

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061219\
 Data File : VU032646.D
 Acq On : 12 Jun 2019 13:02
 Operator : JC/SP
 Sample : K3286-05
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JW3

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	35	rBV	4983	4847	0.43%	0.058%
2	1.392	88	94	107	rBV	87610	93466	8.22%	1.122%
3	1.675	175	182	200	rVB	72975	89174	7.85%	1.071%
4	2.267	356	366	377	rBV	153029	230238	20.26%	2.765%
5	2.322	377	383	399	rVB	8676	14875	1.31%	0.179%
6	2.431	414	417	418	rBV	280	165	0.01%	0.002%
7	2.624	474	477	478	rBV	307	171	0.02%	0.002%
8	2.698	491	500	510	rVB2	6623	11377	1.00%	0.137%
9	2.740	510	513	515	rBV2	254	145	0.01%	0.002%
10	2.765	518	521	524	rBV2	177	132	0.01%	0.002%
11	2.826	536	540	546	rBV3	445	516	0.05%	0.006%
12	2.987	586	590	594	rBV	146	157	0.01%	0.002%
13	3.084	615	620	622	rBV2	198	218	0.02%	0.003%
14	3.183	648	651	653	rBV2	248	172	0.02%	0.002%
15	3.235	663	667	671	rVB2	338	286	0.03%	0.003%
16	3.289	683	684	690	rVB2	223	144	0.01%	0.002%
17	3.321	690	694	698	rBV	344	331	0.03%	0.004%
18	3.379	709	712	717	rVB2	186	154	0.01%	0.002%
19	3.418	717	724	735	rBV5	823	1774	0.16%	0.021%
20	3.460	735	737	741	rVB	452	246	0.02%	0.003%
21	3.521	753	756	760	rBV	164	126	0.01%	0.002%
22	3.550	762	765	770	rBV2	189	141	0.01%	0.002%
23	3.595	775	779	782	rBV	183	128	0.01%	0.002%
24	3.643	788	794	797	rBV2	249	265	0.02%	0.003%
25	3.804	841	844	846	rBV	186	127	0.01%	0.002%
26	3.820	846	849	852	rVB2	178	139	0.01%	0.002%
27	3.900	869	874	878	rBV2	176	197	0.02%	0.002%
28	4.003	901	906	909	rBV2	244	230	0.02%	0.003%
29	4.022	909	912	919	rVB2	156	136	0.01%	0.002%
30	4.087	926	932	933	rBV	174	170	0.01%	0.002%
31	4.170	946	958	989	rBV	60686	159919	14.07%	1.920%
32	4.457	1043	1047	1050	rBV4	318	278	0.02%	0.003%
33	4.476	1050	1053	1055	rVB2	290	151	0.01%	0.002%
34	4.505	1059	1062	1065	rVB	254	171	0.02%	0.002%

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 Title : VOC Analysis

35	4.640	1089	1104	1129	rBV	107172	250018	22.00%	3.002%
36	4.842	1164	1167	1169	rBV	268	171	0.02%	0.002%
37	4.887	1176	1181	1187	rBV3	455	513	0.05%	0.006%
38	4.936	1192	1196	1201	rBV2	212	216	0.02%	0.003%
39	4.987	1209	1212	1214	rBV	265	203	0.02%	0.002%
40	5.183	1269	1273	1278	rVB2	299	266	0.02%	0.003%
41	5.209	1278	1281	1284	rBV2	224	144	0.01%	0.002%
42	5.334	1297	1320	1348	rBV2	219367	639351	56.26%	7.678%
43	5.556	1380	1389	1403	rVB3	3828	7995	0.70%	0.096%
44	5.881	1443	1490	1513	rBV	232898	735363	64.70%	8.831%
45	6.180	1577	1583	1601	rVB3	21769	42054	3.70%	0.505%
46	6.325	1615	1628	1649	rVV	146306	289038	25.43%	3.471%
47	6.421	1652	1658	1683	rVB2	5995	13388	1.18%	0.161%
48	6.579	1701	1707	1715	rBV2	3309	5428	0.48%	0.065%
49	6.698	1733	1744	1772	rBV	645503	1136499	100.00%	13.648%
50	7.103	1868	1870	1874	rBV3	468	374	0.03%	0.004%
51	7.222	1896	1907	1928	rBV	84703	152198	13.39%	1.828%
52	7.415	1956	1967	1990	rBV	114270	196922	17.33%	2.365%
53	7.559	2000	2012	2029	rBV	303239	527898	46.45%	6.339%
54	7.845	2091	2101	2120	rVB2	67950	117698	10.36%	1.413%
55	8.151	2185	2196	2212	rBV	64027	106672	9.39%	1.281%
56	8.257	2214	2229	2235	rVV2	24968	44798	3.94%	0.538%
57	8.305	2235	2244	2265	rVV	223310	376126	33.10%	4.517%
58	8.411	2266	2277	2296	rVB	455362	703894	61.94%	8.453%
59	8.521	2304	2311	2329	rVB	29331	50768	4.47%	0.610%
60	8.900	2417	2429	2456	rBV	307415	479702	42.21%	5.761%
61	9.083	2475	2486	2512	rVB	289844	482484	42.45%	5.794%
62	9.299	2550	2553	2558	rBV3	337	309	0.03%	0.004%
63	9.363	2571	2573	2576	rBV2	311	162	0.01%	0.002%
64	9.463	2601	2604	2606	rBV2	484	333	0.03%	0.004%
65	9.607	2642	2649	2659	rBV3	3189	5468	0.48%	0.066%
66	9.765	2689	2698	2717	rBV2	13848	23689	2.08%	0.284%
67	9.984	2764	2766	2769	rVB2	468	168	0.01%	0.002%
68	10.045	2783	2785	2788	rVB2	354	218	0.02%	0.003%
69	10.064	2788	2791	2793	rBV2	263	195	0.02%	0.002%
70	10.376	2885	2888	2889	rBV2	322	190	0.02%	0.002%
71	10.427	2892	2904	2920	rVV	208411	334876	29.47%	4.021%

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72	10.604	2954	2959	2969	rVB4	1320	1711	0.15%	0.021%
73	10.675	2978	2981	2985	rBV2	332	303	0.03%	0.004%
74	11.025	3088	3090	3095	rVB2	336	242	0.02%	0.003%
75	11.086	3104	3109	3110	rBV2	331	283	0.02%	0.003%
76	11.115	3116	3118	3125	rVB3	400	369	0.03%	0.004%
77	11.299	3172	3175	3176	rBV2	290	172	0.02%	0.002%
78	11.347	3188	3190	3194	rVB	381	189	0.02%	0.002%
79	11.366	3194	3196	3200	rBV	368	283	0.02%	0.003%
80	11.479	3220	3231	3256	rBV	305462	489149	43.04%	5.874%
81	11.755	3313	3317	3319	rBV2	564	479	0.04%	0.006%
82	11.855	3336	3348	3372	rBV	298442	490597	43.17%	5.891%
83	12.176	3443	3448	3453	rBV3	328	474	0.04%	0.006%
84	12.244	3466	3469	3472	rBV	271	179	0.02%	0.002%
85	12.382	3510	3512	3517	rVB2	321	222	0.02%	0.003%
86	12.414	3518	3522	3525	rBV3	362	305	0.03%	0.004%
87	12.472	3533	3540	3551	rBV4	1133	2012	0.18%	0.024%
88	12.710	3611	3614	3617	rBV	423	334	0.03%	0.004%
89	12.855	3657	3659	3661	rBV	227	143	0.01%	0.002%
90	13.032	3711	3714	3718	rVB3	393	343	0.03%	0.004%
91	13.057	3718	3722	3724	rBV2	392	337	0.03%	0.004%
92	13.074	3724	3727	3728	rBV	387	160	0.01%	0.002%
93	13.167	3753	3756	3759	rBV	324	242	0.02%	0.003%
94	13.385	3821	3824	3829	rBV3	364	352	0.03%	0.004%
95	13.864	3969	3973	3975	rBV2	396	306	0.03%	0.004%
96	13.881	3976	3978	3981	rBV2	386	234	0.02%	0.003%
97	14.266	4096	4098	4100	rBV2	428	236	0.02%	0.003%
98	14.373	4129	4131	4133	rBV2	280	155	0.01%	0.002%
99	14.565	4187	4191	4196	rBV2	323	456	0.04%	0.005%
100	14.858	4277	4282	4284	rBV	452	460	0.04%	0.006%

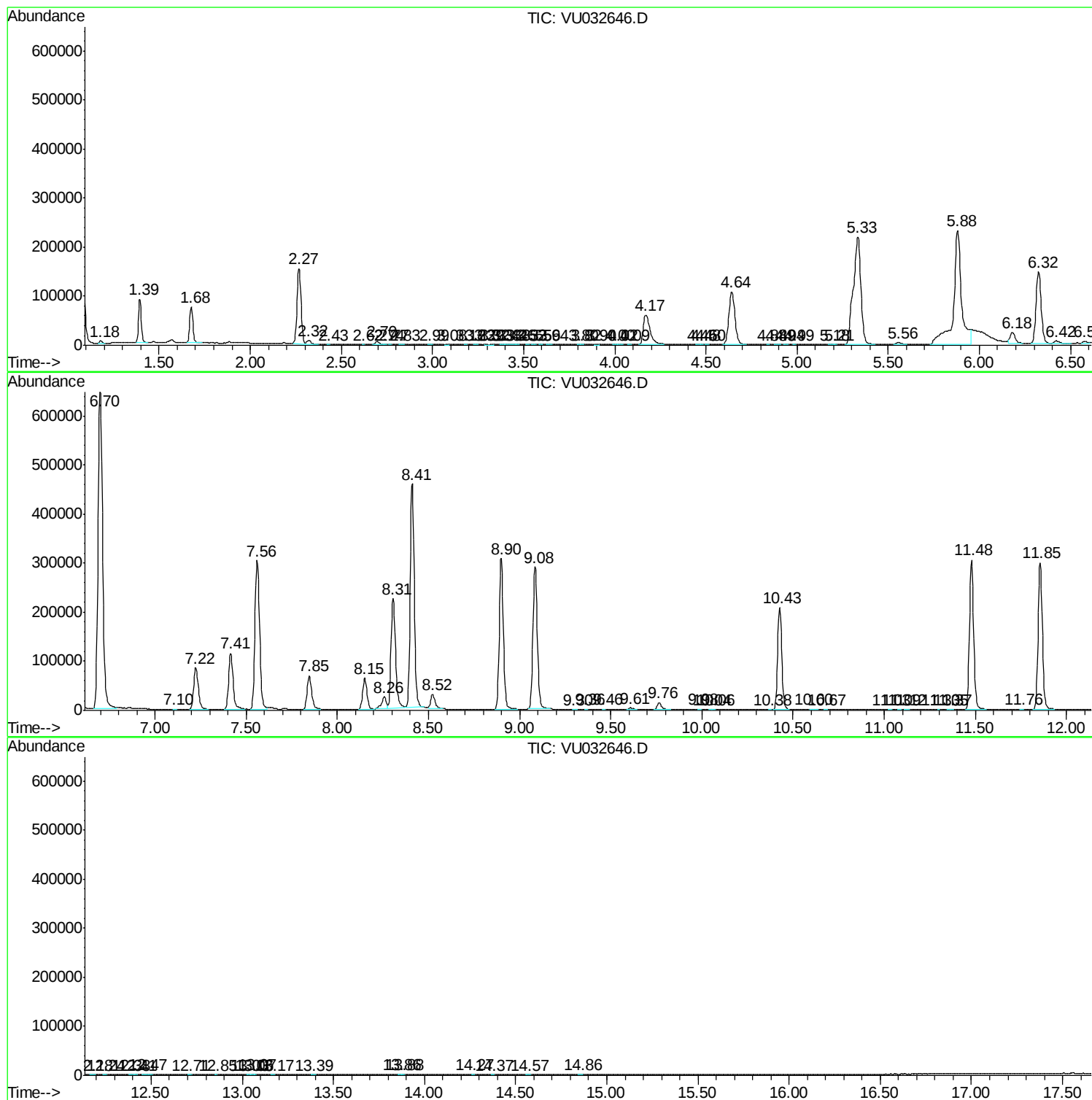
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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



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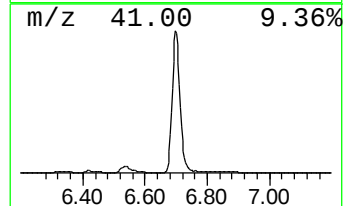
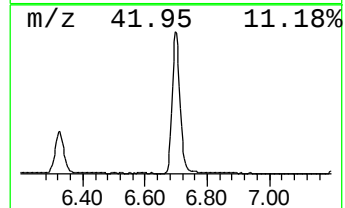
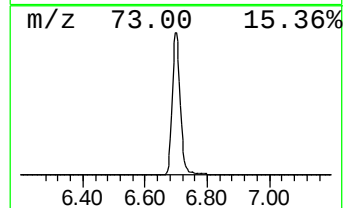
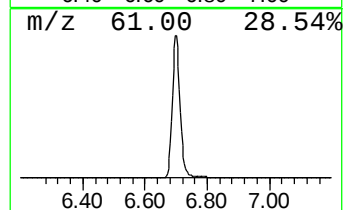
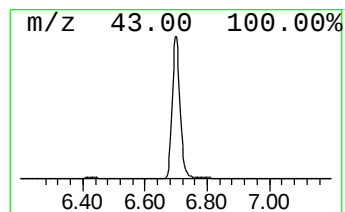
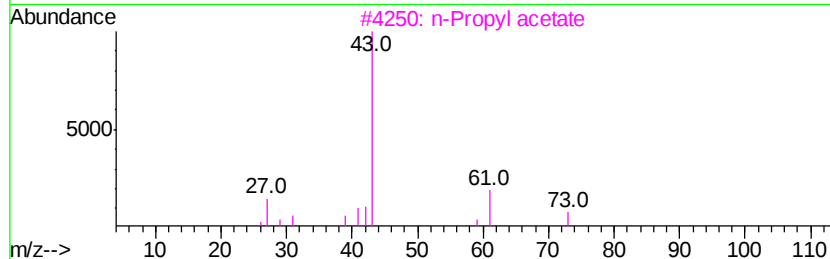
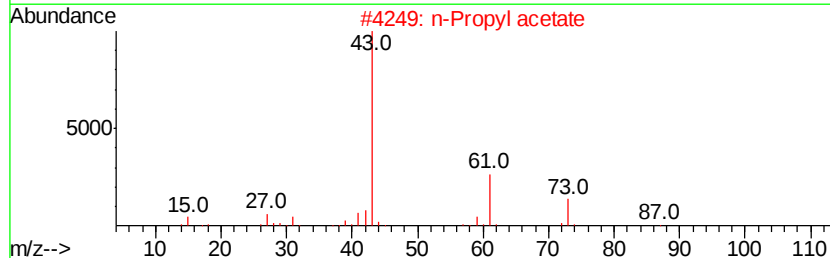
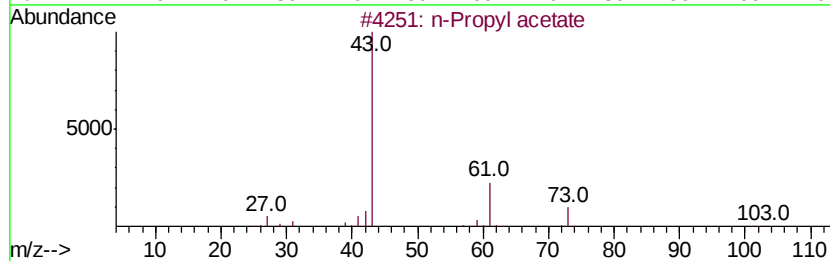
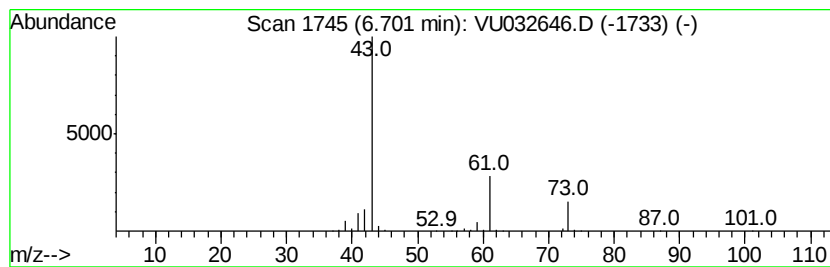
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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	77.27 ug/L	1136500	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		Isobutyl acetate	116	C6H12O2	000110-19-0	9



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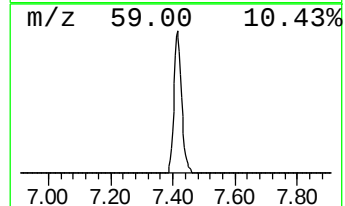
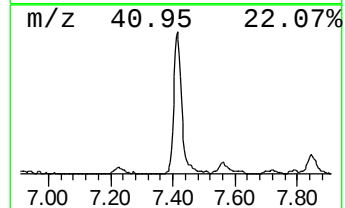
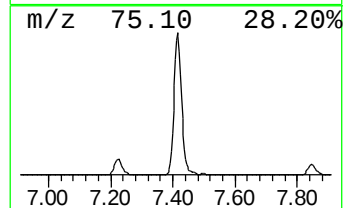
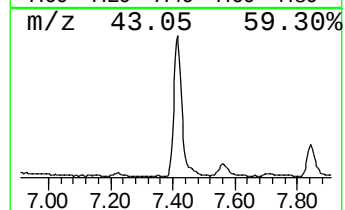
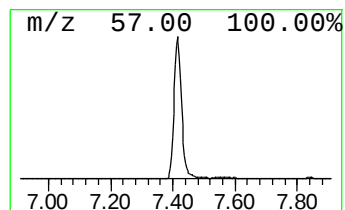
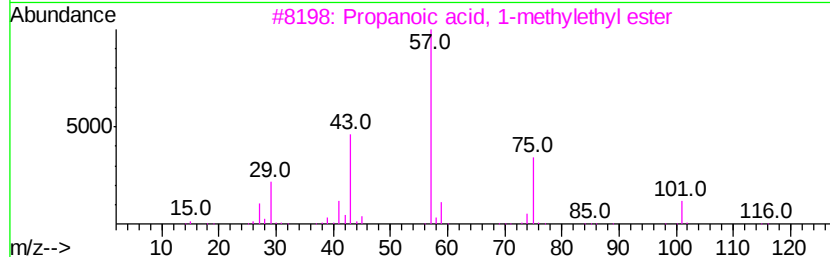
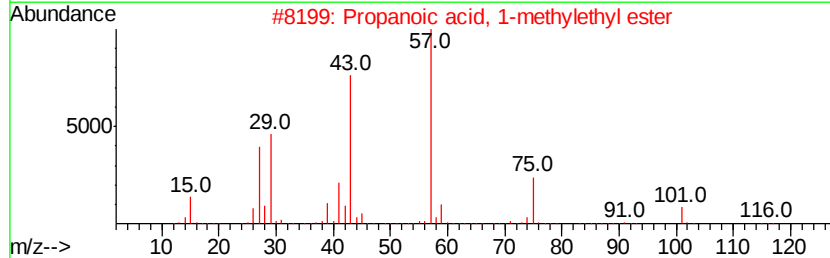
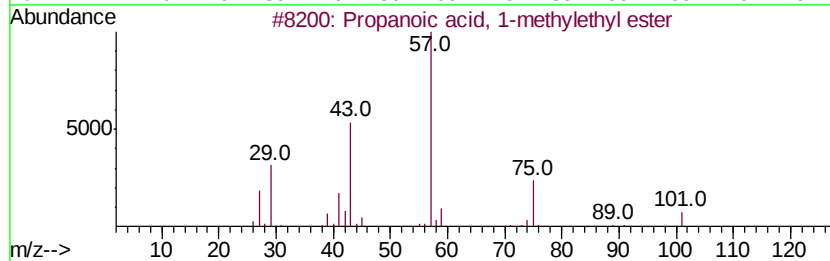
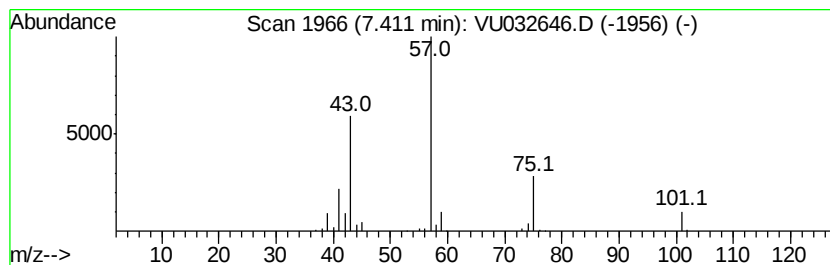
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Quant Title : VOC Analysis

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	13.39 ug/L	196922	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	59	
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40	



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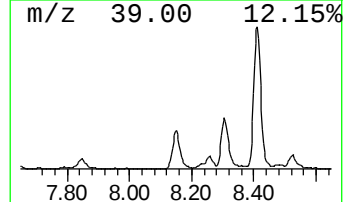
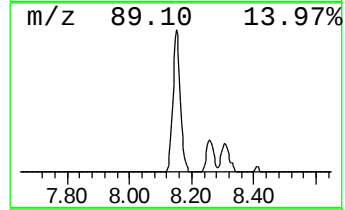
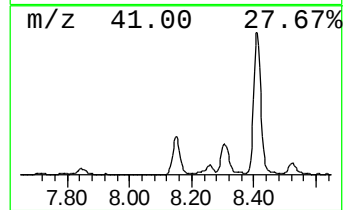
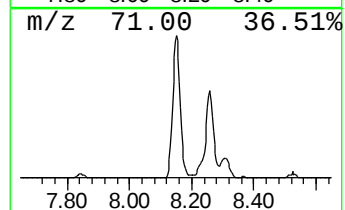
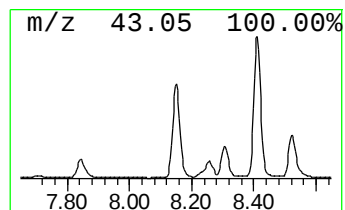
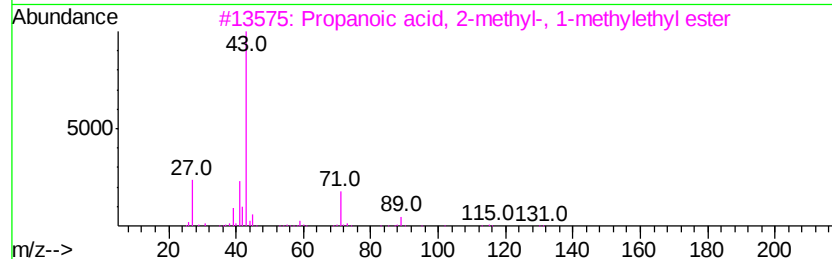
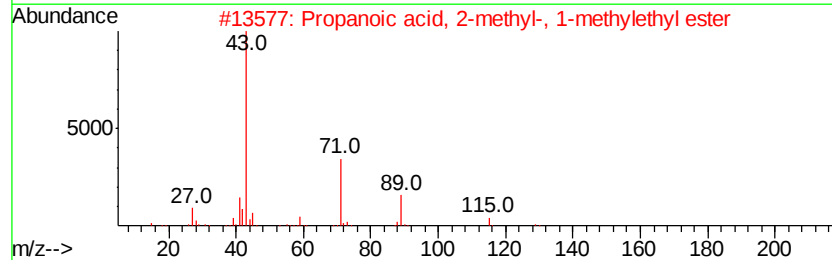
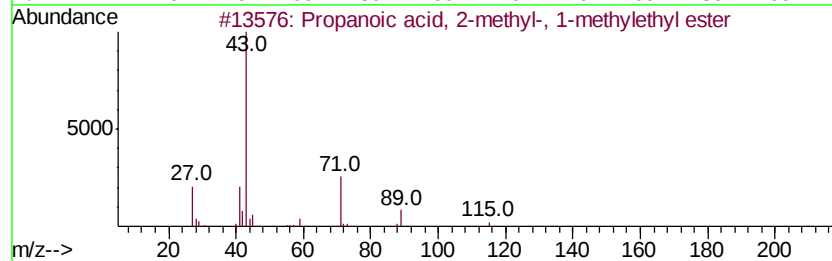
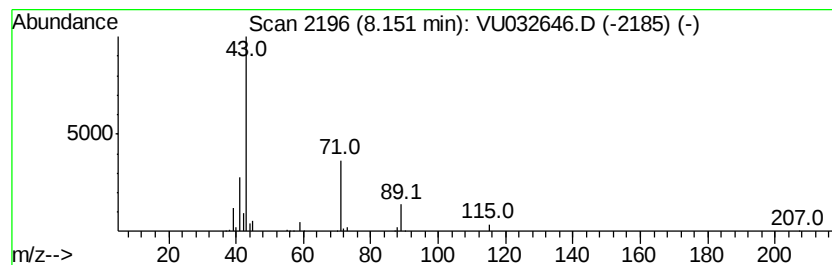
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Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.15	11.05 ug/L	106672	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	78
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032646.D
Acq On : 12 Jun 2019 13:02
Operator : JC/SP
Sample : K3286-05
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
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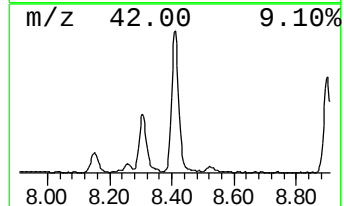
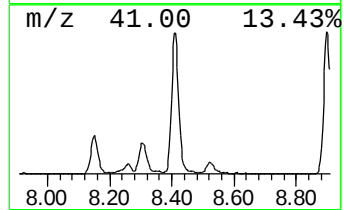
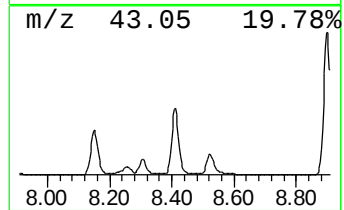
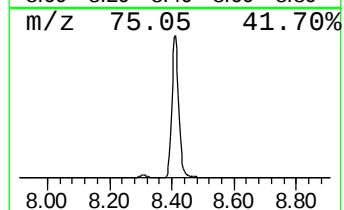
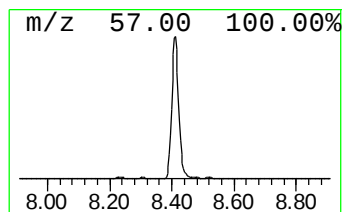
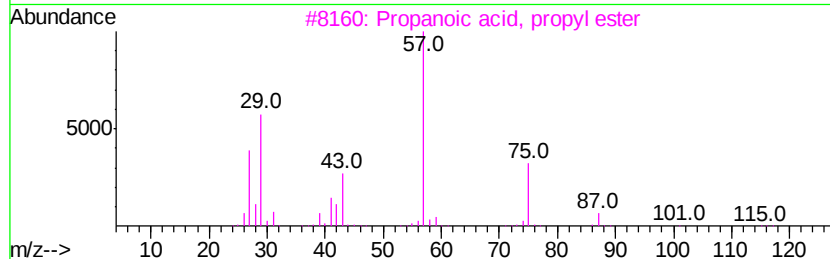
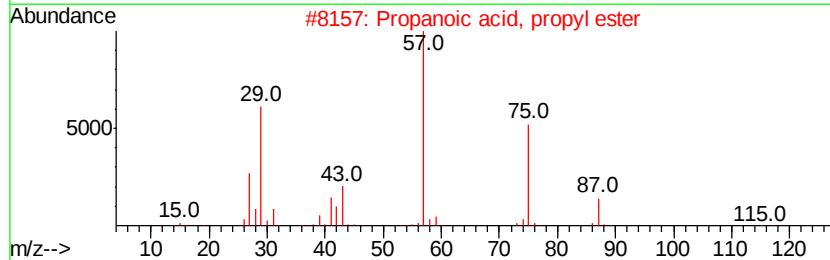
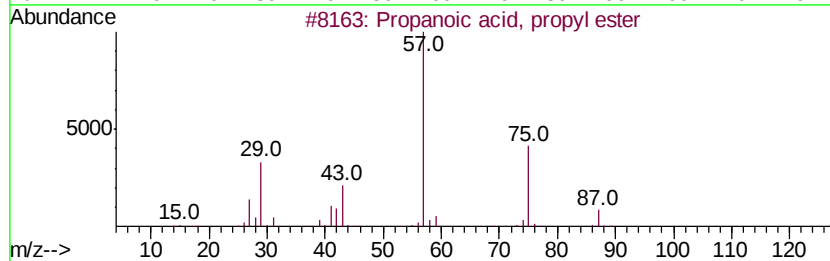
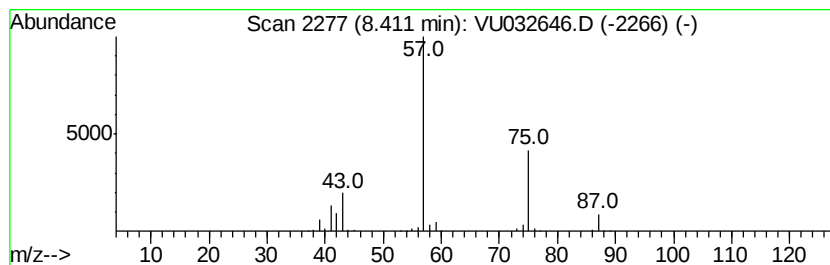
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	72.94 ug/L	703894	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\VU061219\
Data File : VU032646.D
Acq On : 12 Jun 2019 13:02
Operator : JC/SP
Sample : K3286-05
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW3

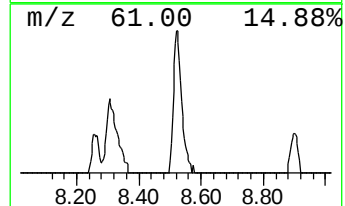
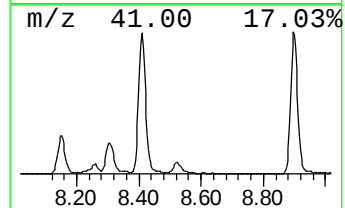
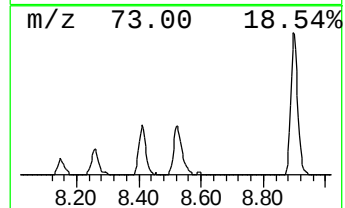
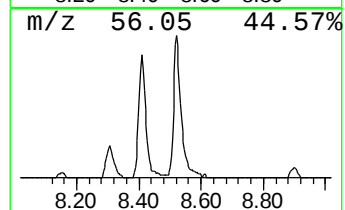
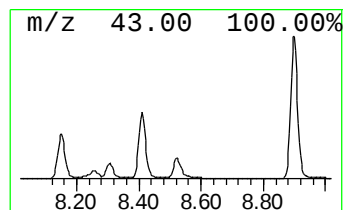
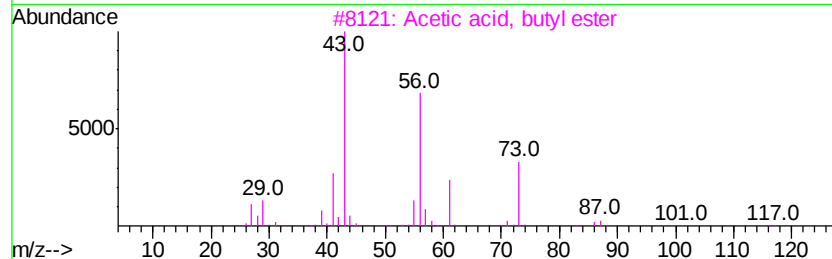
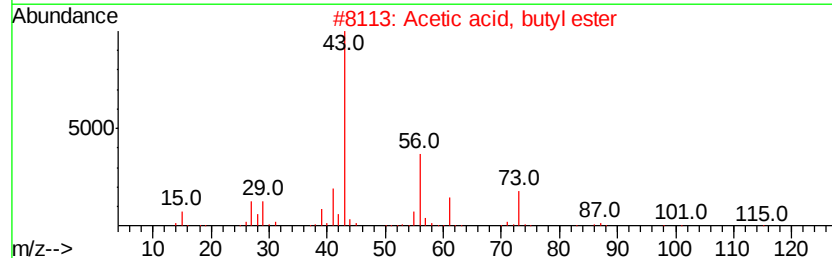
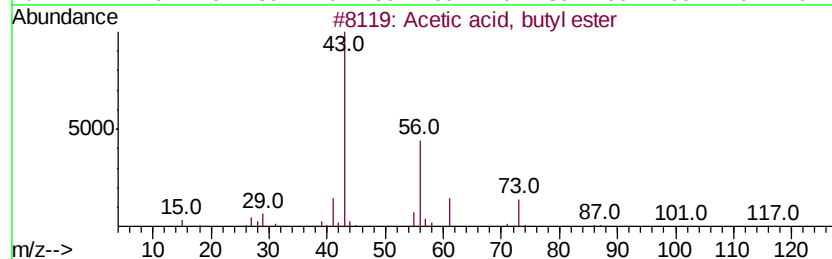
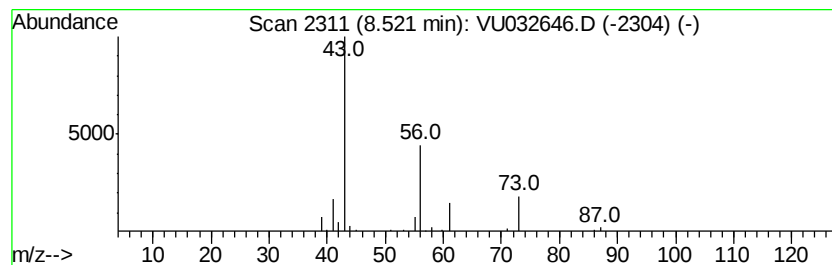
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Quant Title : VOC Analysis

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	5.26 ug/L	50768	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	83	
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72	
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64	
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032646.D
Acq On : 12 Jun 2019 13:02
Operator : JC/SP
Sample : K3286-05
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW3

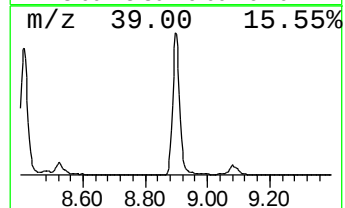
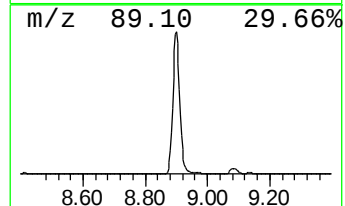
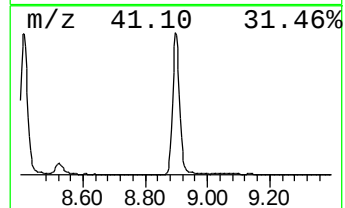
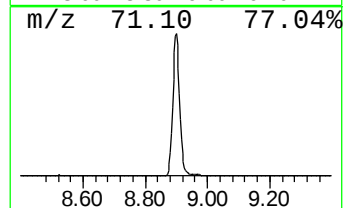
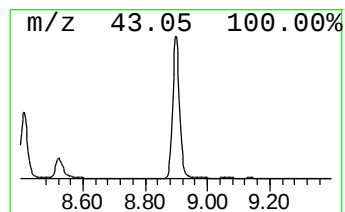
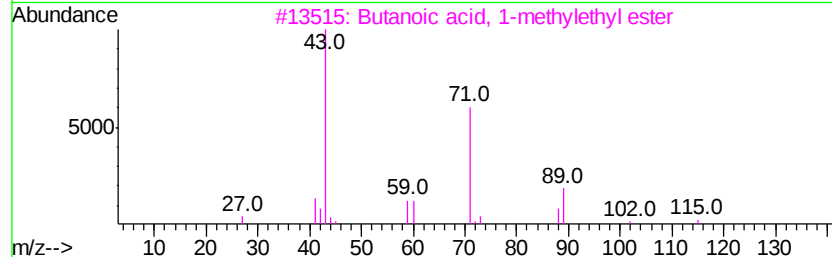
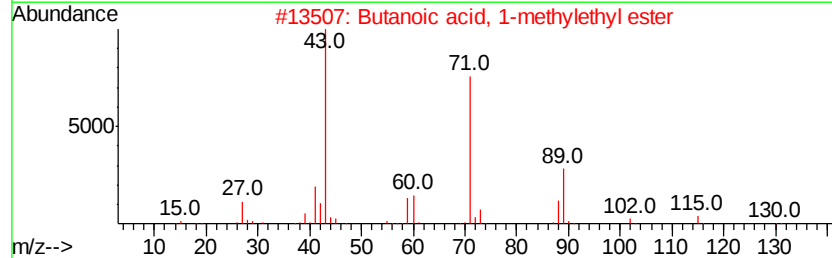
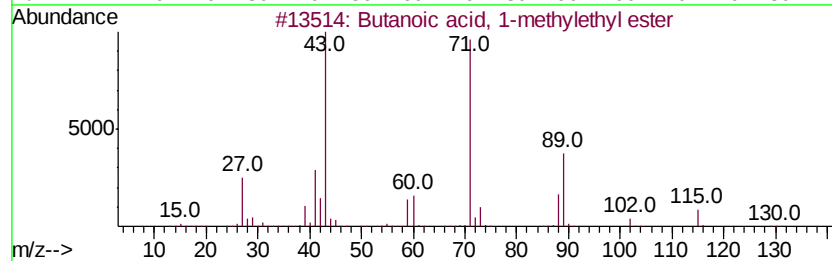
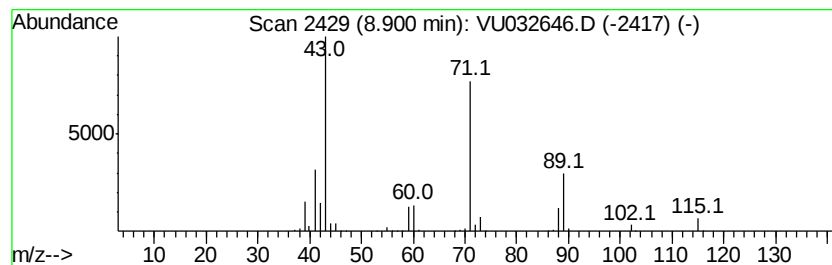
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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	49.71 ug/L	479702	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	90
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-, propy...	130	C7H14O2	000644-49-5	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061219\
Data File : VU032646.D
Acq On : 12 Jun 2019 13:02
Operator : JC/SP
Sample : K3286-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JW3

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	77.3	ug/L	1136500	1	5.88	735363	50.0
Propanoic acid, 1...	7.41	13.4	ug/L	196922	1	5.88	735363	50.0
Propanoic acid, 2...	8.15	11.1	ug/L	106672	2	9.08	482484	50.0
Propanoic acid, p...	8.41	72.9	ug/L	703894	2	9.08	482484	50.0
Acetic acid, buty...	8.52	5.3	ug/L	50768	2	9.08	482484	50.0
Butanoic acid, 1-...	8.90	49.7	ug/L	479702	2	9.08	482484	50.0