

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
 Data File : VU032824.D
 Acq On : 18 Jun 2019 15:09
 Operator : JC/SP
 Sample : K3379-03
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JT4

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\SOMULM061719WMA.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	35	rVB	5883	5269	0.38%	0.049%
2	1.396	88	95	109	rVB	123622	123935	9.03%	1.149%
3	1.470	112	118	128	rVB	18133	19841	1.45%	0.184%
4	1.675	175	182	194	rVB	96040	115114	8.39%	1.067%
5	2.267	355	366	375	rBV	200523	305271	22.25%	2.829%
6	2.315	376	381	399	rVB	25108	40772	2.97%	0.378%
7	2.441	416	420	421	rBV4	606	426	0.03%	0.004%
8	2.569	455	460	462	rBV3	351	337	0.02%	0.003%
9	2.617	466	475	485	rVV	2132	3811	0.28%	0.035%
10	2.695	490	499	514	rVB2	7643	13515	0.99%	0.125%
11	2.778	522	525	528	rBV2	355	252	0.02%	0.002%
12	2.820	533	538	544	rBV4	653	608	0.04%	0.006%
13	2.939	571	575	578	rBV2	375	392	0.03%	0.004%
14	2.958	579	581	585	rVV3	293	247	0.02%	0.002%
15	2.978	585	587	592	rVV2	339	280	0.02%	0.003%
16	3.074	615	617	621	rBV2	341	322	0.02%	0.003%
17	3.129	632	634	638	rBV2	333	286	0.02%	0.003%
18	3.177	641	649	663	rVV7	2448	5402	0.39%	0.050%
19	3.315	689	692	696	rVB2	490	371	0.03%	0.003%
20	3.386	710	714	715	rBV2	358	261	0.02%	0.002%
21	3.405	716	720	721	rBV2	529	291	0.02%	0.003%
22	3.418	721	724	728	rVB5	521	456	0.03%	0.004%
23	3.592	776	778	781	rBV3	368	235	0.02%	0.002%
24	3.659	797	799	802	rVB2	645	381	0.03%	0.004%
25	3.707	812	814	822	rVV2	502	609	0.04%	0.006%
26	3.749	826	827	832	rVB2	429	283	0.02%	0.003%
27	3.807	842	845	850	rVB2	399	326	0.02%	0.003%
28	3.904	867	875	879	rBV3	495	620	0.05%	0.006%
29	3.990	897	902	906	rBV2	412	428	0.03%	0.004%
30	4.080	927	930	938	rBV2	314	365	0.03%	0.003%
31	4.167	945	957	984	rBV	88284	235236	17.15%	2.180%
32	4.415	1032	1034	1043	rVB3	571	630	0.05%	0.006%
33	4.518	1062	1066	1072	rBV2	612	505	0.04%	0.005%
34	4.640	1084	1104	1133	rBV	155461	363284	26.48%	3.367%

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 Title : VOC Analysis

35	5.331	1295	1319	1347	rBV2	306882	905318	65.99%	8.390%
36	5.550	1377	1387	1404	rVB3	6162	13055	0.95%	0.121%
37	5.740	1442	1446	1451	rBV2	549	564	0.04%	0.005%
38	5.881	1476	1490	1514	rBV	279653	548523	39.98%	5.083%
39	6.325	1614	1628	1649	rVV	206416	413332	30.13%	3.831%
40	6.418	1650	1657	1682	rVB2	7358	17356	1.27%	0.161%
41	6.531	1685	1692	1697	rBV2	2929	4329	0.32%	0.040%
42	6.575	1700	1706	1712	rBV	4951	6333	0.46%	0.059%
43	6.698	1731	1744	1774	rBV	772683	1371985	100.00%	12.715%
44	7.000	1834	1838	1840	rBV3	730	582	0.04%	0.005%
45	7.058	1851	1856	1860	rVB3	466	499	0.04%	0.005%
46	7.222	1890	1907	1929	rBV	108903	193267	14.09%	1.791%
47	7.334	1940	1942	1949	rVB5	597	601	0.04%	0.006%
48	7.415	1949	1967	1992	rBV	144484	250841	18.28%	2.325%
49	7.502	1992	1994	1996	rBV2	418	240	0.02%	0.002%
50	7.559	1999	2012	2029	rBV	427616	742233	54.10%	6.879%
51	7.768	2072	2077	2086	rVB7	1052	1490	0.11%	0.014%
52	7.842	2088	2100	2122	rBV2	89554	155719	11.35%	1.443%
53	8.003	2148	2150	2157	rVB3	804	609	0.04%	0.006%
54	8.148	2184	2195	2210	rVV	78527	130089	9.48%	1.206%
55	8.225	2212	2219	2221	rVV2	9058	10776	0.79%	0.100%
56	8.257	2223	2229	2235	rVV2	31518	49319	3.59%	0.457%
57	8.305	2235	2244	2265	rVV	304297	525614	38.31%	4.871%
58	8.408	2266	2276	2302	rVV	576488	912125	66.48%	8.453%
59	8.521	2302	2311	2326	rVB	34812	59161	4.31%	0.548%
60	8.775	2385	2390	2393	rBV3	382	349	0.03%	0.003%
61	8.897	2416	2428	2453	rBV	384525	605122	44.11%	5.608%
62	9.083	2465	2486	2510	rBV	424841	706899	51.52%	6.551%
63	9.299	2551	2553	2558	rVB3	576	374	0.03%	0.003%
64	9.325	2558	2561	2566	rBV5	445	345	0.03%	0.003%
65	9.450	2596	2600	2606	rBV3	472	556	0.04%	0.005%
66	9.601	2636	2647	2661	rBV2	5836	10415	0.76%	0.097%
67	9.762	2686	2697	2708	rBV	20604	33118	2.41%	0.307%
68	9.932	2745	2750	2754	rVB3	375	412	0.03%	0.004%
69	10.038	2779	2783	2786	rBV2	339	268	0.02%	0.002%
70	10.099	2792	2802	2806	rBV4	860	1488	0.11%	0.014%
71	10.186	2825	2829	2831	rBV2	383	278	0.02%	0.003%

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72	10.260	2848	2852	2858	rVB4	243	270	0.02%	0.003%
73	10.308	2865	2867	2873	rVB3	442	341	0.02%	0.003%
74	10.344	2875	2878	2886	rVB2	198	243	0.02%	0.002%
75	10.424	2891	2903	2927	rVB	300347	482061	35.14%	4.467%
76	10.508	2927	2929	2934	rVB3	576	380	0.03%	0.004%
77	10.534	2934	2937	2938	rBV2	471	232	0.02%	0.002%
78	10.669	2975	2979	2984	rBV2	513	365	0.03%	0.003%
79	10.829	3026	3029	3034	rVB3	378	314	0.02%	0.003%
80	10.897	3044	3050	3053	rVV3	467	474	0.03%	0.004%
81	10.942	3059	3064	3070	rVB2	305	332	0.02%	0.003%
82	11.006	3081	3084	3087	rBV2	372	302	0.02%	0.003%
83	11.087	3106	3109	3118	rVB2	455	499	0.04%	0.005%
84	11.177	3134	3137	3143	rVB3	536	420	0.03%	0.004%
85	11.251	3156	3160	3164	rVB3	394	316	0.02%	0.003%
86	11.318	3176	3181	3184	rBV2	331	387	0.03%	0.004%
87	11.479	3218	3231	3255	rBV	431222	690737	50.35%	6.401%
88	11.662	3285	3288	3291	rBV3	407	363	0.03%	0.003%
89	11.794	3325	3329	3334	rVB4	609	530	0.04%	0.005%
90	11.855	3334	3348	3366	rBV	419505	694421	50.61%	6.435%
91	12.058	3409	3411	3414	rBV	455	244	0.02%	0.002%
92	12.170	3440	3446	3449	rBV3	651	625	0.05%	0.006%
93	12.353	3500	3503	3508	rVB2	380	242	0.02%	0.002%
94	12.652	3593	3596	3600	rVB3	464	324	0.02%	0.003%
95	12.685	3600	3606	3612	rBV3	491	566	0.04%	0.005%
96	12.714	3613	3615	3619	rBV2	424	346	0.03%	0.003%
97	12.759	3626	3629	3636	rVB2	351	288	0.02%	0.003%
98	12.823	3646	3649	3652	rBV2	309	270	0.02%	0.003%
99	13.749	3934	3937	3938	rBV	638	317	0.02%	0.003%
100	14.485	4163	4166	4168	rBV3	516	369	0.03%	0.003%

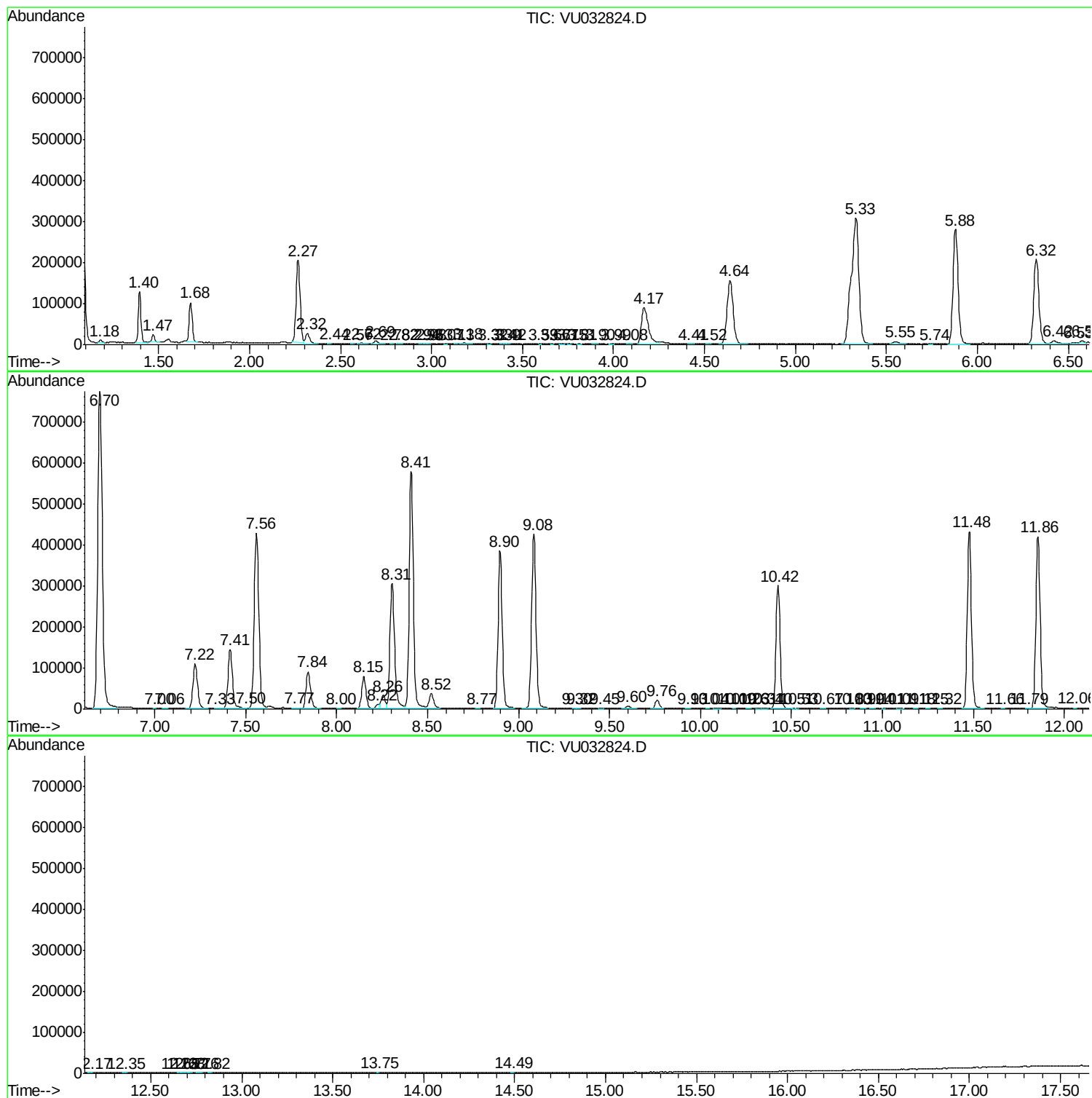
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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



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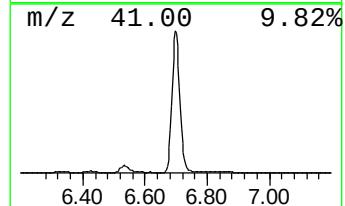
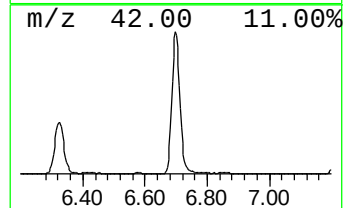
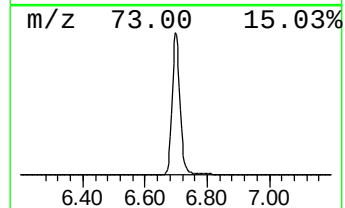
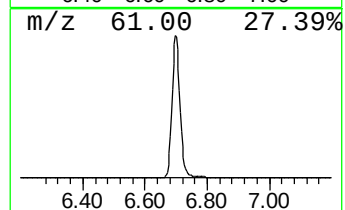
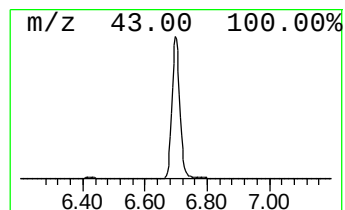
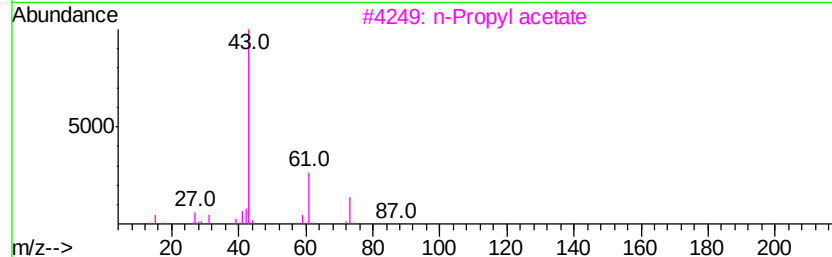
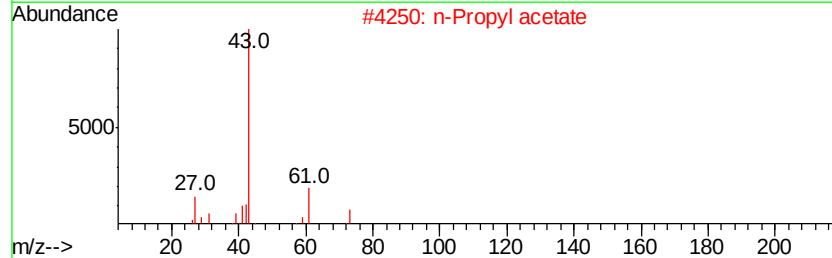
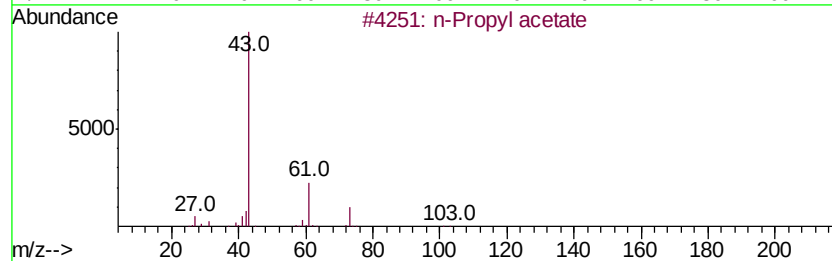
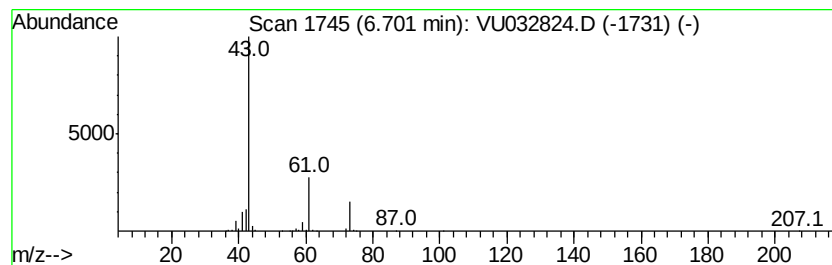
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	125.06 ug/L	1371990	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	9



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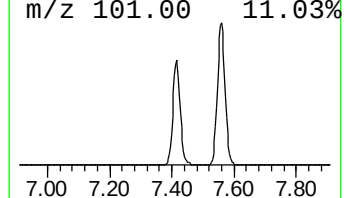
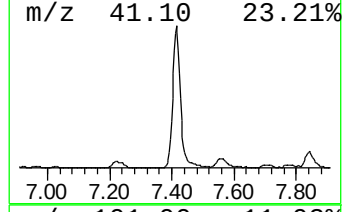
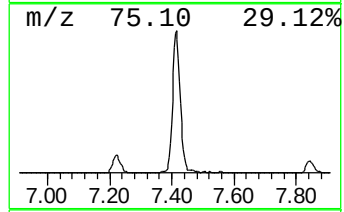
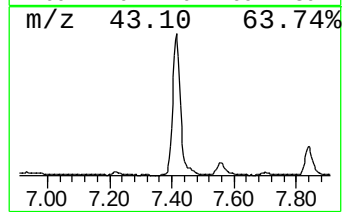
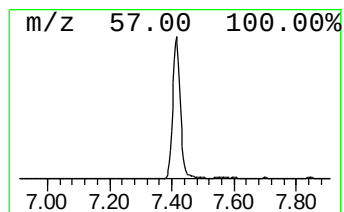
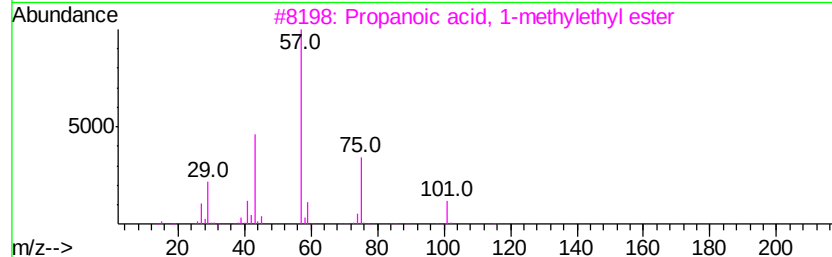
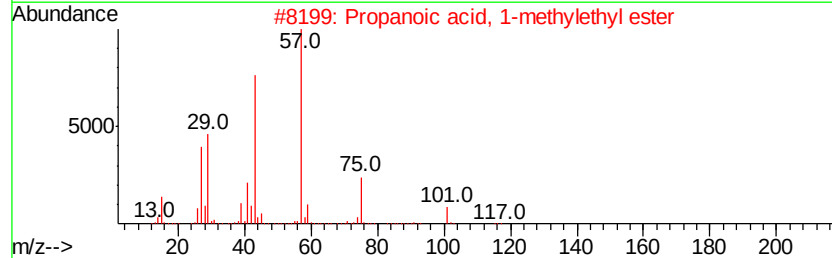
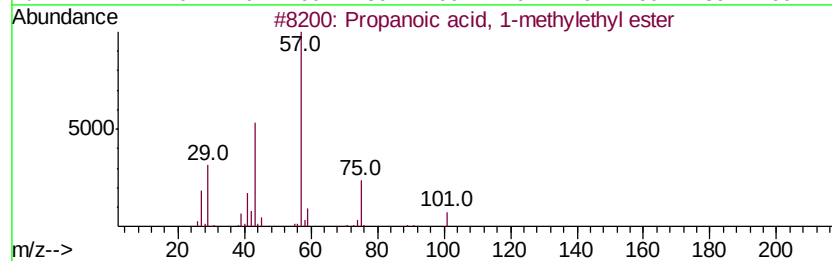
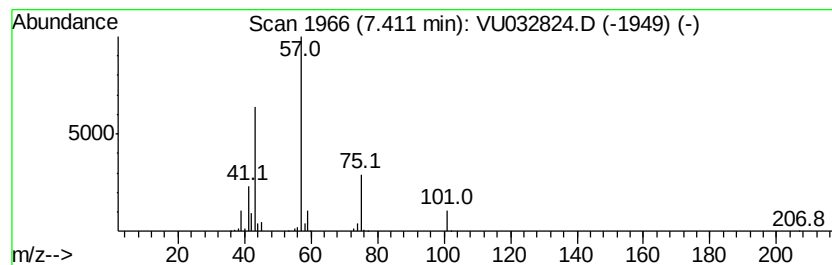
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Quant Title : VOC Analysis

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	22.87 ug/L	250841	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	83
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
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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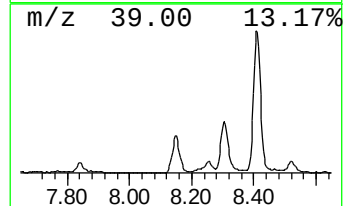
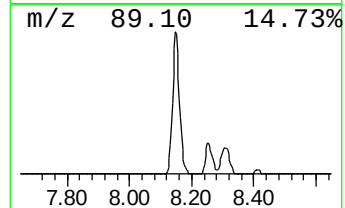
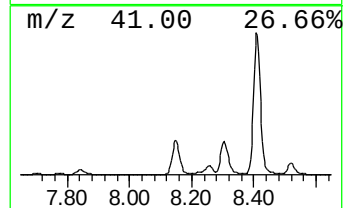
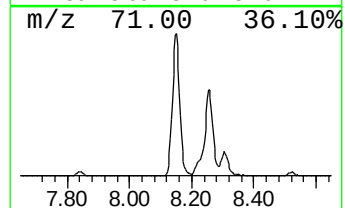
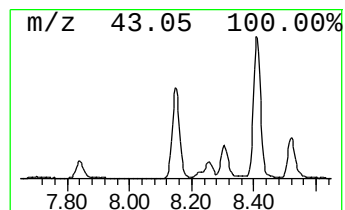
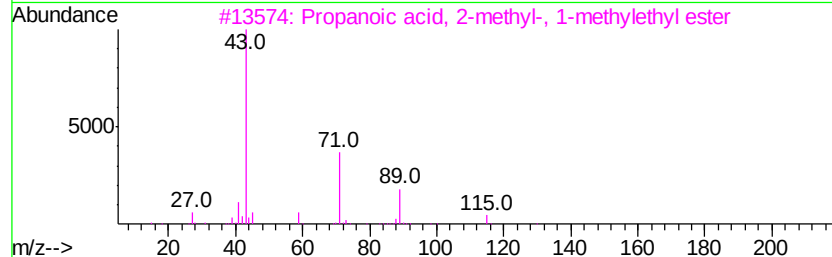
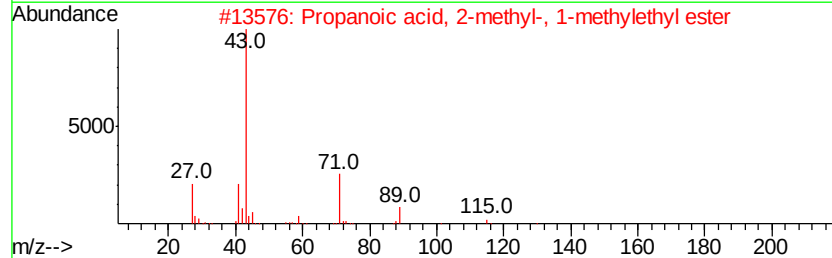
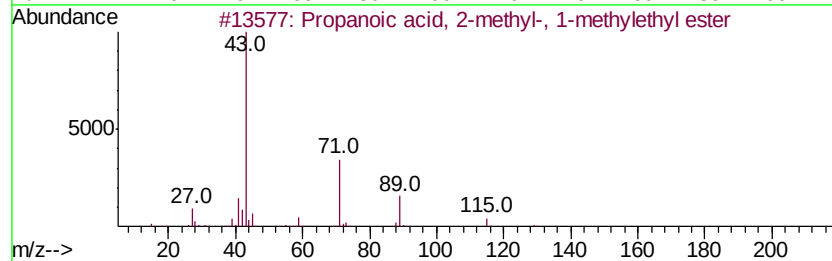
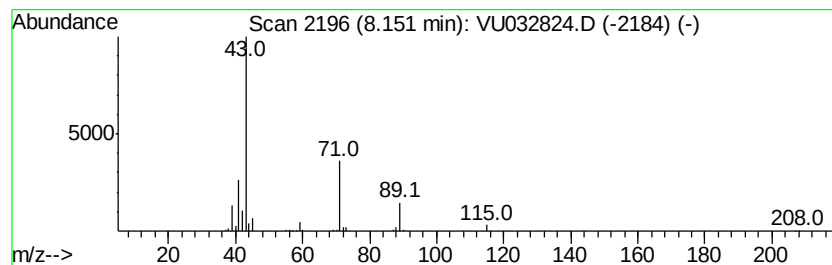
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Quant Title : VOC Analysis

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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	9.20 ug/L	130089	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	72
4		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032824.D
Acq On : 18 Jun 2019 15:09
Operator : JC/SP
Sample : K3379-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JT4

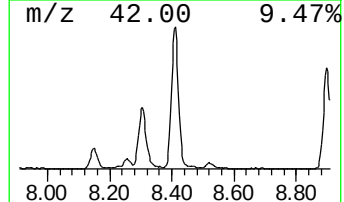
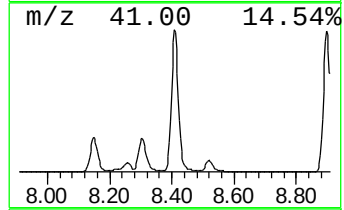
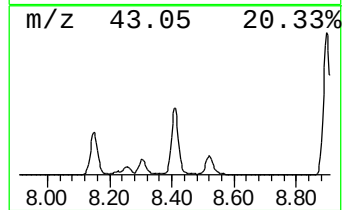
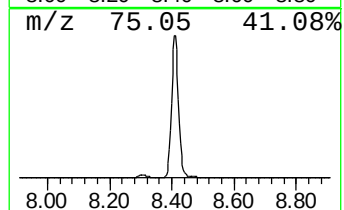
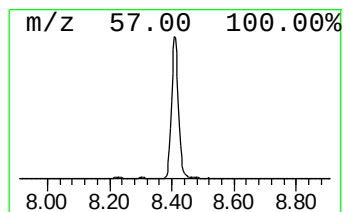
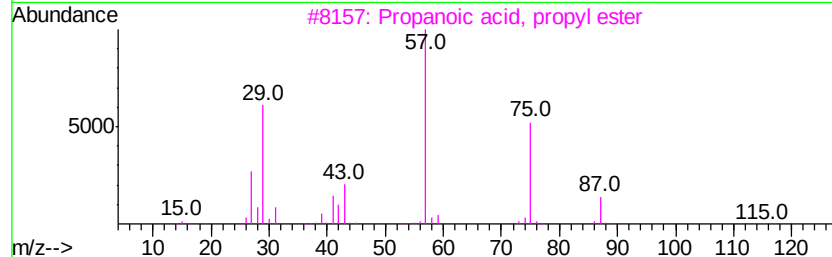
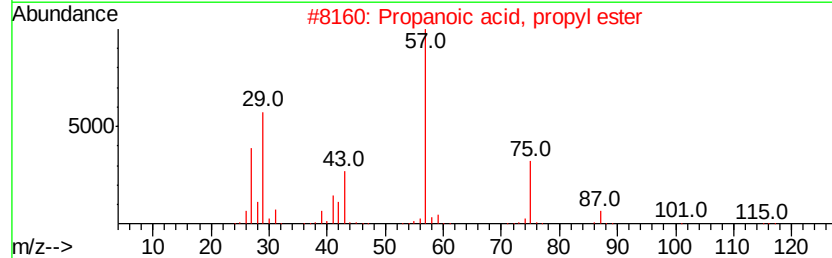
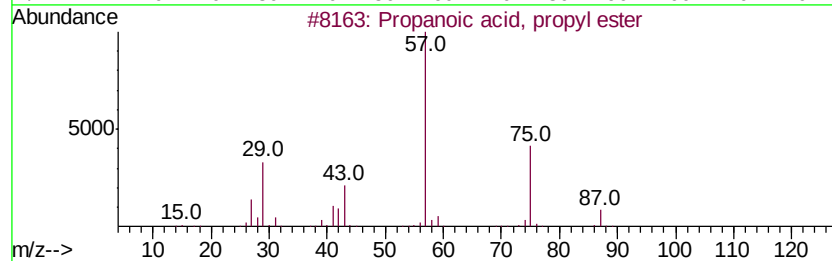
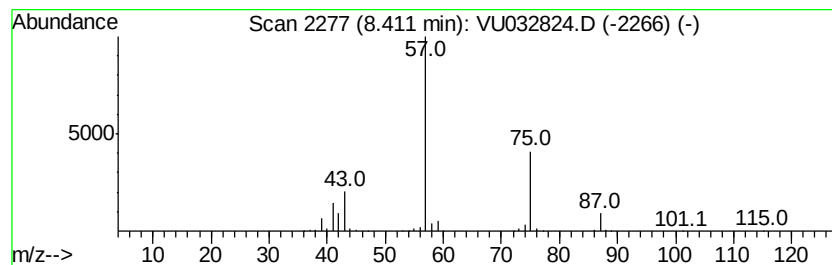
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	64.52 ug/L	912125	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\VU061819\
Data File : VU032824.D
Acq On : 18 Jun 2019 15:09
Operator : JC/SP
Sample : K3379-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JT4

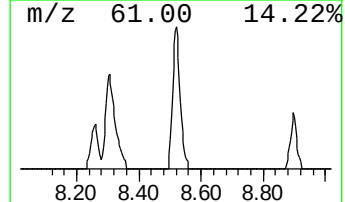
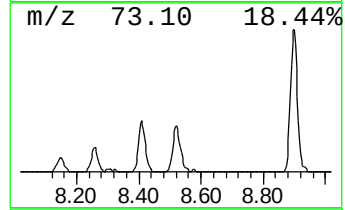
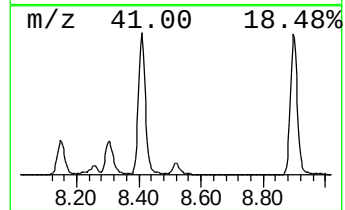
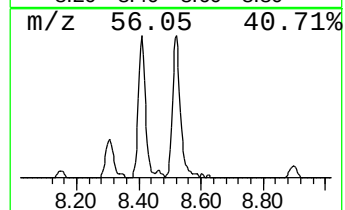
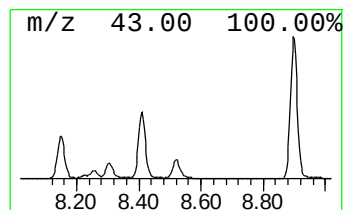
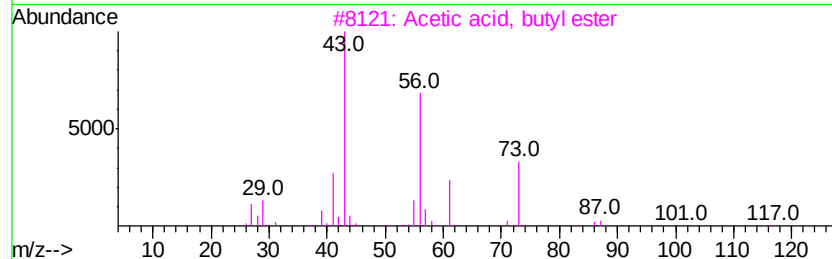
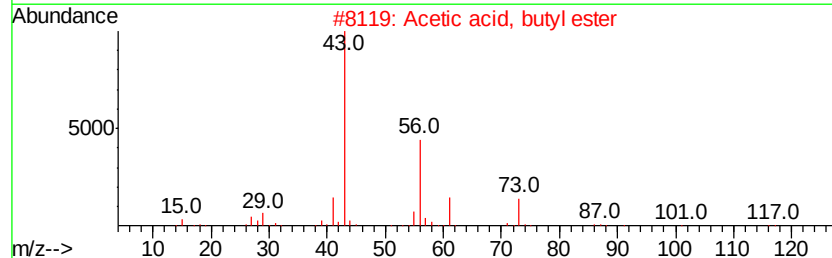
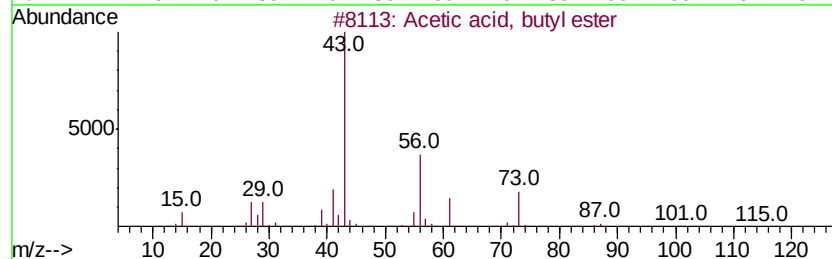
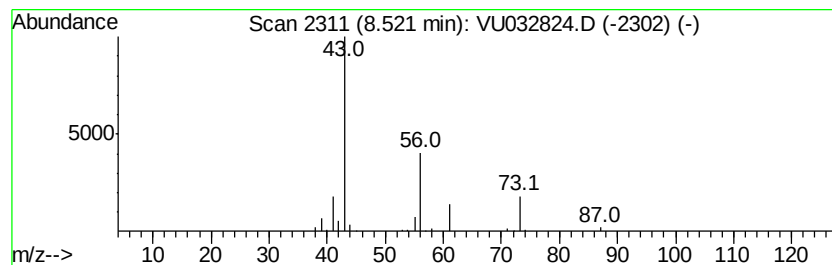
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	4.18 ug/L	59161	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	72
5		Isobutyl acetate	116	C6H12O2	000110-19-0	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032824.D
Acq On : 18 Jun 2019 15:09
Operator : JC/SP
Sample : K3379-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JT4

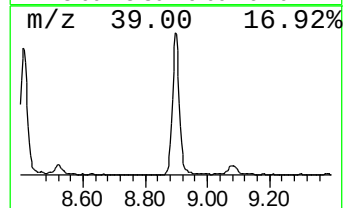
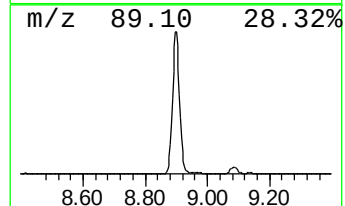
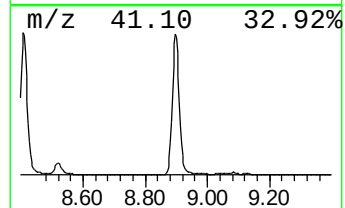
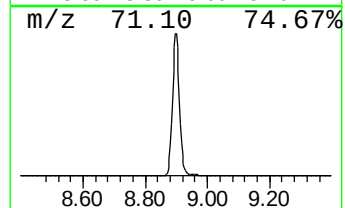
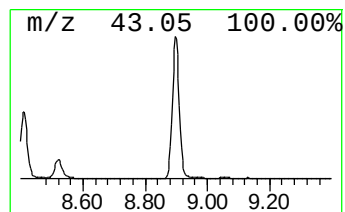
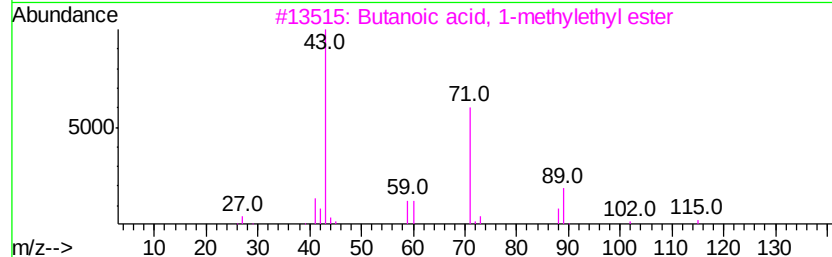
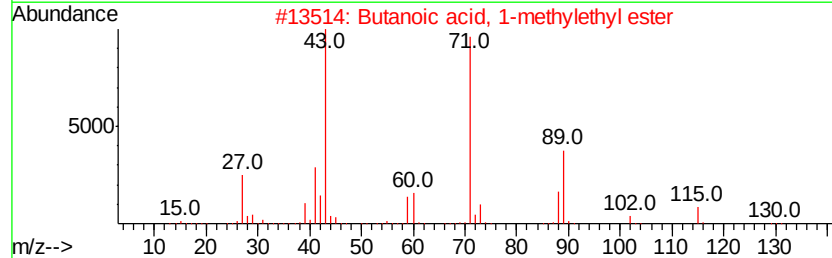
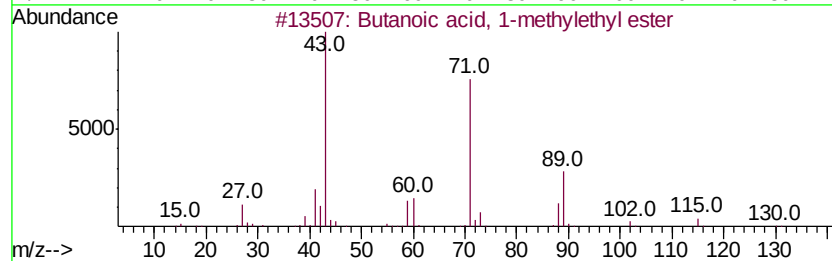
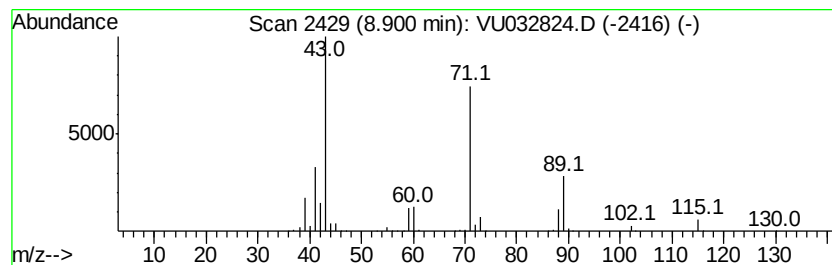
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	42.80 ug/L	605122	Chlorobenzene-d5	9.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	94
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		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032824.D
Acq On : 18 Jun 2019 15:09
Operator : JC/SP
Sample : K3379-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JT4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.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	125.1	ug/L	1371990	1	5.88	548523	50.0
Propanoic acid, 1...	7.41	22.9	ug/L	250841	1	5.88	548523	50.0
Propanoic acid, 2...	8.15	9.2	ug/L	130089	2	9.08	706899	50.0
Propanoic acid, p...	8.41	64.5	ug/L	912125	2	9.08	706899	50.0
Acetic acid, buty...	8.52	4.2	ug/L	59161	2	9.08	706899	50.0
Butanoic acid, 1-...	8.90	42.8	ug/L	605122	2	9.08	706899	50.0