

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091919\
 Data File : VU034663.D
 Acq On : 19 Sep 2019 21:49
 Operator : JC/SP
 Sample : K4895-09
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFDJ2

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\SOMULM091919WMA.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	1.177	24	27	34	rVB4	7804	7050	0.30%	0.034%
2	1.396	88	95	107	rVB	366499	382325	16.12%	1.820%
3	1.672	174	181	196	rVB	287839	362722	15.30%	1.727%
4	2.257	354	363	374	rVB	492568	746502	31.48%	3.555%
5	2.428	410	416	425	rVB	12725	19528	0.82%	0.093%
6	2.688	487	497	507	rVV3	13676	24227	1.02%	0.115%
7	2.727	507	509	515	rVB6	2024	1589	0.07%	0.008%
8	2.772	520	523	531	rBV8	2315	2276	0.10%	0.011%
9	2.968	572	584	596	rBV2	71394	133803	5.64%	0.637%
10	3.039	604	606	609	rVB4	2258	1241	0.05%	0.006%
11	3.058	609	612	615	rBV4	1586	1301	0.05%	0.006%
12	3.203	655	657	663	rBV6	1283	1243	0.05%	0.006%
13	3.244	666	670	676	rBV7	1827	2165	0.09%	0.010%
14	3.296	682	686	688	rVB5	1662	1244	0.05%	0.006%
15	3.344	699	701	707	rVB7	2402	1806	0.08%	0.009%
16	3.386	707	714	717	rBV7	1373	1626	0.07%	0.008%
17	3.434	724	729	730	rVV4	1580	1089	0.05%	0.005%
18	3.466	734	739	743	rBV6	1412	1270	0.05%	0.006%
19	3.611	776	784	785	rBV7	3341	4162	0.18%	0.020%
20	3.753	825	828	837	rVB10	1949	2308	0.10%	0.011%
21	3.830	848	852	854	rBV5	1366	1137	0.05%	0.005%
22	3.865	861	863	873	rVB9	1482	2272	0.10%	0.011%
23	4.010	905	908	911	rBV4	1422	1044	0.04%	0.005%
24	4.035	913	916	917	rBV2	2267	1070	0.05%	0.005%
25	4.151	939	952	959	rBV	224888	497954	21.00%	2.371%
26	4.537	1069	1072	1073	rBV3	1908	1210	0.05%	0.006%
27	4.621	1082	1098	1121	rBV	374976	897715	37.86%	4.275%
28	4.833	1161	1164	1169	rBV5	1495	1193	0.05%	0.006%
29	5.315	1290	1314	1347	rBV2	791991	2371045	100.00%	11.290%
30	5.531	1372	1381	1402	rVB	42077	89388	3.77%	0.426%
31	5.865	1471	1485	1504	rBV	598364	1201038	50.65%	5.719%
32	6.164	1566	1578	1599	rVB	240272	474181	20.00%	2.258%
33	6.309	1610	1623	1642	rBV	541163	1077403	45.44%	5.130%
34	6.563	1696	1702	1708	rBV2	10703	16744	0.71%	0.080%

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 Title : VOC Analysis

35	6.688	1731	1741	1768	rBV	241249	465104	19.62%	2.215%
36	7.026	1844	1846	1850	rBV3	1885	1599	0.07%	0.008%
37	7.206	1890	1902	1923	rVV	318169	591683	24.95%	2.817%
38	7.402	1952	1963	1972	rBV	94252	159269	6.72%	0.758%
39	7.543	1995	2007	2021	rBV	1047092	1829069	77.14%	8.709%
40	7.617	2024	2030	2044	rVB2	68124	118341	4.99%	0.563%
41	7.830	2084	2096	2120	rBV	213626	408707	17.24%	1.946%
42	8.135	2179	2191	2205	rBV	264702	452071	19.07%	2.153%
43	8.212	2209	2215	2229	rVB9	25365	45095	1.90%	0.215%
44	8.289	2229	2239	2265	rBV	816362	1506953	63.56%	7.175%
45	8.804	2396	2399	2404	rBV6	1904	2079	0.09%	0.010%
46	8.884	2412	2424	2445	rBV2	202785	353495	14.91%	1.683%
47	9.067	2462	2481	2510	rBV	908369	1605460	67.71%	7.645%
48	9.231	2522	2532	2546	rVB3	26721	46846	1.98%	0.223%
49	9.357	2559	2571	2587	rVB2	39915	77198	3.26%	0.368%
50	9.463	2602	2604	2610	rVB6	2258	1566	0.07%	0.007%
51	9.511	2616	2619	2625	rVB7	2140	2094	0.09%	0.010%
52	9.543	2625	2629	2630	rBV2	2082	1316	0.06%	0.006%
53	9.592	2635	2644	2657	rVV2	13659	26305	1.11%	0.125%
54	9.759	2685	2696	2710	rBV2	127582	212468	8.96%	1.012%
55	9.865	2725	2729	2733	rVB6	1888	1753	0.07%	0.008%
56	9.900	2738	2740	2744	rBV5	1464	1157	0.05%	0.006%
57	9.923	2744	2747	2749	rVV3	1780	1166	0.05%	0.006%
58	9.936	2749	2751	2754	rVB4	1964	1162	0.05%	0.006%
59	10.038	2781	2783	2787	rVB4	2143	1324	0.06%	0.006%
60	10.058	2787	2789	2794	rBV4	2304	2423	0.10%	0.012%
61	10.148	2808	2817	2828	rVB6	7260	12295	0.52%	0.059%
62	10.193	2828	2831	2834	rBV5	1439	1118	0.05%	0.005%
63	10.299	2861	2864	2865	rBV3	2447	1497	0.06%	0.007%
64	10.408	2886	2898	2919	rBV	674502	1108656	46.76%	5.279%
65	10.508	2926	2929	2933	rBV5	1695	1338	0.06%	0.006%
66	10.569	2940	2948	2955	rBV3	8534	12567	0.53%	0.060%
67	10.662	2968	2977	2981	rBV2	27194	42631	1.80%	0.203%
68	10.749	2996	3004	3017	rVB3	43307	68430	2.89%	0.326%
69	10.952	3057	3067	3081	rVB2	45268	77954	3.29%	0.371%
70	11.058	3095	3100	3102	rBV4	1859	1627	0.07%	0.008%
71	11.128	3113	3122	3137	rVB3	39371	67670	2.85%	0.322%

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72	11.196	3137	3143	3145	rBV6	2515	2781	0.12%	0.013%
73	11.299	3172	3175	3186	rVB9	3574	4089	0.17%	0.019%
74	11.405	3201	3208	3214	rBV6	9058	12408	0.52%	0.059%
75	11.460	3214	3225	3244	rVV	817796	1372270	57.88%	6.534%
76	11.550	3244	3253	3266	rVB	77848	125863	5.31%	0.599%
77	11.665	3286	3289	3292	rBV5	2121	1514	0.06%	0.007%
78	11.746	3305	3314	3324	rBV2	27872	51913	2.19%	0.247%
79	11.836	3331	3342	3361	rBV	915347	1554961	65.58%	7.404%
80	12.199	3452	3455	3458	rBV5	2045	1957	0.08%	0.009%
81	12.231	3458	3465	3473	rBV2	14859	23876	1.01%	0.114%
82	12.334	3488	3497	3505	rBV3	16926	29788	1.26%	0.142%
83	12.630	3584	3589	3596	rVB4	9082	12556	0.53%	0.060%
84	12.681	3598	3605	3615	rVB	19614	30601	1.29%	0.146%
85	12.759	3625	3629	3632	rBV6	1990	1662	0.07%	0.008%
86	12.775	3632	3634	3638	rBV4	1876	1667	0.07%	0.008%
87	12.839	3650	3654	3657	rBV4	2698	2805	0.12%	0.013%
88	12.945	3679	3687	3689	rBV8	8349	9856	0.42%	0.047%
89	13.000	3701	3704	3708	rBV7	2142	1693	0.07%	0.008%
90	13.103	3726	3736	3755	rVB3	33078	64387	2.72%	0.307%
91	13.177	3755	3759	3762	rBV5	2801	2322	0.10%	0.011%
92	13.495	3852	3858	3859	rBV5	4450	4206	0.18%	0.020%
93	13.733	3925	3932	3941	rBV4	11991	25616	1.08%	0.122%
94	13.820	3957	3959	3963	rBV5	2370	1711	0.07%	0.008%
95	14.112	4047	4050	4051	rBV3	2160	1148	0.05%	0.005%
96	14.148	4059	4061	4065	rVB4	2953	1507	0.06%	0.007%
97	14.222	4082	4084	4089	rVB5	2423	1951	0.08%	0.009%
98	14.257	4089	4095	4100	rBV9	2911	3742	0.16%	0.018%
99	15.054	4338	4343	4346	rBV6	5996	6878	0.29%	0.033%
100	15.334	4427	4430	4431	rBV2	2362	1285	0.05%	0.006%

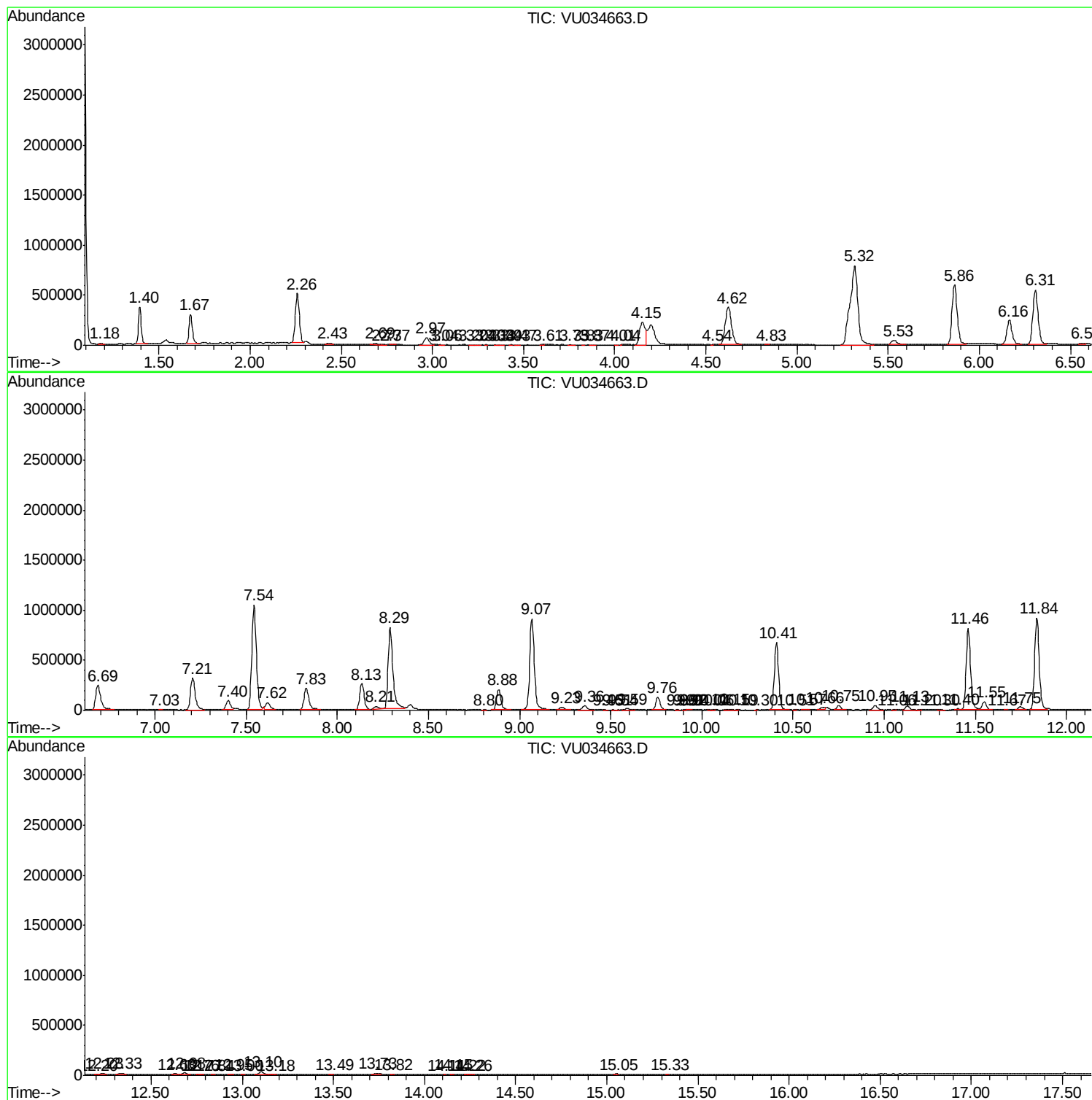
Sum of corrected areas: 21001370

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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



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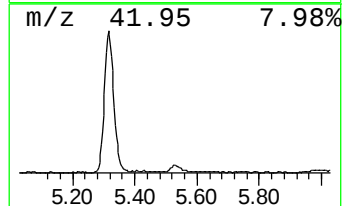
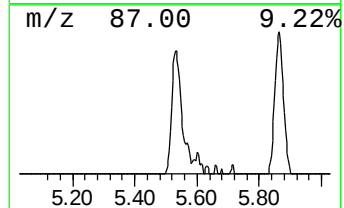
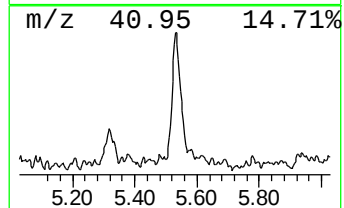
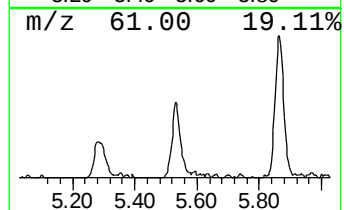
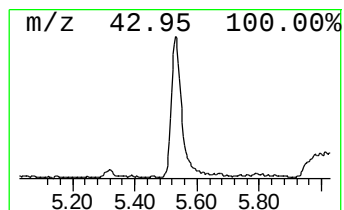
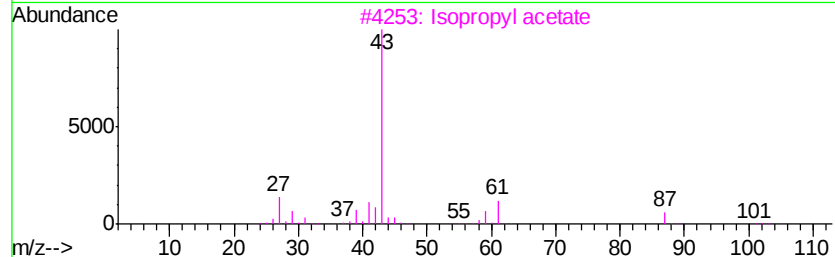
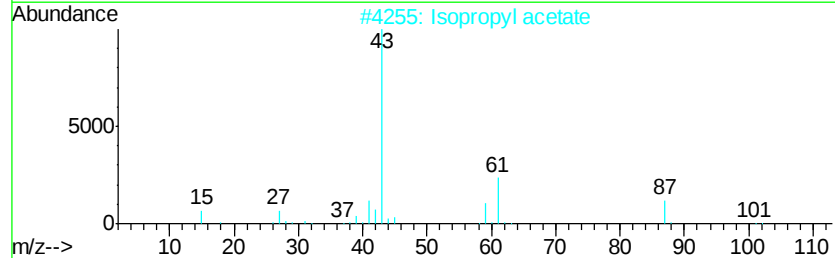
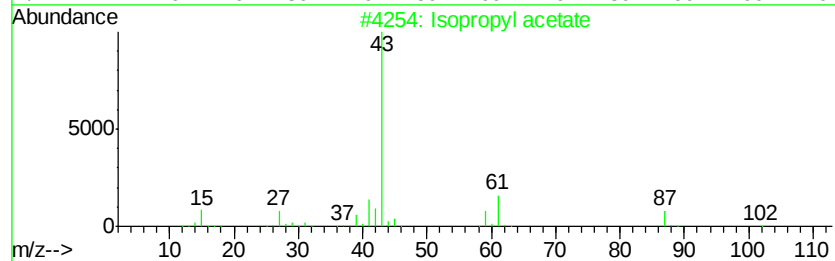
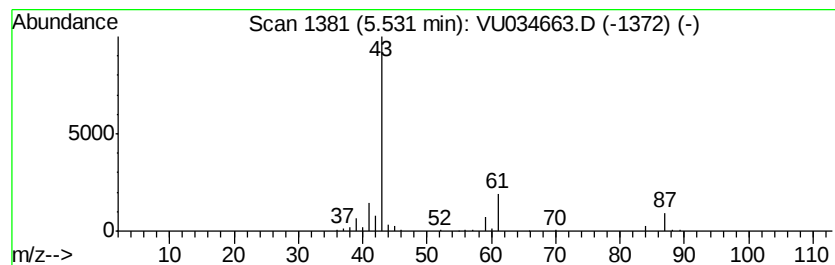
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.53	3.72 ug/L	89388	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl acetate	102	C5H10O2	000108-21-4	59
2		Isopropyl acetate	102	C5H10O2	000108-21-4	36
3		Isopropyl acetate	102	C5H10O2	000108-21-4	28
4		Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	10
5		Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9



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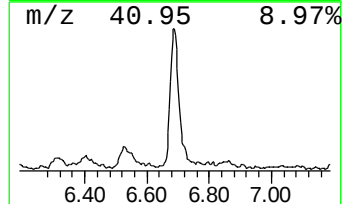
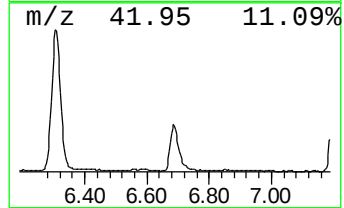
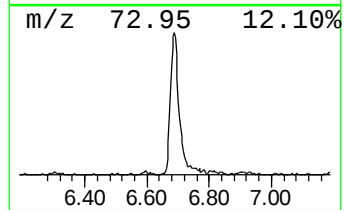
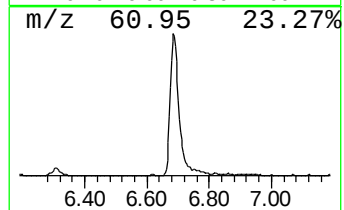
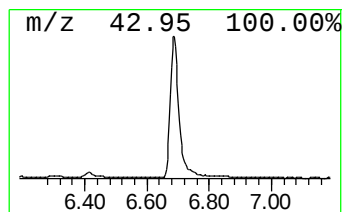
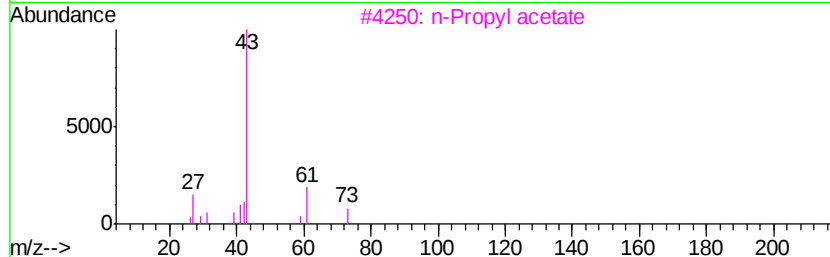
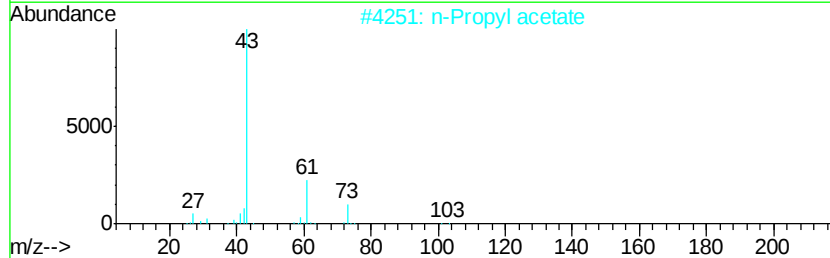
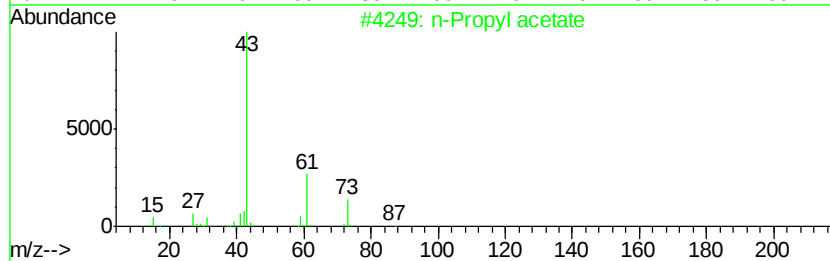
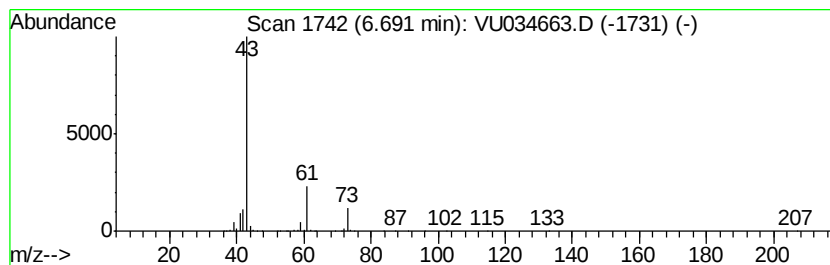
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Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	19.36 ug/L	465104	1,4-Difluorobenzene	5.86

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	83
3		n-Propyl acetate	102	C5H10O2	000109-60-4	78
4		Isopropyl acetate	102	C5H10O2	000108-21-4	9
5		Isopropyl acetate	102	C5H10O2	000108-21-4	9



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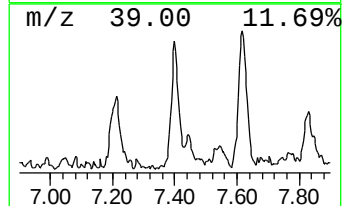
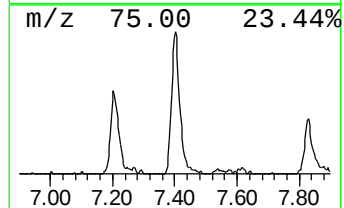
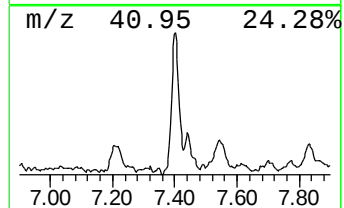
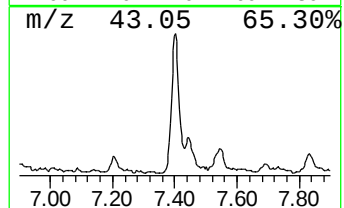
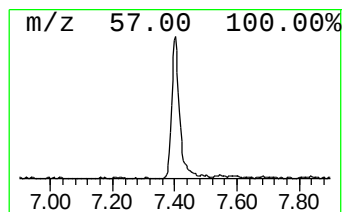
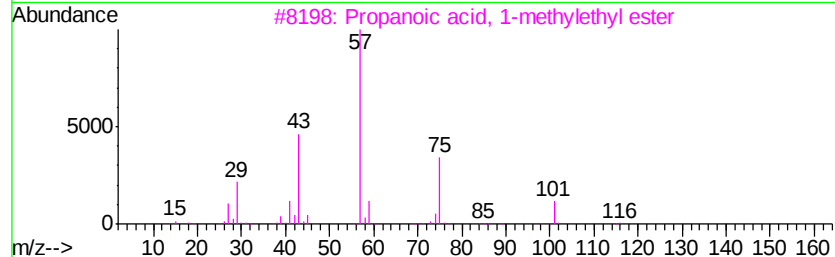
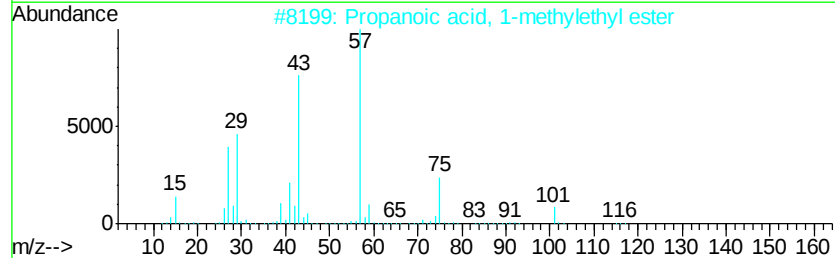
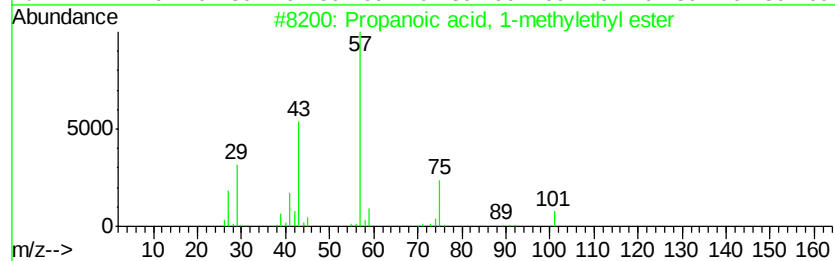
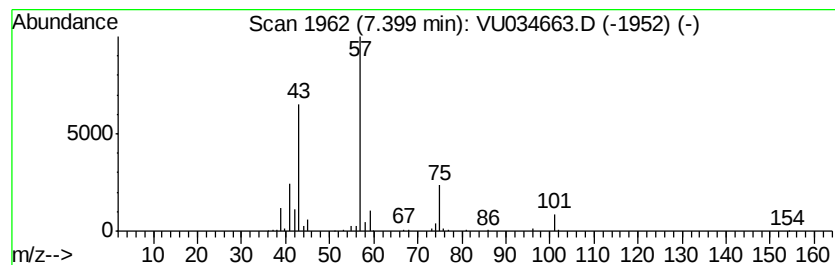
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Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	6.63 ug/L	159269	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
4		Propionic acid, 4-hydroxy-3-hexyl...	174	C9H18O3	1000151-16-9	50
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU091919\
Data File : VU034663.D
Acq On : 19 Sep 2019 21:49
Operator : JC/SP
Sample : K4895-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDJ2

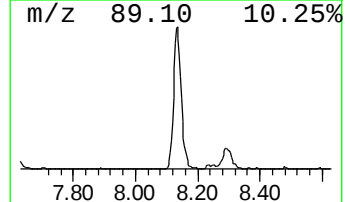
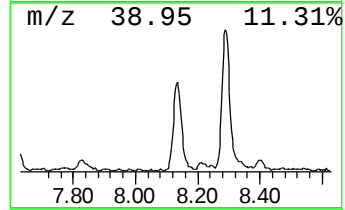
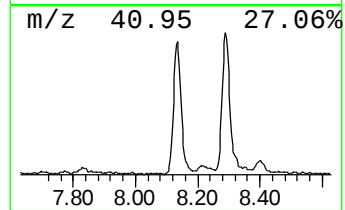
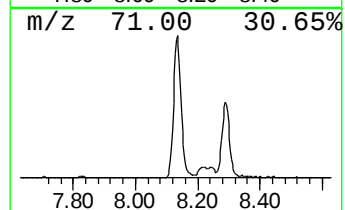
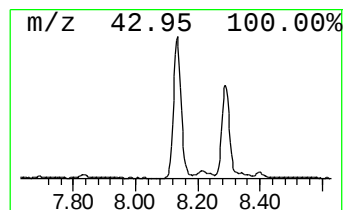
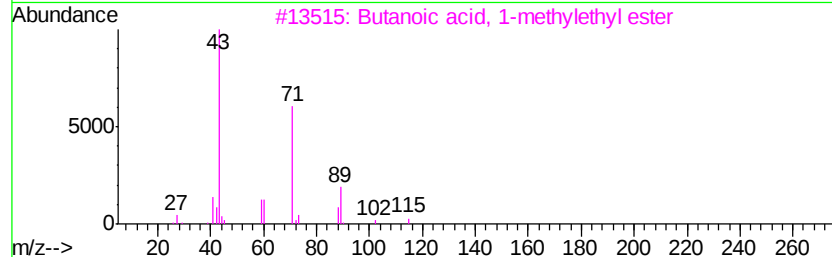
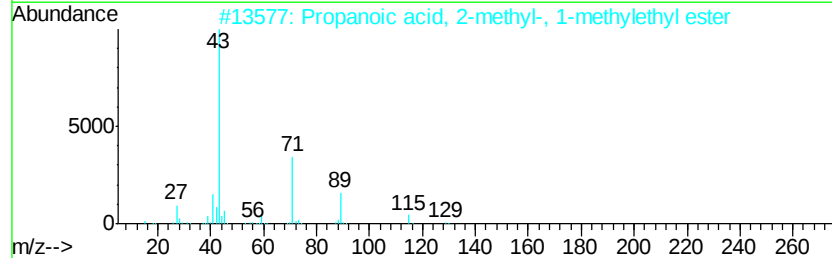
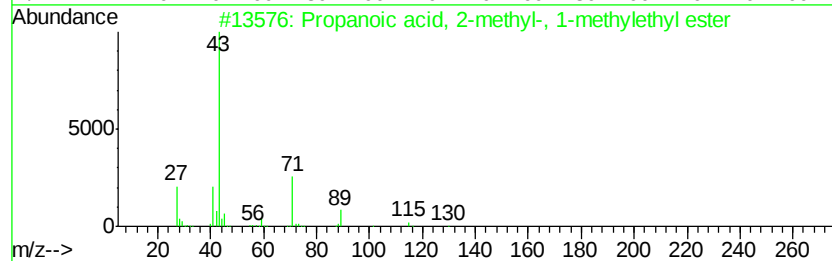
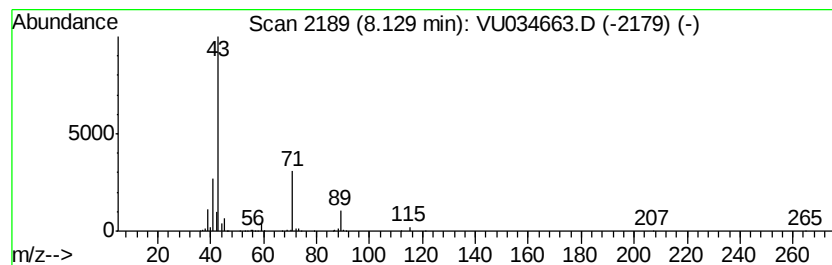
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.13	14.08 ug/L	452071	Chlorobenzene-d5	9.07

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		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	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU091919\
Data File : VU034663.D
Acq On : 19 Sep 2019 21:49
Operator : JC/SP
Sample : K4895-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDJ2

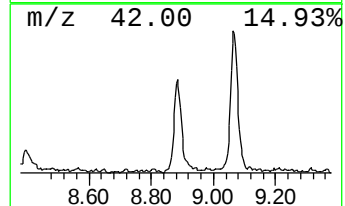
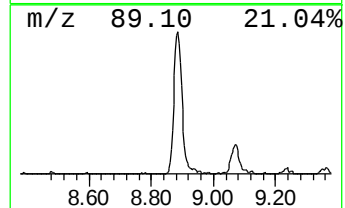
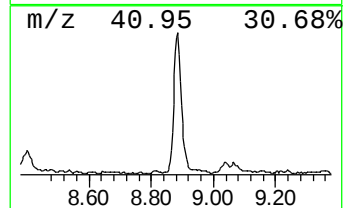
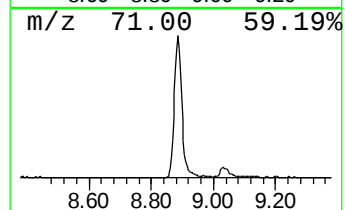
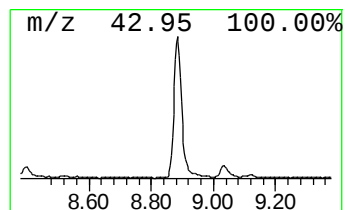
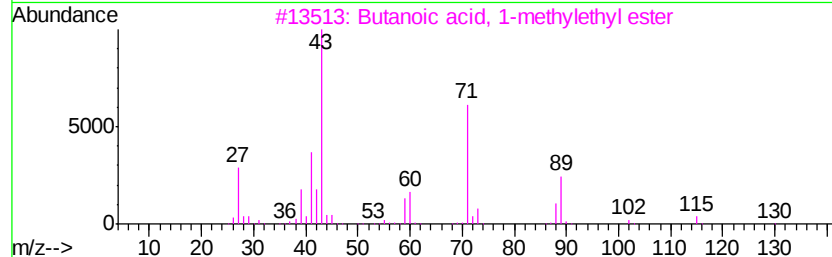
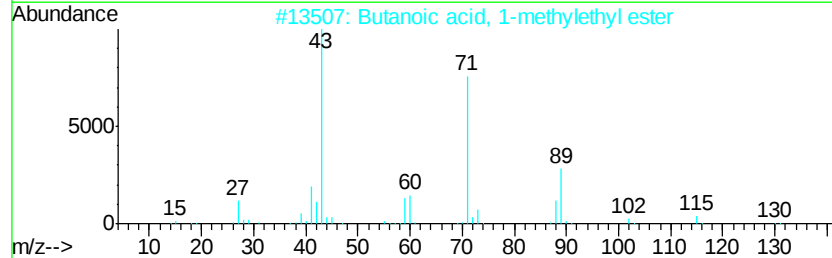
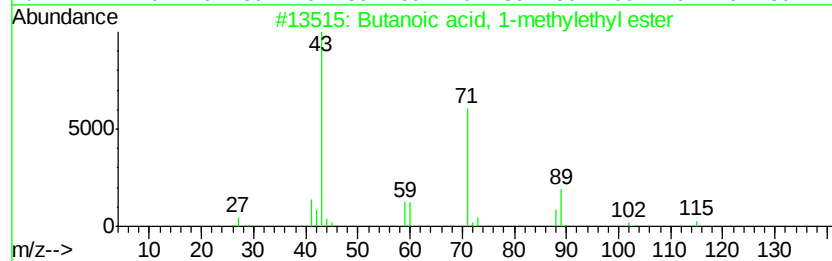
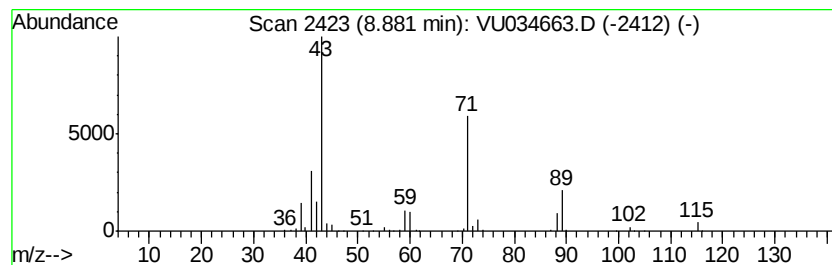
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Quant Title : VOC Analysis

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

Peak Number 6 Butanoic acid, 1-methylethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	11.01 ug/L	353495	Chlorobenzene-d5	9.07

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	78
4		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	78
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU091919\
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Acq On : 19 Sep 2019 21:49
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Sample : K4895-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDJ2

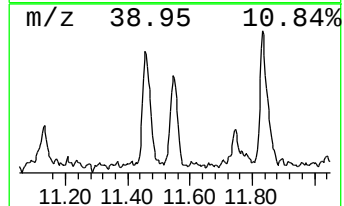
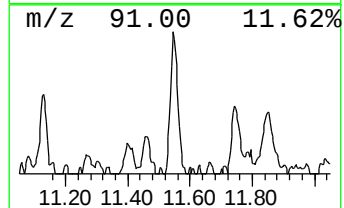
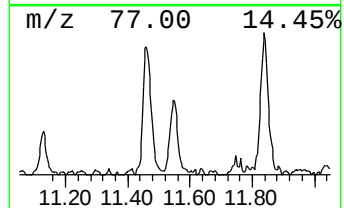
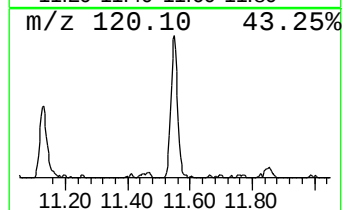
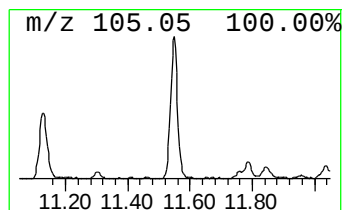
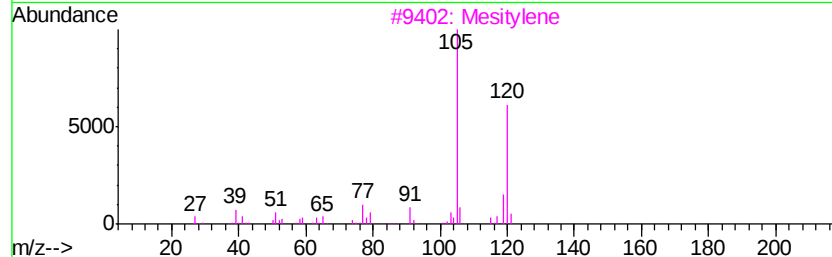
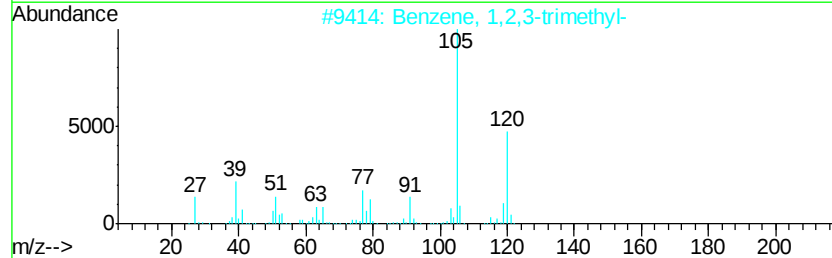
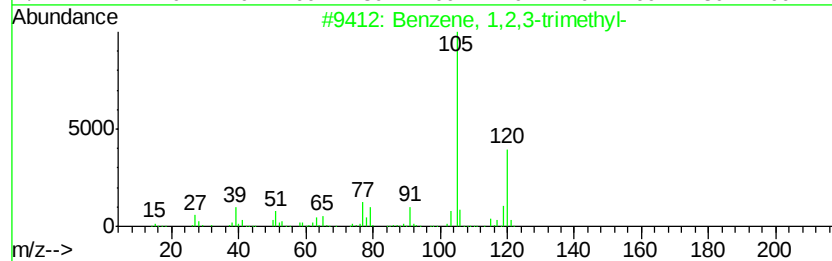
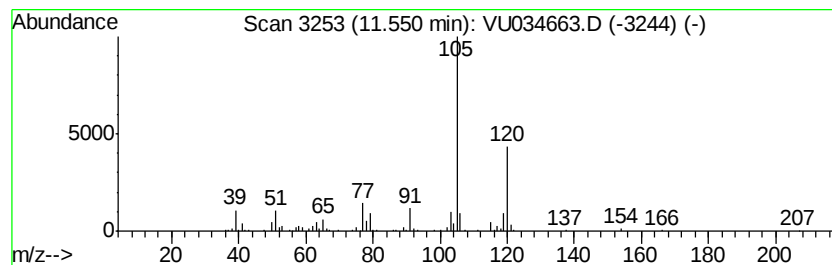
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	4.59 ug/L	125863	1,4-Dichlorobenzene-d4	11.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	93
3		Mesitylene	120	C9H12	000108-67-8	93
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87



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Data File : VU034663.D
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Sample : K4895-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDJ2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.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
Isopropyl acetate	5.53	3.7	ug/L	89388	1	5.86	1201040	50.0
n-Propyl acetate	6.69	19.4	ug/L	465104	1	5.86	1201040	50.0
Propanoic acid, 1...	7.40	6.6	ug/L	159269	1	5.86	1201040	50.0
Propanoic acid, 2...	8.13	14.1	ug/L	452071	2	9.07	1605460	50.0
Butanoic acid, 1-...	8.88	11.0	ug/L	353495	2	9.07	1605460	50.0
Benzene, 1,2,3-tr...	11.55	4.6	ug/L	125863	3	11.46	1372270	50.0