

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061319\
 Data File : VU032691.D
 Acq On : 13 Jun 2019 13:58
 Operator : JC/SP
 Sample : K3286-18
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JQ7

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	38	rVB2	3985	3678	0.35%	0.049%
2	1.395	89	95	108	rVB	70750	70153	6.62%	0.927%
3	1.678	175	183	198	rVB	60843	72884	6.87%	0.963%
4	2.267	356	366	377	rBV	117064	175396	16.54%	2.318%
5	2.694	490	499	510	rVB2	7242	11976	1.13%	0.158%
6	2.820	534	538	546	rVB3	295	403	0.04%	0.005%
7	2.910	563	566	570	rVB2	239	178	0.02%	0.002%
8	3.048	606	609	614	rBV2	171	154	0.01%	0.002%
9	3.257	670	674	677	rBV2	204	185	0.02%	0.002%
10	3.350	700	703	706	rBV2	201	145	0.01%	0.002%
11	3.421	717	725	733	rVV4	814	1817	0.17%	0.024%
12	3.807	841	845	850	rVV2	139	155	0.01%	0.002%
13	3.868	861	864	868	rVV2	196	146	0.01%	0.002%
14	3.945	885	888	892	rBV2	189	150	0.01%	0.002%
15	4.054	916	922	925	rBV2	201	254	0.02%	0.003%
16	4.170	942	958	982	rBV2	61038	157995	14.90%	2.088%
17	4.389	1024	1026	1031	rVB2	316	163	0.02%	0.002%
18	4.469	1048	1051	1054	rVB	256	145	0.01%	0.002%
19	4.546	1072	1075	1080	rVB2	295	269	0.03%	0.004%
20	4.572	1080	1083	1087	rBV2	198	166	0.02%	0.002%
21	4.643	1087	1105	1129	rBV	99883	232963	21.97%	3.079%
22	4.791	1148	1151	1154	rBV	217	153	0.01%	0.002%
23	4.807	1154	1156	1163	rVB2	443	460	0.04%	0.006%
24	5.141	1257	1260	1264	rVV2	218	206	0.02%	0.003%
25	5.173	1267	1270	1273	rVV2	239	166	0.02%	0.002%
26	5.334	1290	1320	1347	rBV2	190929	571144	53.87%	7.548%
27	5.556	1381	1389	1402	rVV3	3284	6848	0.65%	0.091%
28	5.797	1462	1464	1466	rBV	282	196	0.02%	0.003%
29	5.881	1472	1490	1517	rBV2	213668	448537	42.31%	5.928%
30	6.324	1615	1628	1649	rBV2	132469	262829	24.79%	3.473%
31	6.427	1653	1660	1671	rVB3	4952	8688	0.82%	0.115%
32	6.533	1686	1693	1700	rBV2	1652	2863	0.27%	0.038%
33	6.578	1702	1707	1715	rVV2	3007	4734	0.45%	0.063%
34	6.697	1732	1744	1781	rBV	587993	1060185	100.00%	14.011%

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 Title : VOC Analysis

35	7.170	1889	1891	1897	rVB3	378	307	0.03%	0.004%
36	7.225	1897	1908	1937	rBV	72051	134272	12.66%	1.775%
37	7.340	1943	1944	1948	rVB2	399	154	0.01%	0.002%
38	7.414	1956	1967	1996	rBV	104912	186136	17.56%	2.460%
39	7.559	2000	2012	2033	rBV	254952	447407	42.20%	5.913%
40	7.787	2077	2083	2084	rBV3	466	386	0.04%	0.005%
41	7.845	2091	2101	2125	rBV2	56881	103140	9.73%	1.363%
42	8.151	2182	2196	2214	rBV	58266	98682	9.31%	1.304%
43	8.257	2214	2229	2235	rVV2	25231	47425	4.47%	0.627%
44	8.305	2235	2244	2266	rVV	211536	383321	36.16%	5.066%
45	8.411	2266	2277	2303	rVV	426407	700363	66.06%	9.256%
46	8.521	2304	2311	2340	rVB	27882	52690	4.97%	0.696%
47	8.646	2347	2350	2351	rBV2	378	157	0.01%	0.002%
48	8.681	2357	2361	2365	rVB3	325	239	0.02%	0.003%
49	8.900	2417	2429	2464	rBV	289256	465658	43.92%	6.154%
50	9.083	2475	2486	2514	rBV	314244	524386	49.46%	6.930%
51	9.257	2539	2540	2546	rVB	335	191	0.02%	0.003%
52	9.286	2546	2549	2551	rBV	245	171	0.02%	0.002%
53	9.511	2614	2619	2623	rBV2	318	388	0.04%	0.005%
54	9.546	2627	2630	2633	rBV2	224	143	0.01%	0.002%
55	9.607	2639	2649	2661	rBV3	3330	6302	0.59%	0.083%
56	9.720	2682	2684	2687	rVB	337	172	0.02%	0.002%
57	9.765	2687	2698	2717	rBV	14594	25357	2.39%	0.335%
58	9.842	2720	2722	2726	rVB2	287	134	0.01%	0.002%
59	9.864	2726	2729	2734	rVB	318	240	0.02%	0.003%
60	9.893	2734	2738	2740	rBV3	294	294	0.03%	0.004%
61	9.951	2752	2756	2761	rVB3	250	201	0.02%	0.003%
62	9.993	2761	2769	2775	rBV3	327	606	0.06%	0.008%
63	10.041	2781	2784	2786	rBV2	333	197	0.02%	0.003%
64	10.154	2813	2819	2824	rBV	196	291	0.03%	0.004%
65	10.183	2824	2828	2831	rVB3	283	235	0.02%	0.003%
66	10.215	2836	2838	2843	rVB2	417	266	0.03%	0.004%
67	10.241	2843	2846	2848	rBV2	248	177	0.02%	0.002%
68	10.331	2872	2874	2881	rVB	361	238	0.02%	0.003%
69	10.379	2884	2889	2890	rBV2	225	168	0.02%	0.002%
70	10.427	2892	2904	2923	rVV	203928	328805	31.01%	4.345%
71	10.527	2932	2935	2938	rVB2	460	281	0.03%	0.004%

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72	10.588	2952	2954	2960	rVB2	220	161	0.02%	0.002%
73	11.109	3111	3116	3119	rVB	249	262	0.02%	0.003%
74	11.215	3146	3149	3151	rBV	206	154	0.01%	0.002%
75	11.254	3158	3161	3164	rVB	244	140	0.01%	0.002%
76	11.331	3183	3185	3192	rVB2	267	181	0.02%	0.002%
77	11.479	3219	3231	3254	rBV	312074	505217	47.65%	6.677%
78	11.717	3303	3305	3309	rVB2	245	144	0.01%	0.002%
79	11.797	3326	3330	3331	rBV2	266	139	0.01%	0.002%
80	11.855	3337	3348	3372	rBV	272228	449676	42.41%	5.943%
81	12.279	3476	3480	3487	rBV2	227	273	0.03%	0.004%
82	12.395	3513	3516	3522	rVB2	269	211	0.02%	0.003%
83	12.421	3522	3524	3531	rBV2	262	241	0.02%	0.003%
84	12.498	3545	3548	3550	rBV2	289	192	0.02%	0.003%
85	12.643	3590	3593	3596	rBV	301	214	0.02%	0.003%
86	12.794	3637	3640	3645	rBV2	256	297	0.03%	0.004%
87	12.884	3665	3668	3670	rBV2	214	146	0.01%	0.002%
88	13.096	3732	3734	3739	rVB	259	196	0.02%	0.003%
89	13.128	3739	3744	3748	rBV2	376	376	0.04%	0.005%
90	13.205	3765	3768	3776	rVB2	312	332	0.03%	0.004%
91	13.241	3776	3779	3782	rBV	215	176	0.02%	0.002%
92	13.601	3889	3891	3898	rVB2	232	184	0.02%	0.002%
93	13.861	3968	3972	3973	rBV	251	175	0.02%	0.002%
94	13.906	3983	3986	3992	rVB2	485	451	0.04%	0.006%
95	13.938	3992	3996	3997	rBV2	331	213	0.02%	0.003%
96	13.999	4012	4015	4017	rBV2	241	158	0.01%	0.002%
97	14.250	4091	4093	4096	rBV	247	169	0.02%	0.002%
98	14.527	4176	4179	4181	rBV2	276	182	0.02%	0.002%
99	14.697	4229	4232	4235	rBV3	228	186	0.02%	0.002%
100	15.205	4387	4390	4393	rVB	463	285	0.03%	0.004%

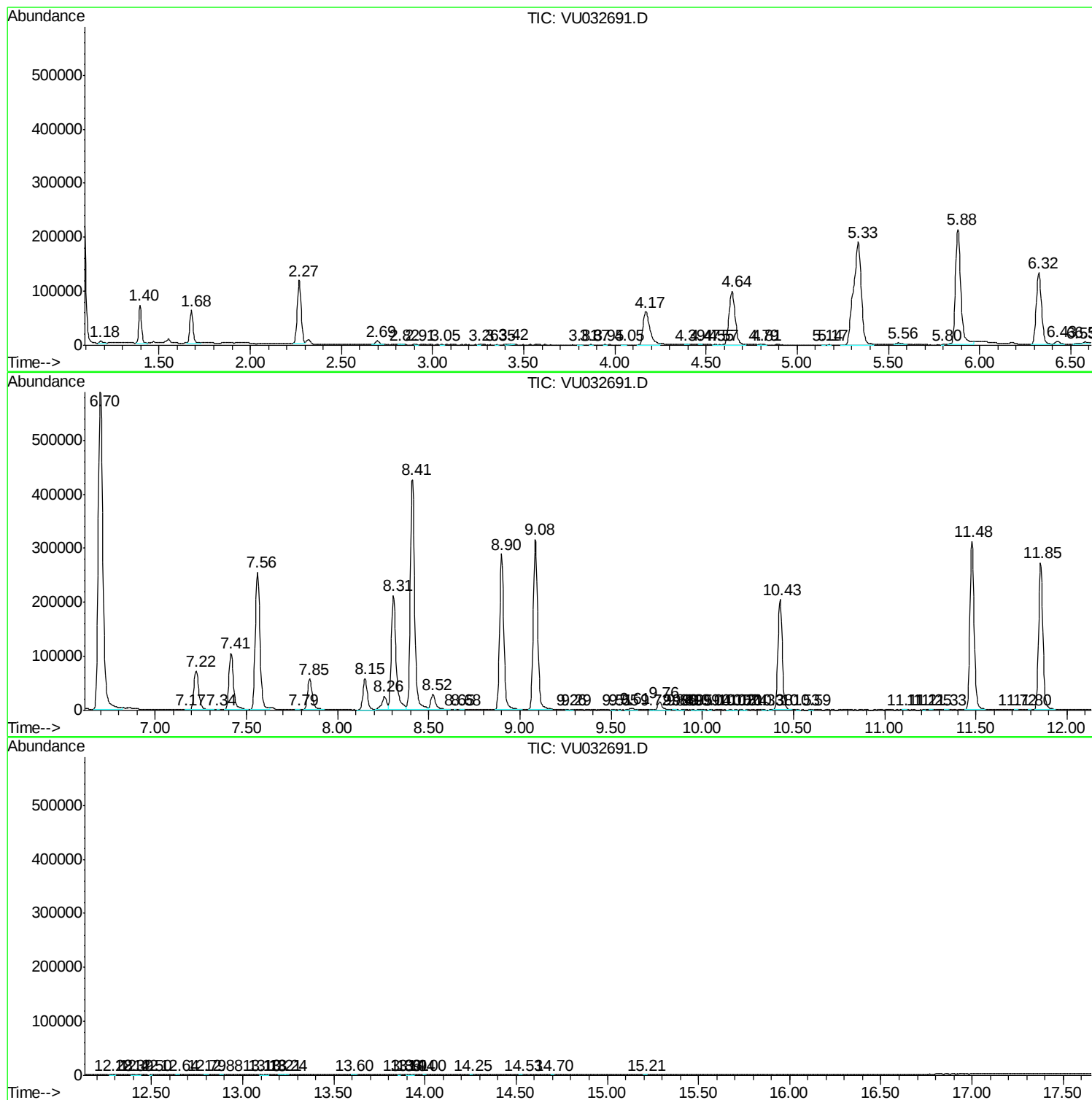
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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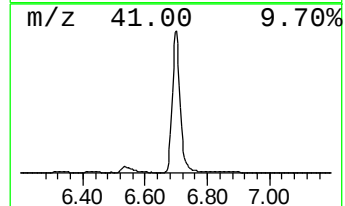
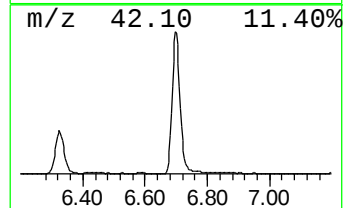
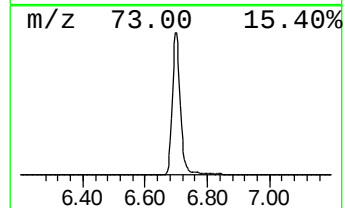
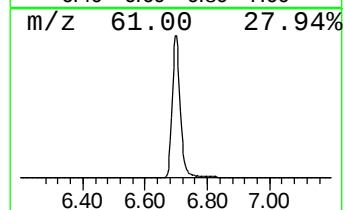
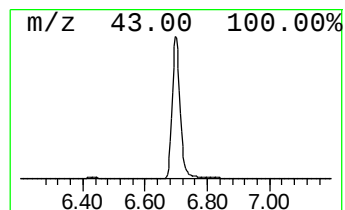
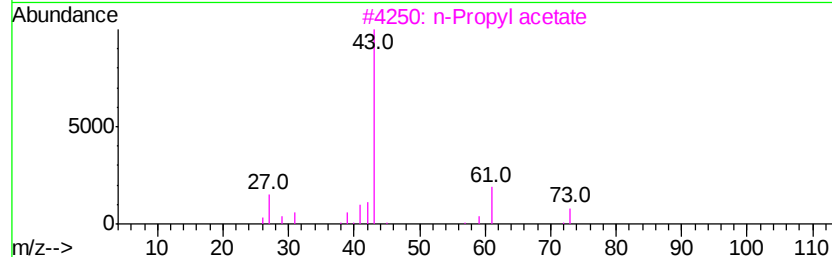
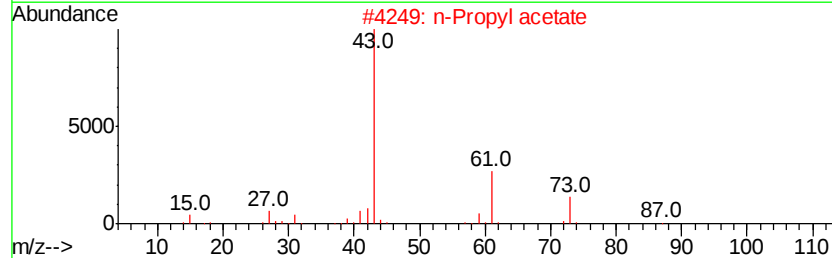
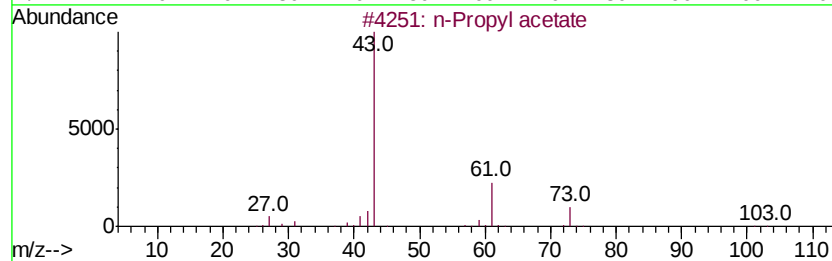
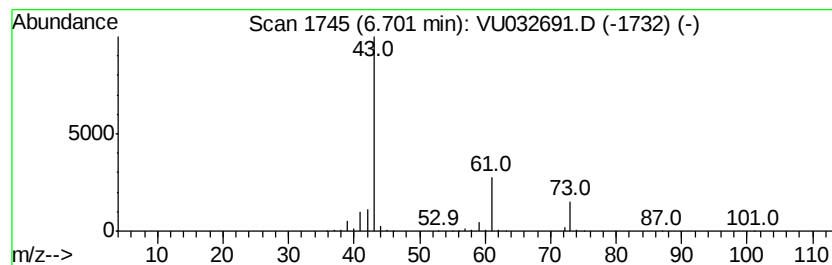
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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	118.18 ug/L	1060190	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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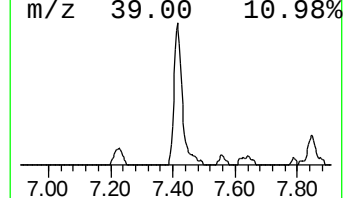
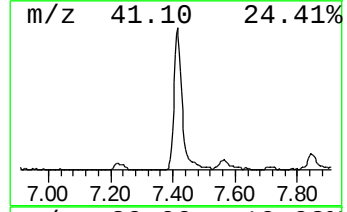
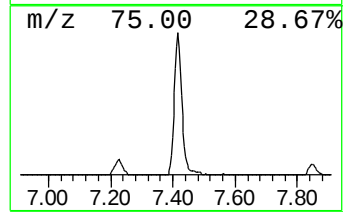
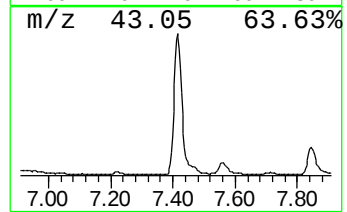
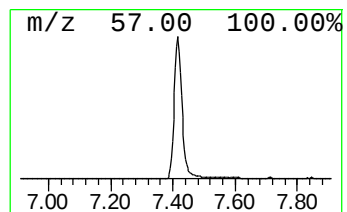
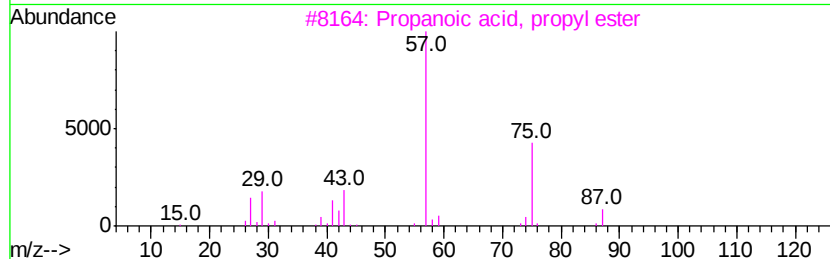
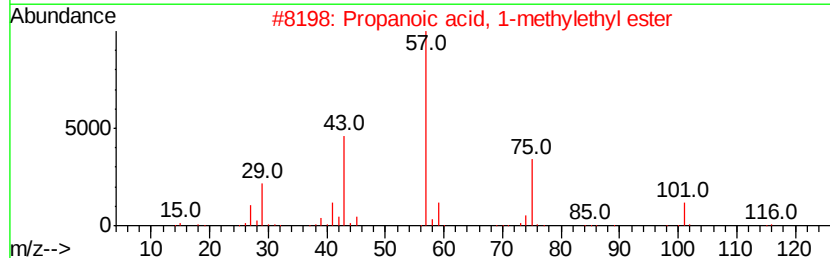
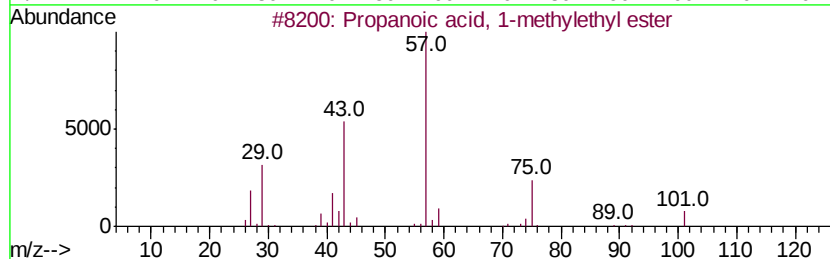
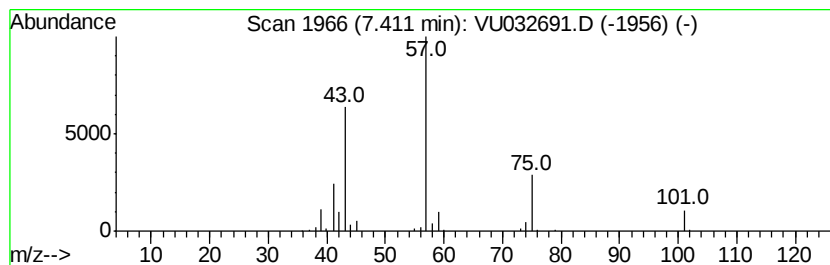
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Quant Title : VOC Analysis

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	20.75 ug/L	186136	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, propyl ester	116	C6H12O2	000106-36-5	59
4		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



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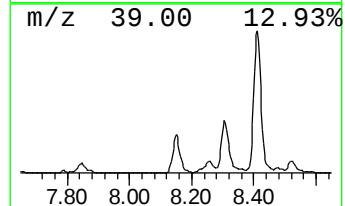
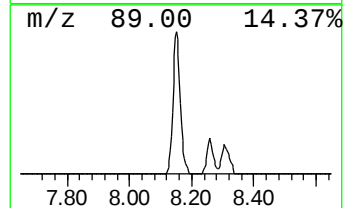
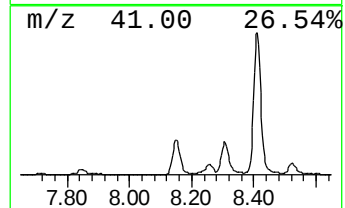
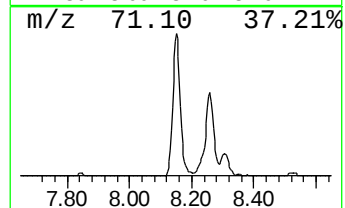
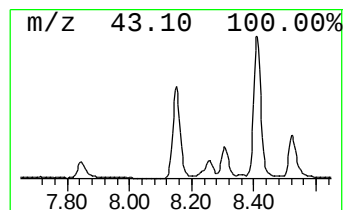
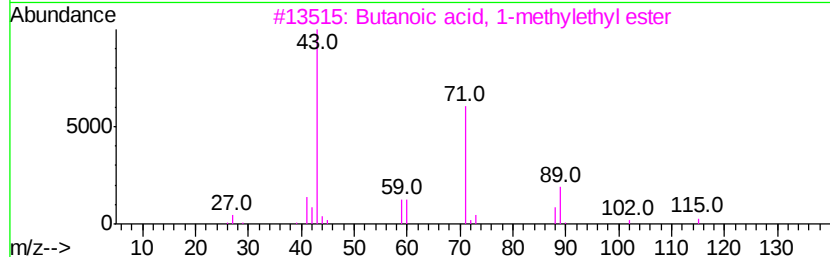
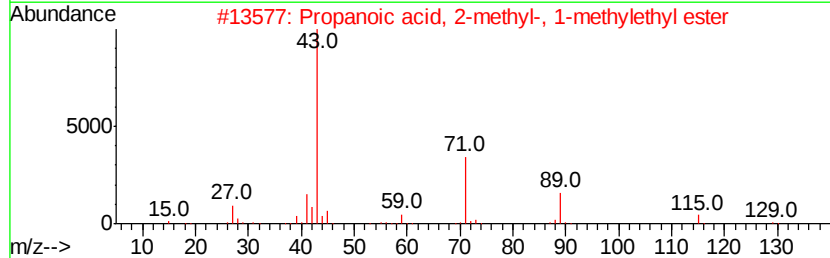
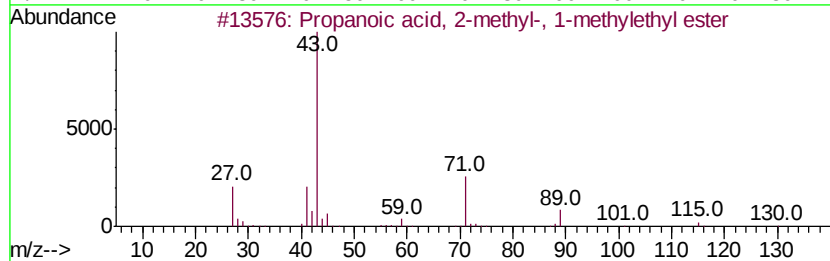
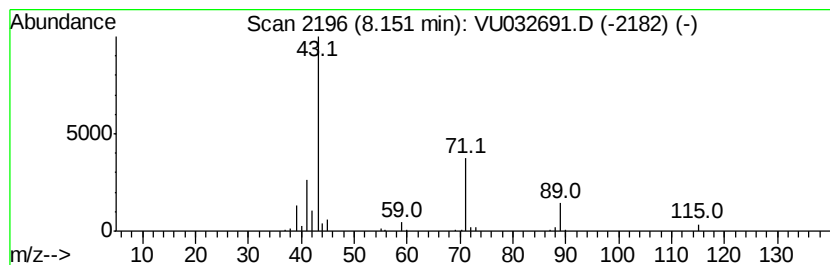
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.41 ug/L	98682	Chlorobenzene-d5	9.09

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	78
3			Butanoic acid, 1-methyl-ethyl ester	130	C7H14O2	000638-11-9	72
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	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061319\
Data File : VU032691.D
Acq On : 13 Jun 2019 13:58
Operator : JC/SP
Sample : K3286-18
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
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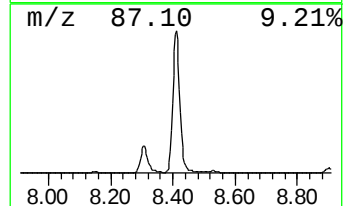
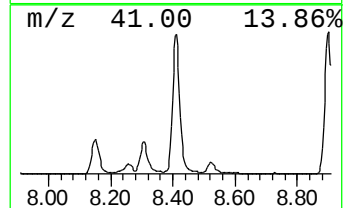
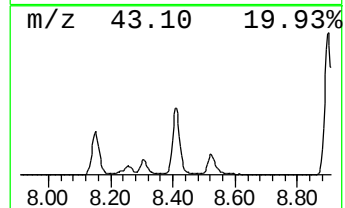
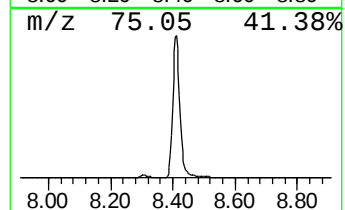
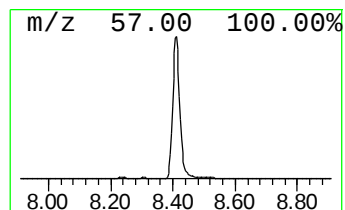
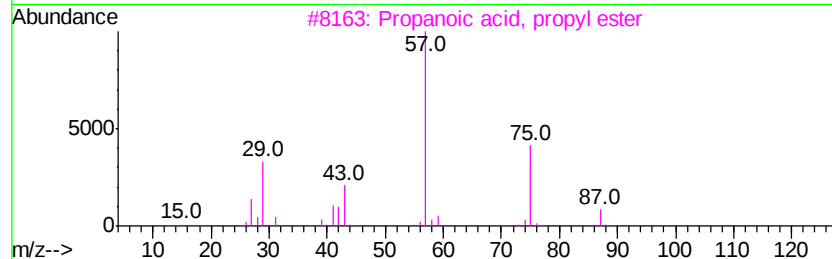
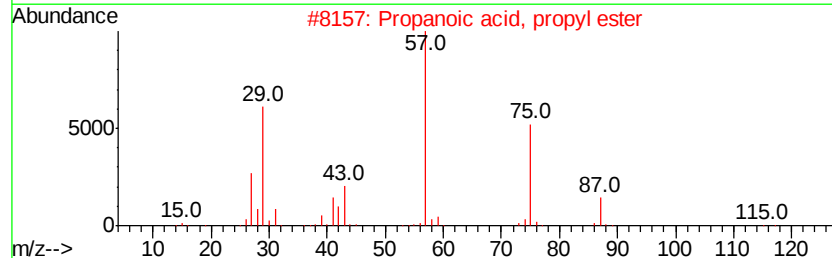
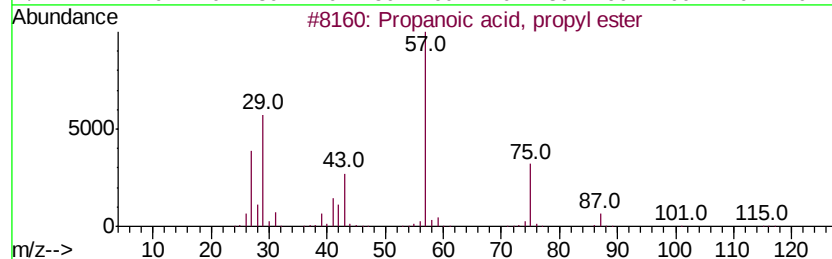
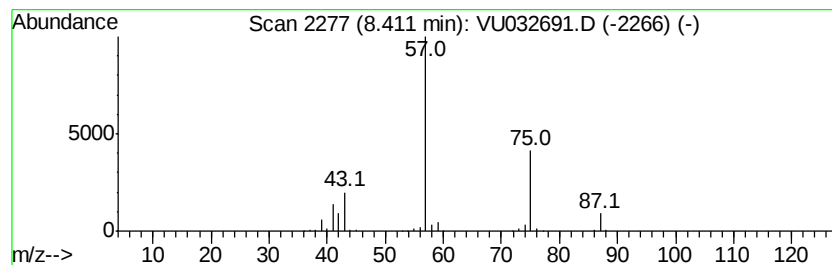
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Quant Title : VOC Analysis

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	66.78 ug/L	700363	Chlorobenzene-d5	9.09

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\VU061319\
Data File : VU032691.D
Acq On : 13 Jun 2019 13:58
Operator : JC/SP
Sample : K3286-18
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JQ7

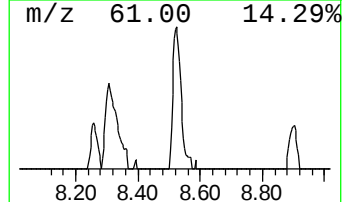
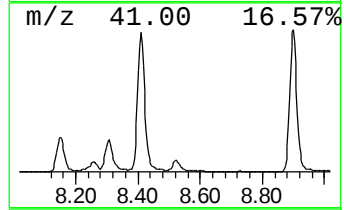
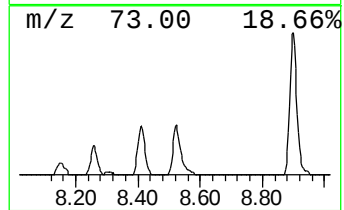
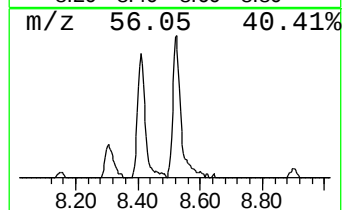
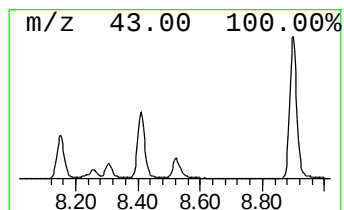
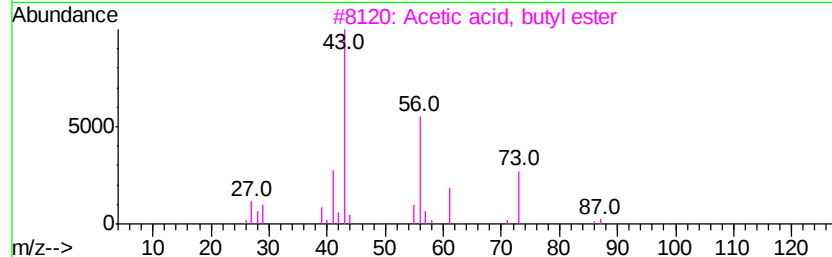
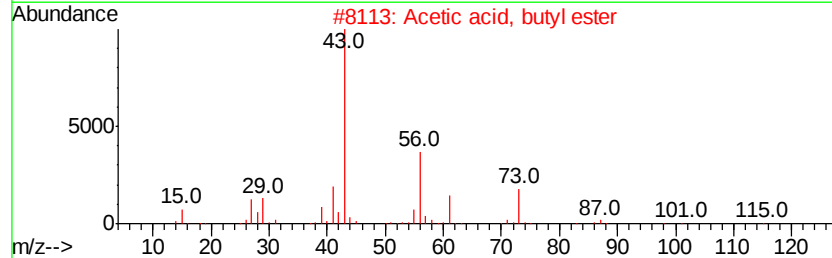
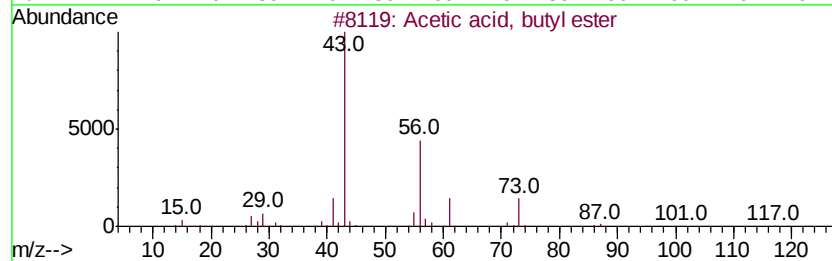
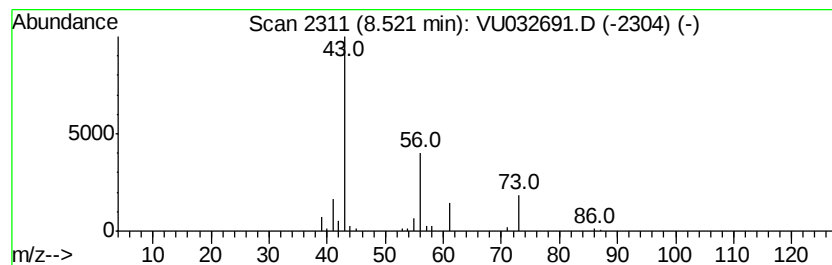
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Quant Title : VOC Analysis

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	5.02 ug/L	52690	Chlorobenzene-d5	9.09

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	56		
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	38		



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061319\
Data File : VU032691.D
Acq On : 13 Jun 2019 13:58
Operator : JC/SP
Sample : K3286-18
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JQ7

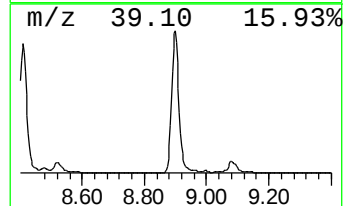
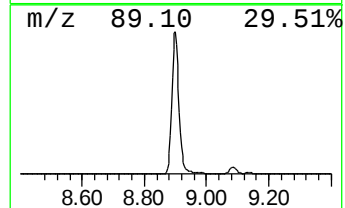
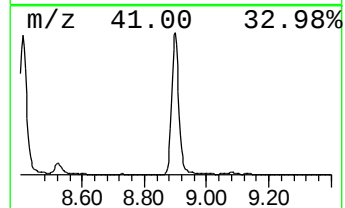
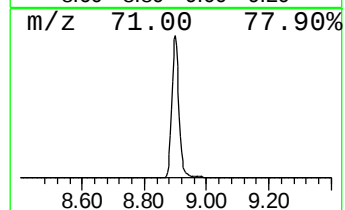
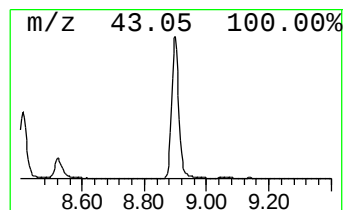
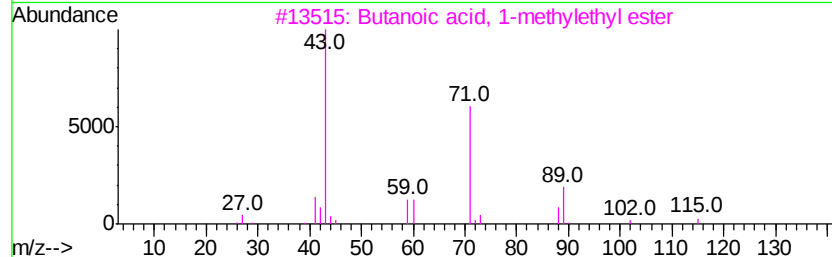
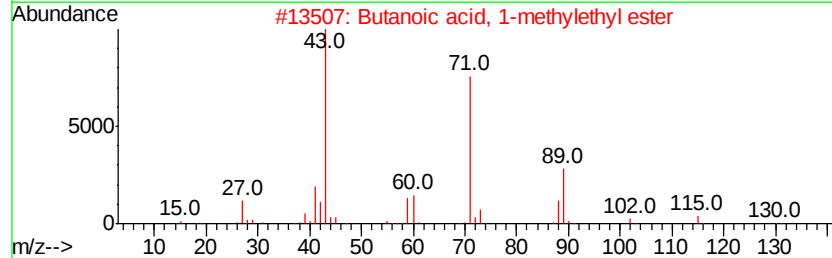
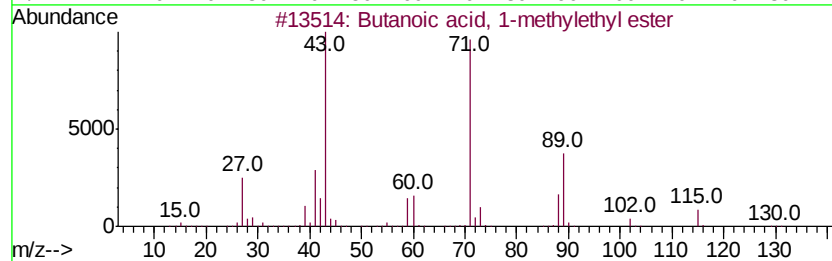
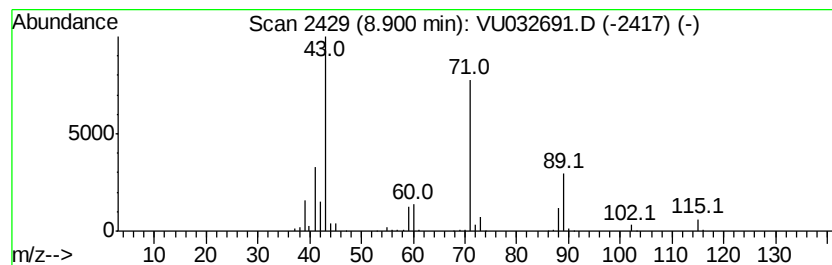
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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	44.40 ug/L	465658	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	72
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032691.D
Acq On : 13 Jun 2019 13:58
Operator : JC/SP
Sample : K3286-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JQ7

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	118.2	ug/L	1060190	1	5.88	448537	50.0
Propanoic acid, 1...	7.41	20.8	ug/L	186136	1	5.88	448537	50.0
Propanoic acid, 2...	8.15	9.4	ug/L	98682	2	9.09	524386	50.0
Propanoic acid, p...	8.41	66.8	ug/L	700363	2	9.09	524386	50.0
Acetic acid, buty...	8.52	5.0	ug/L	52690	2	9.09	524386	50.0
Butanoic acid, 1-...	8.90	44.4	ug/L	465658	2	9.09	524386	50.0