	272	264	0.03%	0.004%
17	3.714	810	816	818	rBV	292	214	0.02%	0.003%
18	3.749	821	827	833	rVB2	350	432	0.05%	0.006%
19	3.990	898	902	910	rVB	377	416	0.05%	0.006%
20	4.054	918	922	925	rBV2	253	245	0.03%	0.003%
21	4.170	946	958	982	rBV	59020	151431	16.48%	2.095%
22	4.434	1037	1040	1047	rVB	258	244	0.03%	0.003%
23	4.643	1087	1105	1126	rBV	104365	247207	26.91%	3.421%
24	4.813	1155	1158	1161	rVB2	453	270	0.03%	0.004%
25	4.852	1167	1170	1174	rBV2	275	258	0.03%	0.004%
26	4.884	1174	1180	1184	rBV2	669	805	0.09%	0.011%
27	5.006	1214	1218	1220	rVB2	359	206	0.02%	0.003%
28	5.196	1274	1277	1280	rBV2	304	217	0.02%	0.003%
29	5.334	1295	1320	1345	rBV2	215406	624608	67.98%	8.643%
30	5.553	1378	1388	1402	rVV2	3617	7663	0.83%	0.106%
31	5.640	1412	1415	1421	rVB	300	220	0.02%	0.003%
32	5.833	1454	1475	1476	rBV4	8887	26064	2.84%	0.361%
33	5.881	1479	1490	1507	rVV	194642	393927	42.88%	5.451%
34	6.180	1572	1583	1602	rVB	85178	166462	18.12%	2.303%

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Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
 Title : VOC Analysis

35	6.324	1615	1628	1650	rBV	141179	280978	30.58%	3.888%
36	6.421	1652	1658	1672	rVB2	4541	8697	0.95%	0.120%
37	6.533	1686	1693	1700	rBV3	1748	3306	0.36%	0.046%
38	6.578	1702	1707	1714	rVV2	2648	3963	0.43%	0.055%
39	6.697	1733	1744	1780	rBV	514707	918771	100.00%	12.713%
40	7.222	1897	1907	1933	rVB	82717	147235	16.03%	2.037%
41	7.414	1955	1967	1997	rBV	96832	169869	18.49%	2.351%
42	7.559	2000	2012	2041	rBV	298413	517801	56.36%	7.165%
43	7.787	2079	2083	2085	rBV2	540	324	0.04%	0.004%
44	7.845	2090	2101	2120	rBV	64411	115668	12.59%	1.601%
45	7.977	2140	2142	2147	rVB4	387	226	0.02%	0.003%
46	8.057	2165	2167	2174	rVB4	387	318	0.03%	0.004%
47	8.151	2184	2196	2211	rBV	48271	82077	8.93%	1.136%
48	8.228	2211	2220	2223	rBV4	9995	14356	1.56%	0.199%
49	8.305	2235	2244	2266	rVV	202068	341821	37.20%	4.730%
50	8.411	2267	2277	2299	rVB	285966	453743	49.39%	6.279%
51	8.524	2305	2312	2331	rVB2	16408	30667	3.34%	0.424%
52	8.636	2344	2347	2352	rVB5	459	433	0.05%	0.006%
53	8.829	2403	2407	2412	rBV3	312	456	0.05%	0.006%
54	8.900	2417	2429	2456	rBV	193560	313730	34.15%	4.341%
55	9.032	2466	2470	2472	rBV2	337	291	0.03%	0.004%
56	9.083	2473	2486	2516	rVV	280420	472084	51.38%	6.532%
57	9.363	2570	2573	2576	rBV	323	272	0.03%	0.004%
58	9.392	2580	2582	2588	rVV2	405	429	0.05%	0.006%
59	9.437	2591	2596	2598	rVV3	228	229	0.02%	0.003%
60	9.540	2625	2628	2635	rBV3	320	390	0.04%	0.005%
61	9.614	2644	2651	2661	rBV3	1388	2297	0.25%	0.032%
62	9.652	2661	2663	2670	rVB3	570	519	0.06%	0.007%
63	9.691	2670	2675	2678	rBV2	382	399	0.04%	0.006%
64	9.768	2691	2699	2709	rBV5	5092	8368	0.91%	0.116%
65	9.868	2728	2730	2736	rVB2	518	461	0.05%	0.006%
66	9.900	2736	2740	2741	rBV	352	260	0.03%	0.004%
67	9.955	2751	2757	2758	rBV2	253	206	0.02%	0.003%
68	10.057	2783	2789	2795	rBV3	233	362	0.04%	0.005%
69	10.090	2795	2799	2802	rVB3	380	327	0.04%	0.005%
70	10.135	2809	2813	2816	rBV3	427	292	0.03%	0.004%
71	10.160	2816	2821	2823	rVB	311	238	0.03%	0.003%

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 Title : VOC Analysis

72	10.186	2827	2829	2834	rVV2	307	287	0.03%	0.004%
73	10.209	2834	2836	2840	rVB	335	204	0.02%	0.003%
74	10.279	2855	2858	2861	rVB2	417	271	0.03%	0.004%
75	10.305	2861	2866	2872	rBV2	236	301	0.03%	0.004%
76	10.427	2891	2904	2924	rVV	203282	326419	35.53%	4.517%
77	10.604	2952	2959	2971	rBV4	1191	1747	0.19%	0.024%
78	10.672	2975	2980	2985	rVB2	445	363	0.04%	0.005%
79	10.909	3051	3054	3058	rBV3	242	243	0.03%	0.003%
80	10.987	3074	3078	3081	rVV	311	238	0.03%	0.003%
81	11.019	3081	3088	3090	rVV2	215	229	0.02%	0.003%
82	11.048	3094	3097	3102	rVB3	416	364	0.04%	0.005%
83	11.099	3110	3113	3119	rBV	362	298	0.03%	0.004%
84	11.479	3219	3231	3254	rBV	289124	465189	50.63%	6.437%
85	11.758	3313	3318	3323	rVB3	241	283	0.03%	0.004%
86	11.855	3334	3348	3371	rBV	285847	474937	51.69%	6.572%
87	12.106	3423	3426	3430	rVB2	454	291	0.03%	0.004%
88	12.154	3438	3441	3444	rBV2	234	207	0.02%	0.003%
89	12.469	3534	3539	3540	rBV3	738	615	0.07%	0.009%
90	12.800	3637	3642	3644	rVV2	340	268	0.03%	0.004%
91	12.913	3674	3677	3683	rVV2	293	269	0.03%	0.004%
92	13.080	3724	3729	3732	rVB2	275	214	0.02%	0.003%
93	13.369	3813	3819	3824	rBV	362	341	0.04%	0.005%
94	13.559	3875	3878	3881	rBV2	374	257	0.03%	0.004%
95	13.851	3963	3969	3973	rBV4	486	606	0.07%	0.008%
96	14.273	4094	4100	4106	rBV3	783	1296	0.14%	0.018%
97	14.424	4143	4147	4149	rBV2	260	225	0.02%	0.003%
98	14.488	4163	4167	4174	rVB2	353	468	0.05%	0.006%
99	14.527	4174	4179	4182	rBV2	476	437	0.05%	0.006%
100	15.999	4635	4637	4640	rVB2	457	234	0.03%	0.003%

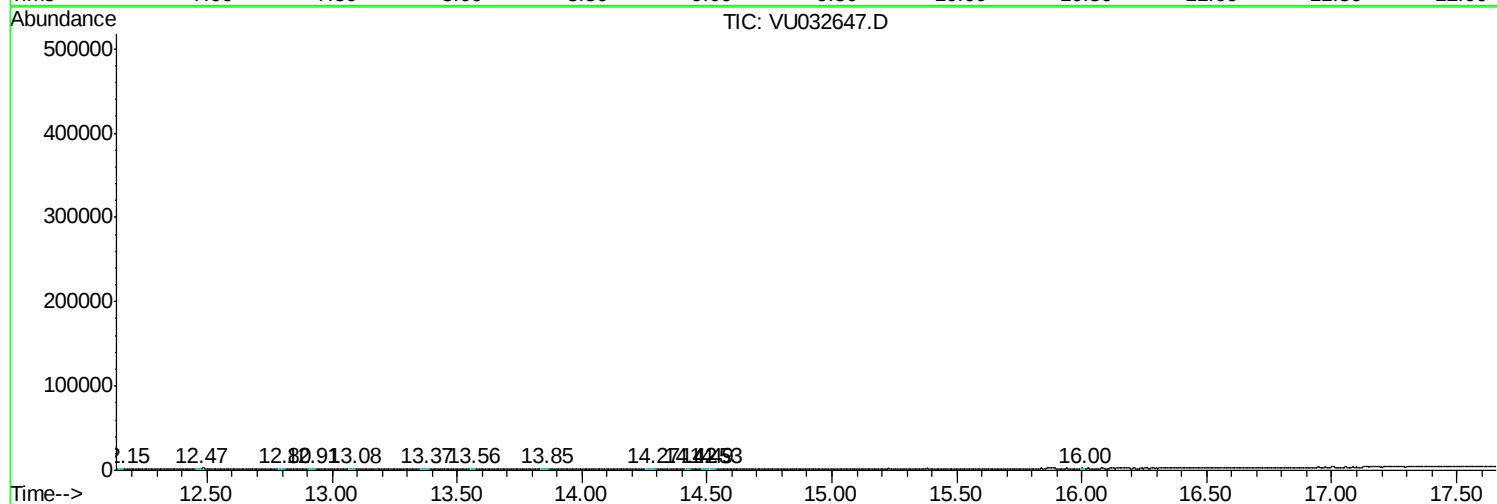
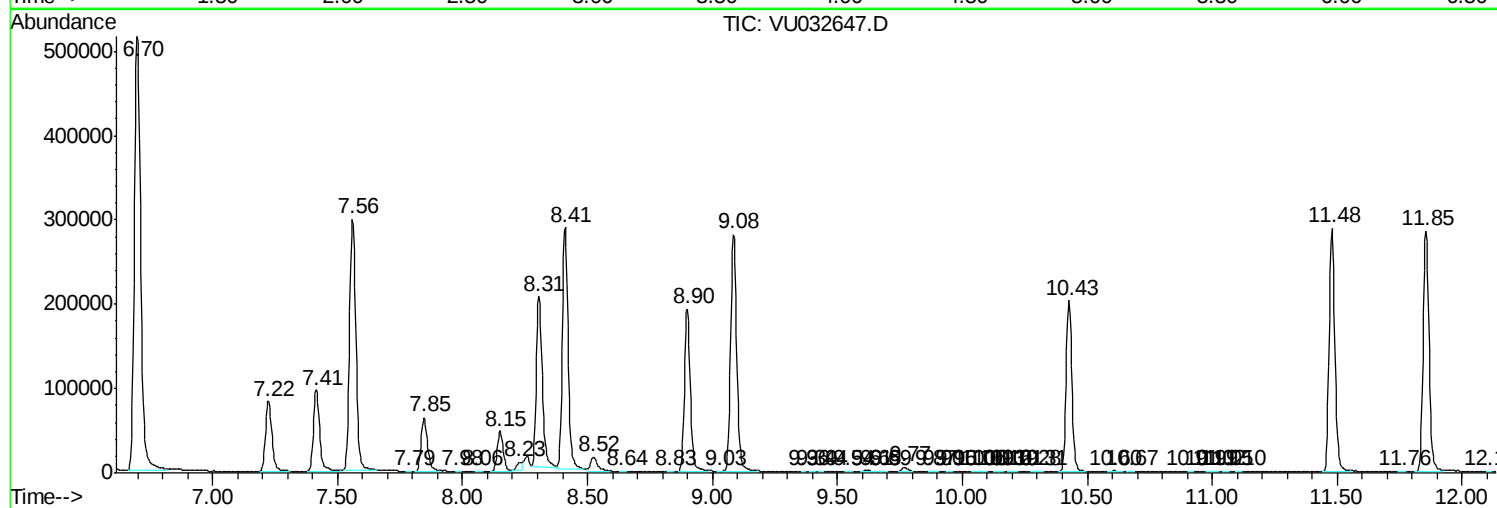
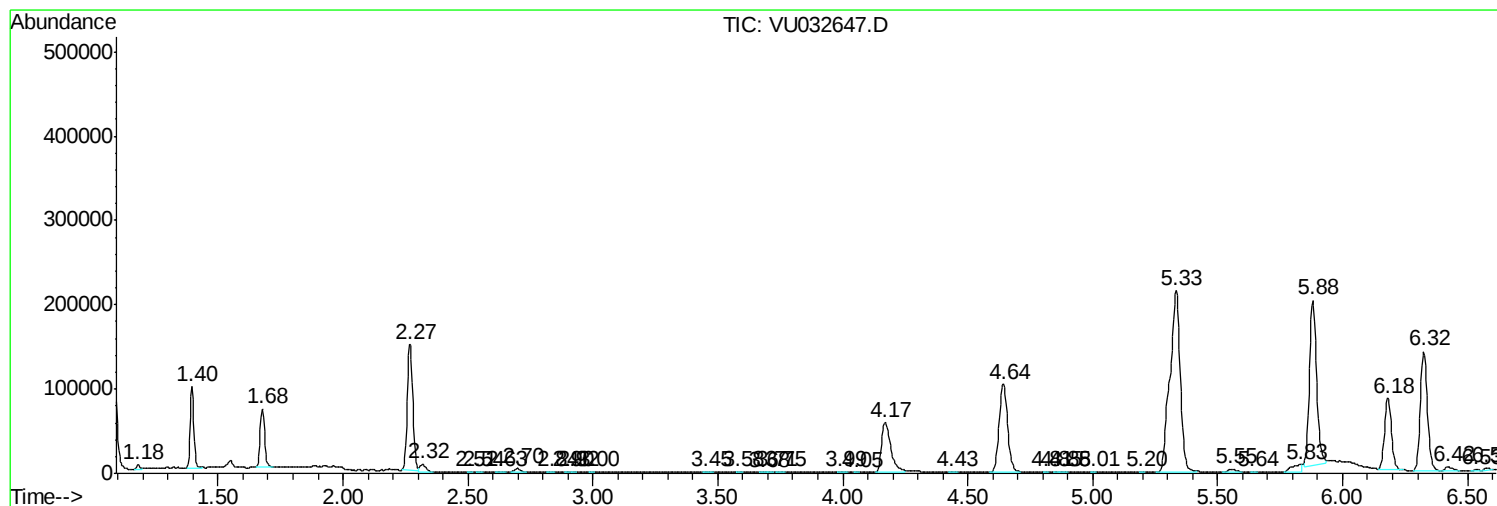
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ALS Vial : 12 Sample Multiplier: 1

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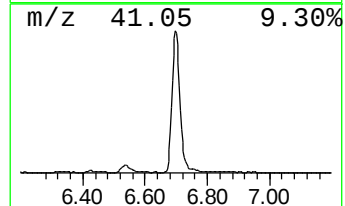
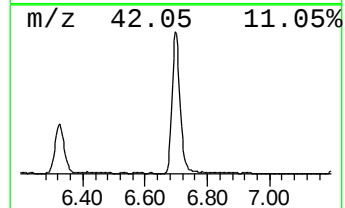
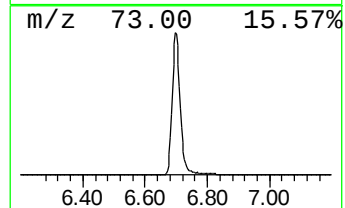
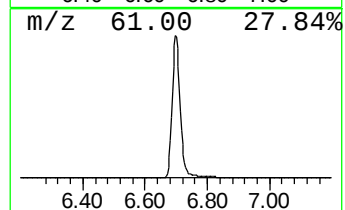
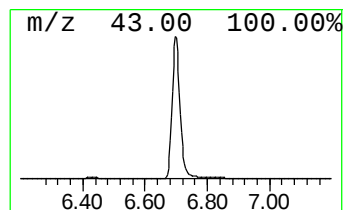
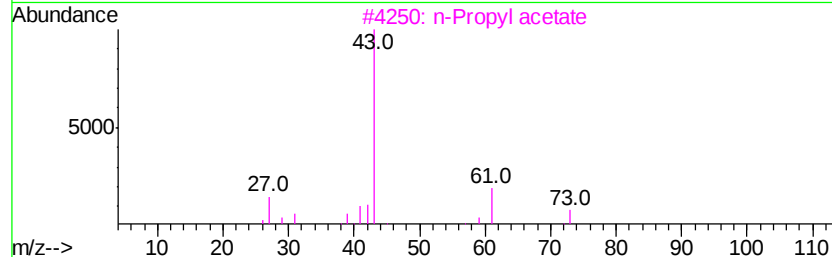
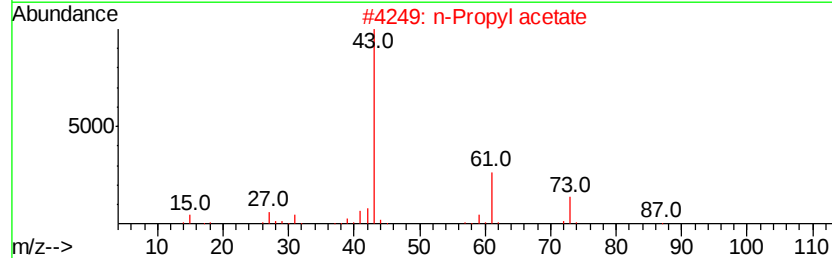
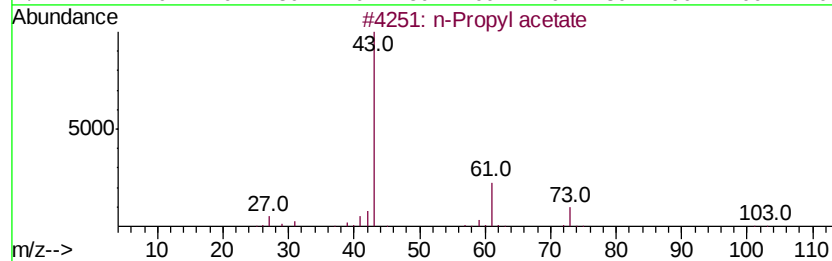
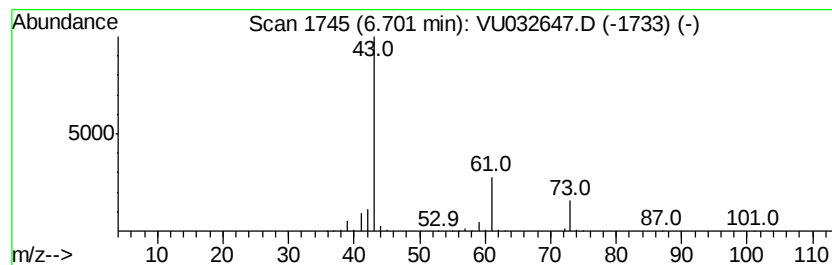
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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	116.62 ug/L	918771	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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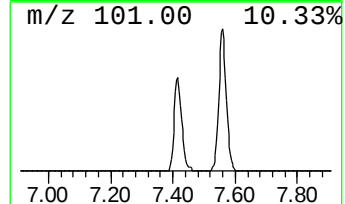
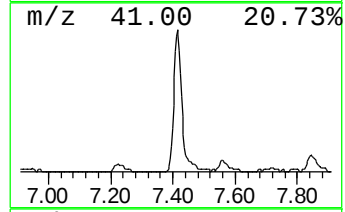
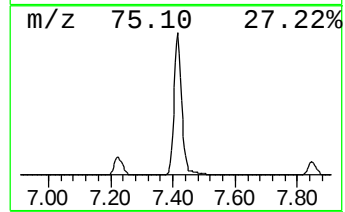
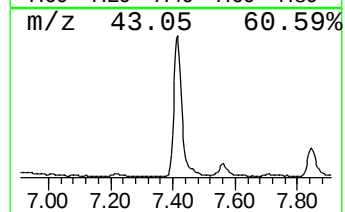
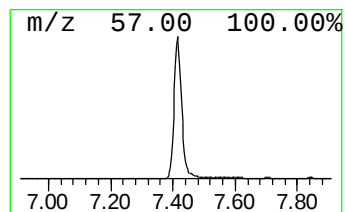
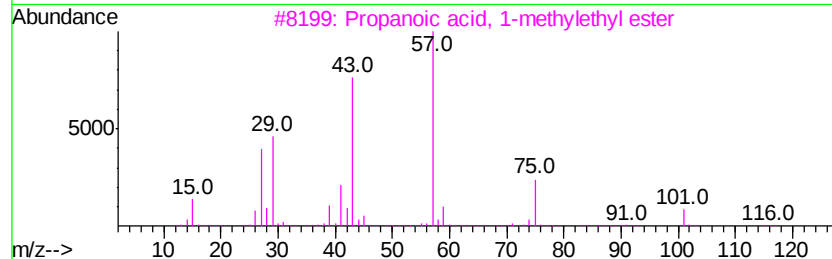
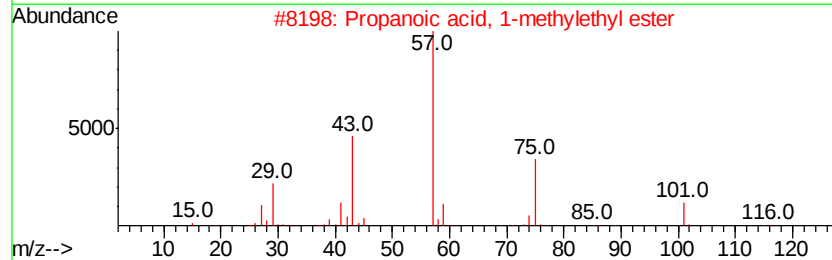
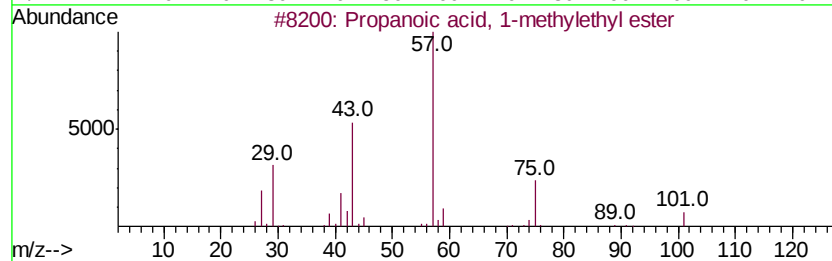
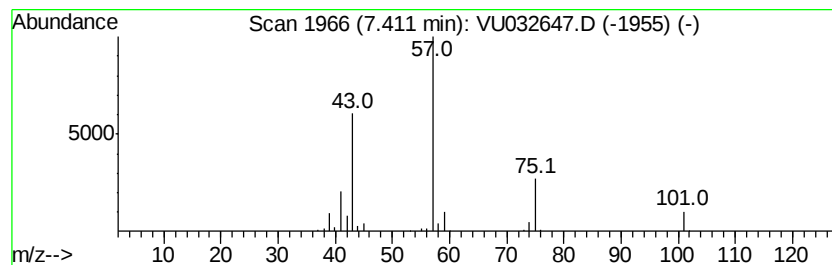
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Quant Title : VOC Analysis

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	21.56 ug/L	169869	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	64
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
4		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42



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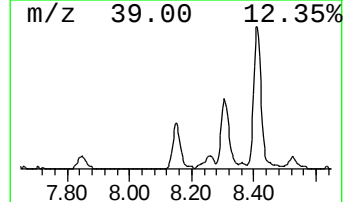
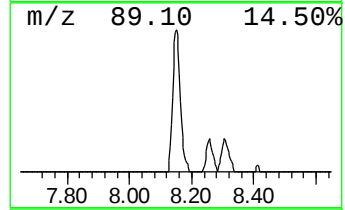
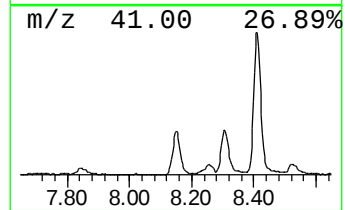
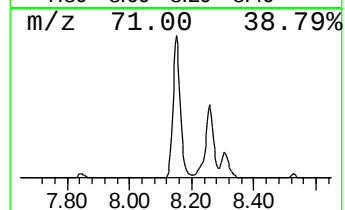
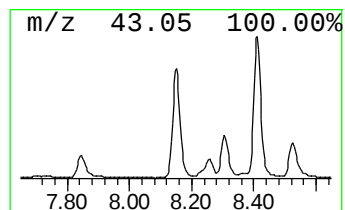
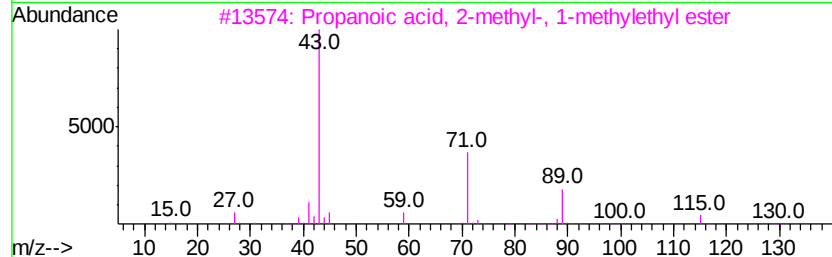
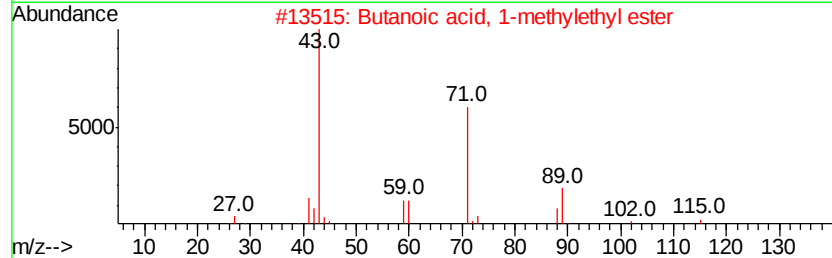
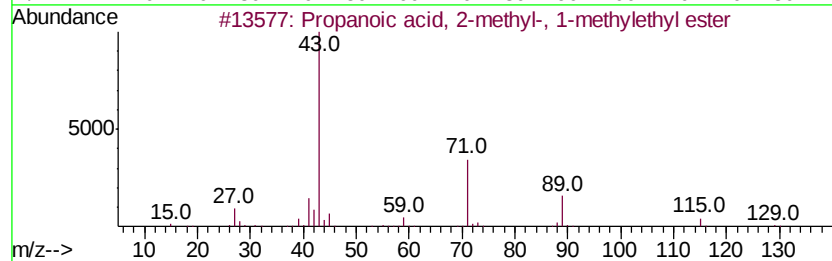
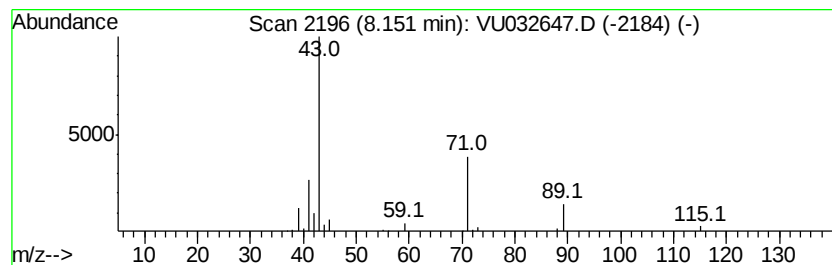
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.15	8.69 ug/L	82077	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	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	78	
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78	
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	74	
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032647.D
Acq On : 12 Jun 2019 13:25
Operator : JC/SP
Sample : K3286-06
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JW4

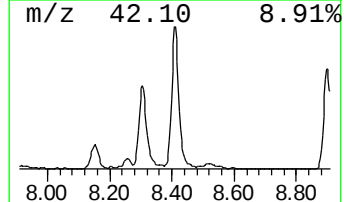
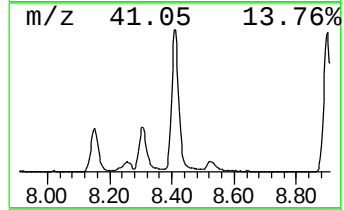
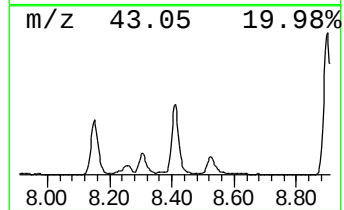
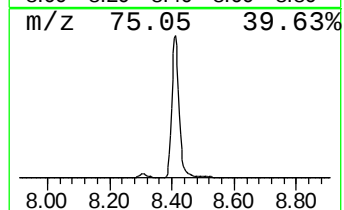
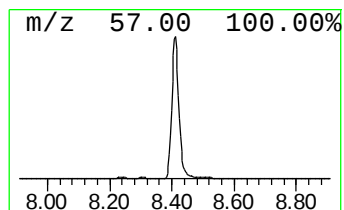
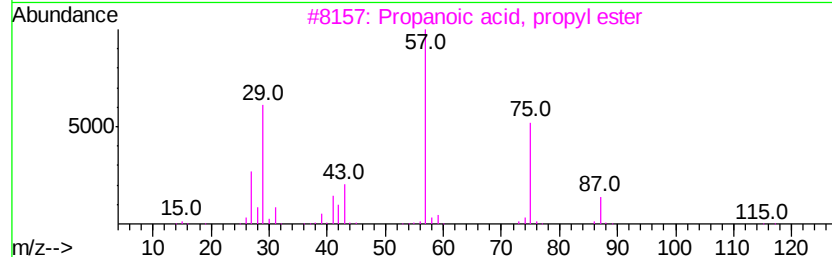
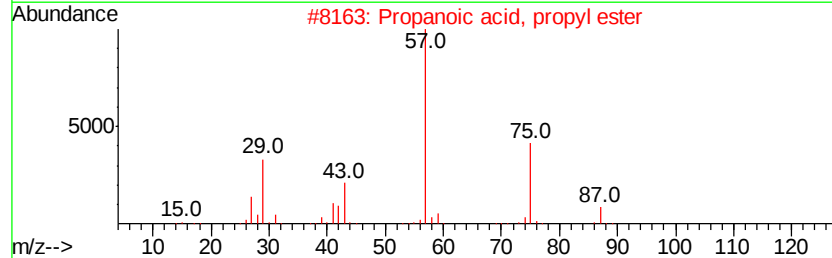
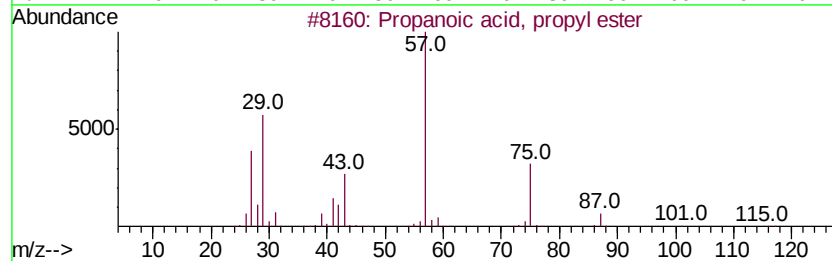
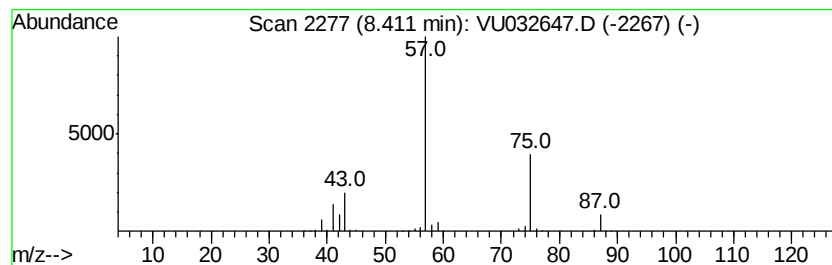
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Quant Title : VOC Analysis

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	48.06 ug/L	453743	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	39



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032647.D
Acq On : 12 Jun 2019 13:25
Operator : JC/SP
Sample : K3286-06
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW4

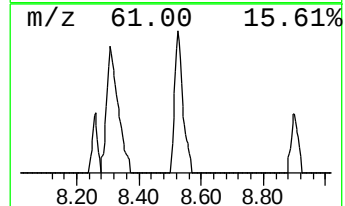
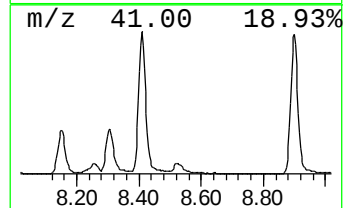
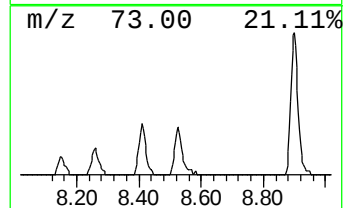
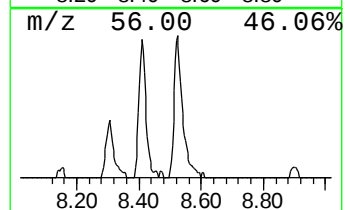
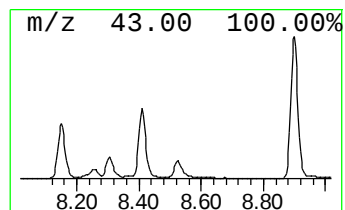
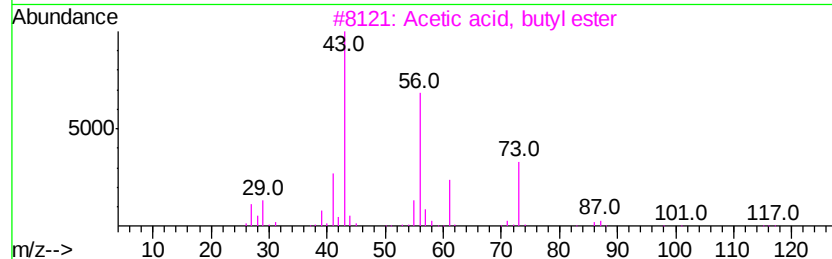
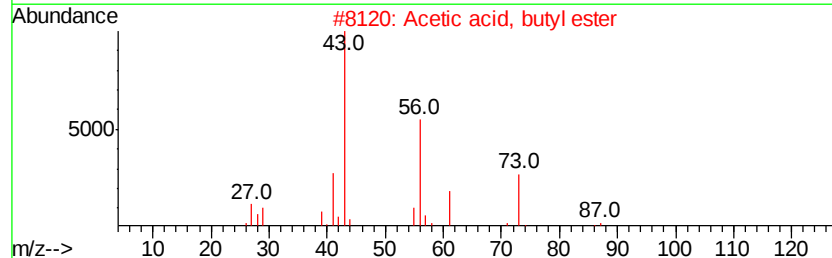
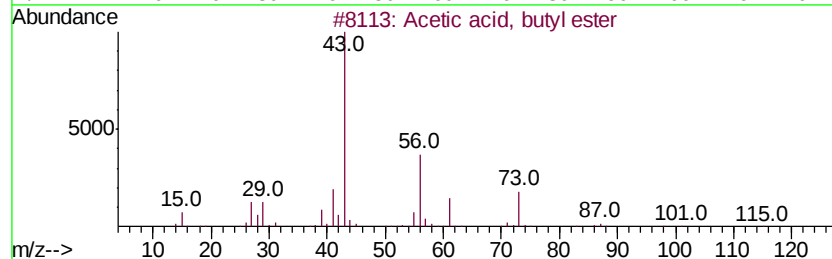
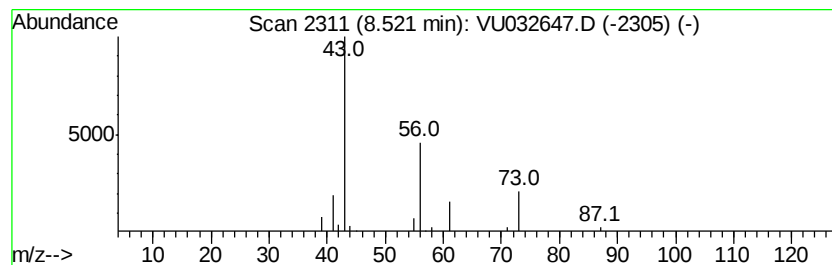
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Quant Title : VOC Analysis

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	3.25 ug/L	30667	Chlorobenzene-d5	9.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
5			Isobutyl acetate	116	C6H12O2	000110-19-0	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032647.D
Acq On : 12 Jun 2019 13:25
Operator : JC/SP
Sample : K3286-06
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW4

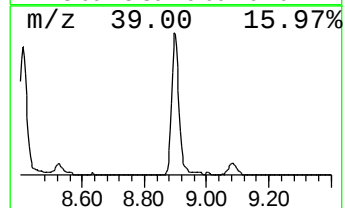
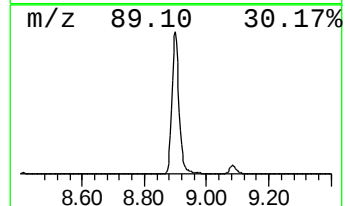
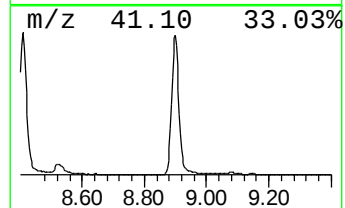
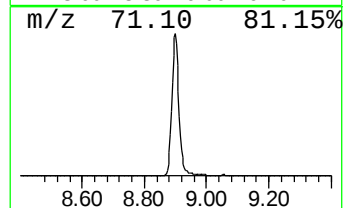
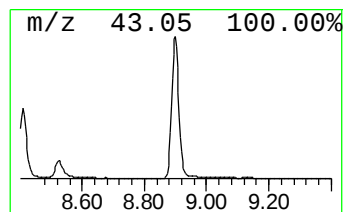
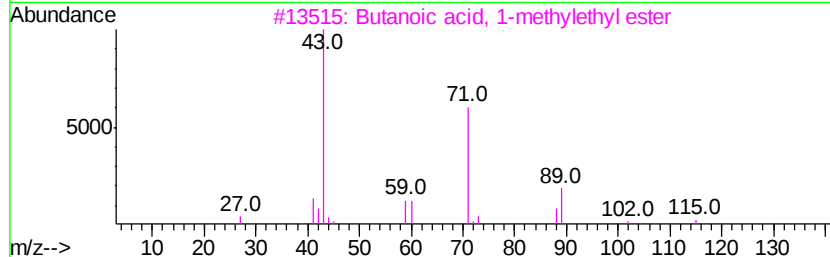
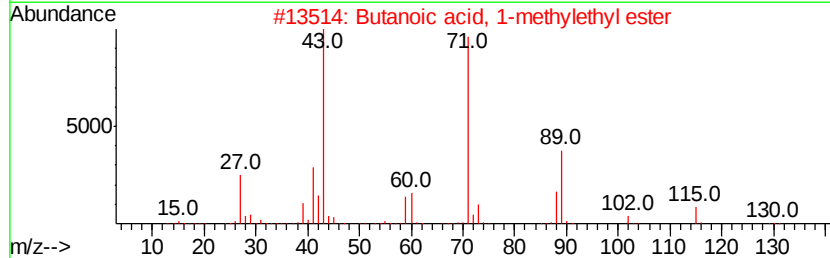
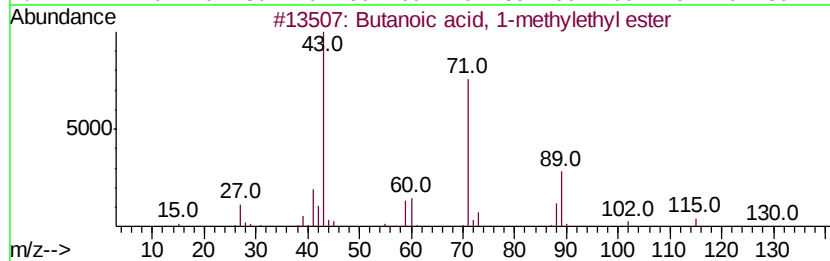
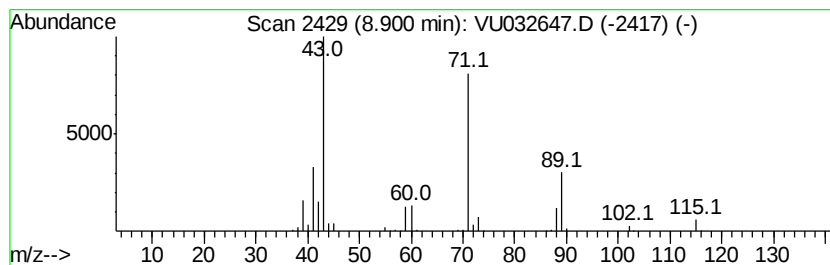
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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	33.23 ug/L	313730	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
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, propyl ester	130	C7H14O2	000105-66-8	72
5		Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061219\
Data File : VU032647.D
Acq On : 12 Jun 2019 13:25
Operator : JC/SP
Sample : K3286-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW4

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	116.6	ug/L	918771	1	5.88	393927	50.0
Propanoic acid, 1...	7.41	21.6	ug/L	169869	1	5.88	393927	50.0
Propanoic acid, 2...	8.15	8.7	ug/L	82077	2	9.08	472084	50.0
Propanoic acid, p...	8.41	48.1	ug/L	453743	2	9.08	472084	50.0
Acetic acid, buty...	8.52	3.3	ug/L	30667	2	9.08	472084	50.0
Butanoic acid, 1-...	8.90	33.2	ug/L	313730	2	9.08	472084	50.0