

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
 Data File : VU025603.D
 Acq On : 23 Jul 2018 15:35
 Operator : MD/SY
 Sample : PB111343ZHE#09
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PB111343ZHE#09

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\SOMULM072018WMA.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	0.613	4	7	12	rVB	351	279	0.03%	0.003%
2	0.670	17	25	29	rBV2	534	670	0.06%	0.007%
3	0.860	80	84	88	rBV2	326	269	0.03%	0.003%
4	0.960	113	115	119	rVB3	477	310	0.03%	0.003%
5	1.002	124	128	133	rVB2	403	418	0.04%	0.004%
6	1.060	134	146	147	rBV2	1065	1289	0.12%	0.013%
7	1.088	148	155	175	rBV	156539	178709	17.33%	1.848%
8	1.404	245	253	264	rBV	103571	107976	10.47%	1.117%
9	1.683	332	340	353	rVB	88440	110165	10.68%	1.139%
10	2.275	514	524	534	rBV	199411	294329	28.54%	3.044%
11	2.445	570	577	584	rBV2	4081	5592	0.54%	0.058%
12	2.619	624	631	641	rVB2	3706	6368	0.62%	0.066%
13	2.703	648	657	668	rBV	7097	12458	1.21%	0.129%
14	2.825	689	695	697	rBV2	1070	1082	0.10%	0.011%
15	2.895	712	717	722	rVB3	492	615	0.06%	0.006%
16	3.146	787	795	799	rBV3	411	608	0.06%	0.006%
17	3.166	799	801	804	rVV4	594	382	0.04%	0.004%
18	3.178	804	805	808	rVV	365	246	0.02%	0.003%
19	3.195	808	810	814	rVV2	445	295	0.03%	0.003%
20	3.404	869	875	876	rBV3	896	831	0.08%	0.009%
21	3.590	931	933	937	rVV2	382	266	0.03%	0.003%
22	3.825	999	1006	1010	rBV3	413	549	0.05%	0.006%
23	3.867	1013	1019	1023	rBV3	307	417	0.04%	0.004%
24	3.973	1049	1052	1055	rBV2	311	262	0.03%	0.003%
25	4.182	1098	1117	1139	rBV2	97907	261549	25.36%	2.705%
26	4.461	1202	1204	1207	rVV2	558	317	0.03%	0.003%
27	4.654	1246	1264	1298	rBV	184865	434953	42.17%	4.499%
28	4.860	1320	1328	1330	rBV2	522	599	0.06%	0.006%
29	4.886	1333	1336	1348	rVB4	1181	1759	0.17%	0.018%
30	4.989	1361	1368	1371	rBV3	708	767	0.07%	0.008%
31	5.346	1454	1479	1500	rBV2	347120	1031439	100.00%	10.669%
32	5.484	1520	1522	1528	rVB3	560	578	0.06%	0.006%
33	5.551	1528	1543	1560	rBV2	98170	202588	19.64%	2.095%
34	5.725	1594	1597	1601	rBV2	512	365	0.04%	0.004%

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 Title : VOC Analysis

35	5.792	1611	1618	1623	rBV3	467	708	0.07%	0.007%
36	5.892	1623	1649	1666	rBV	398824	858658	83.25%	8.882%
37	6.336	1773	1787	1807	rVB	237724	477095	46.26%	4.935%
38	6.580	1857	1863	1870	rVB2	3828	5817	0.56%	0.060%
39	6.709	1891	1903	1919	rBV	148045	262720	25.47%	2.717%
40	6.850	1942	1947	1959	rVB5	2788	4525	0.44%	0.047%
41	7.230	2051	2065	2082	rBV	142690	252564	24.49%	2.612%
42	7.352	2099	2103	2104	rBV2	852	585	0.06%	0.006%
43	7.426	2116	2126	2133	rBV2	6448	10504	1.02%	0.109%
44	7.571	2157	2171	2188	rBV	487803	846632	82.08%	8.757%
45	7.728	2217	2220	2221	rBV3	880	541	0.05%	0.006%
46	7.853	2246	2259	2275	rBV2	104368	179466	17.40%	1.856%
47	8.098	2331	2335	2337	rBV2	439	352	0.03%	0.004%
48	8.185	2345	2362	2371	rBV3	12137	31707	3.07%	0.328%
49	8.313	2392	2402	2423	rVB	340054	569633	55.23%	5.892%
50	8.419	2425	2435	2447	rVB	74558	115955	11.24%	1.199%
51	8.525	2460	2468	2481	rVB	24007	37652	3.65%	0.389%
52	8.596	2489	2490	2497	rVB3	605	438	0.04%	0.005%
53	8.908	2575	2587	2598	rBV	87398	136051	13.19%	1.407%
54	9.091	2627	2644	2664	rBV	540683	890489	86.33%	9.211%
55	9.242	2687	2691	2692	rBV4	604	380	0.04%	0.004%
56	9.255	2692	2695	2698	rVB4	598	475	0.05%	0.005%
57	9.448	2747	2755	2758	rBV3	558	721	0.07%	0.007%
58	9.506	2771	2773	2777	rVB2	502	276	0.03%	0.003%
59	9.577	2792	2795	2797	rBV2	473	370	0.04%	0.004%
60	9.593	2797	2800	2802	rVB2	389	270	0.03%	0.003%
61	9.638	2812	2814	2819	rVB4	392	302	0.03%	0.003%
62	9.728	2839	2842	2845	rBV3	644	409	0.04%	0.004%
63	9.770	2849	2855	2861	rBV6	2307	3020	0.29%	0.031%
64	9.866	2880	2885	2888	rBV	377	454	0.04%	0.005%
65	9.898	2892	2895	2900	rBV2	558	482	0.05%	0.005%
66	9.927	2901	2904	2912	rVB4	403	449	0.04%	0.005%
67	10.101	2955	2958	2961	rVB2	554	389	0.04%	0.004%
68	10.143	2968	2971	2975	rVB2	580	394	0.04%	0.004%
69	10.172	2977	2980	2984	rBV2	351	271	0.03%	0.003%
70	10.381	3043	3045	3048	rBV	396	270	0.03%	0.003%
71	10.435	3050	3062	3079	rVV	351649	559043	54.20%	5.782%

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72	10.615	3110	3118	3132	rVB3	3353	6661	0.65%	0.069%
73	10.725	3147	3152	3153	rBV2	489	308	0.03%	0.003%
74	10.776	3161	3168	3178	rVB3	3268	4825	0.47%	0.050%
75	10.818	3178	3181	3183	rBV2	532	338	0.03%	0.003%
76	10.866	3193	3196	3199	rVV2	416	350	0.03%	0.004%
77	10.943	3216	3220	3222	rBV2	323	266	0.03%	0.003%
78	11.069	3257	3259	3265	rVB2	318	247	0.02%	0.003%
79	11.107	3267	3271	3274	rVB3	375	317	0.03%	0.003%
80	11.201	3294	3300	3302	rBV3	477	481	0.05%	0.005%
81	11.487	3377	3389	3405	rBV	573379	894305	86.70%	9.250%
82	11.596	3420	3423	3429	rVB5	600	616	0.06%	0.006%
83	11.689	3449	3452	3455	rBV	371	287	0.03%	0.003%
84	11.863	3493	3506	3527	rBV	527078	842817	81.71%	8.718%
85	12.156	3594	3597	3600	rBV3	638	440	0.04%	0.005%
86	12.249	3623	3626	3628	rBV3	469	306	0.03%	0.003%
87	12.445	3685	3687	3689	rBV2	580	273	0.03%	0.003%
88	12.519	3707	3710	3713	rBV3	500	410	0.04%	0.004%
89	12.619	3738	3741	3745	rBV2	407	361	0.03%	0.004%
90	12.638	3745	3747	3752	rVB4	809	702	0.07%	0.007%
91	12.934	3836	3839	3842	rBV2	423	283	0.03%	0.003%
92	12.992	3854	3857	3859	rBV2	428	326	0.03%	0.003%
93	13.358	3965	3971	3972	rBV2	441	405	0.04%	0.004%
94	13.384	3976	3979	3982	rVB2	559	312	0.03%	0.003%
95	13.541	4025	4028	4031	rBV	579	466	0.05%	0.005%
96	14.371	4282	4286	4289	rBV2	581	476	0.05%	0.005%
97	14.435	4303	4306	4308	rBV2	603	348	0.03%	0.004%
98	14.493	4320	4324	4327	rBV3	446	470	0.05%	0.005%
99	14.557	4341	4344	4346	rBV3	499	290	0.03%	0.003%
100	15.336	4583	4586	4590	rBV3	872	837	0.08%	0.009%

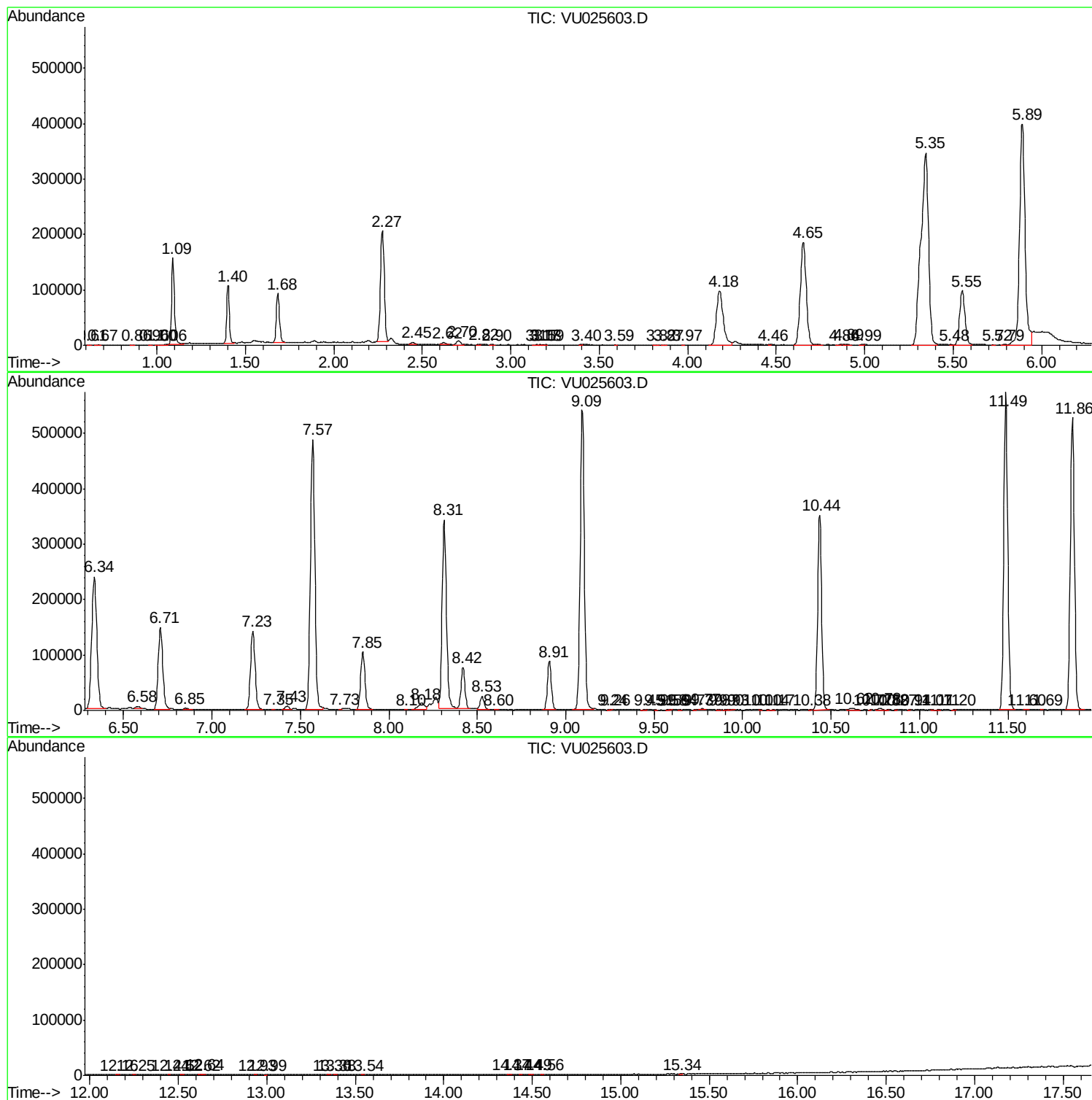
Sum of corrected areas: 9667889

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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



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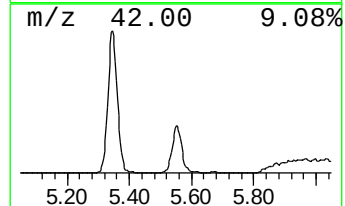
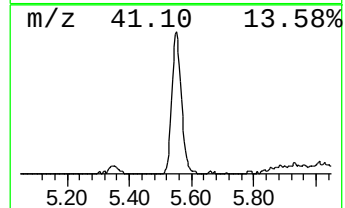
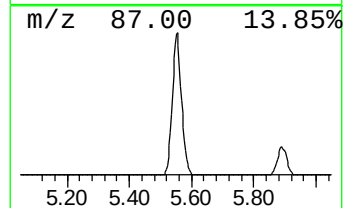
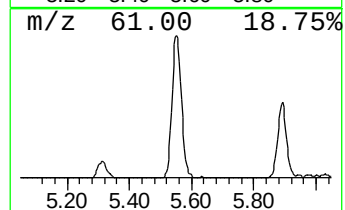
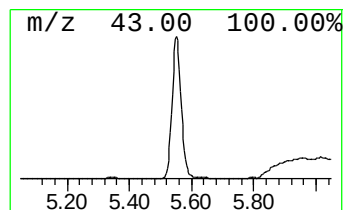
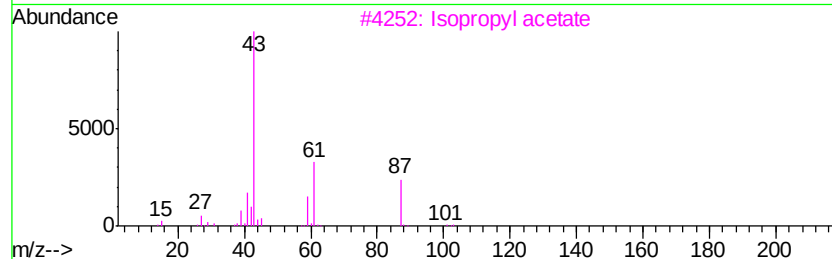
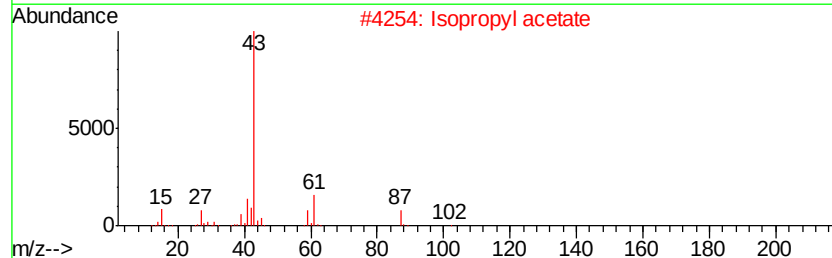
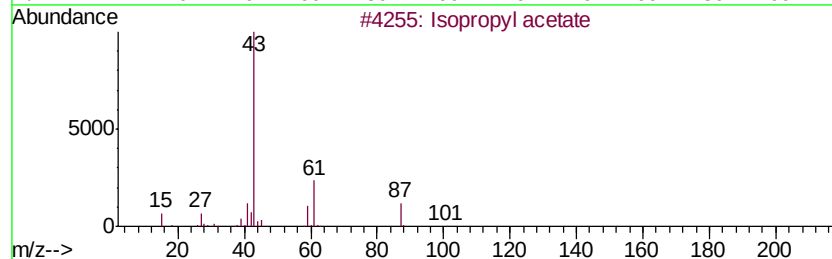
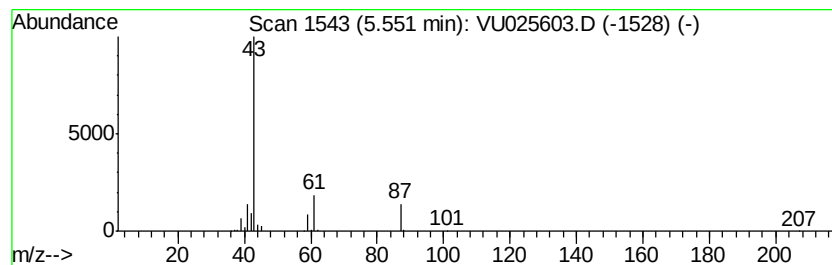
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.55	11.80 ug/L	202588	1,4-Difluorobenzene	5.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Isopropyl acetate	102 C5H10O2	000108-21-4	83
2	Isopropyl acetate	102 C5H10O2	000108-21-4	78
3	Isopropyl acetate	102 C5H10O2	000108-21-4	59
4	2-Pentanol, acetate	130 C7H14O2	000626-38-0	36
5	Propane, 1-(1-methylethoxy)-	102 C6H14O	000627-08-7	36



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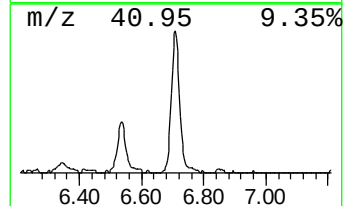
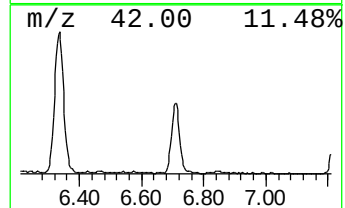
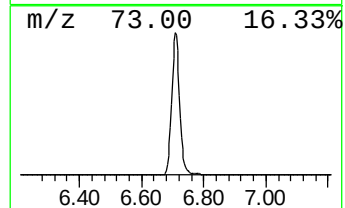
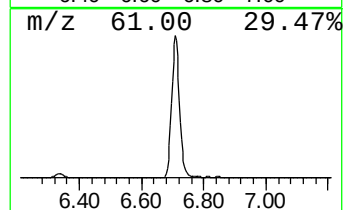
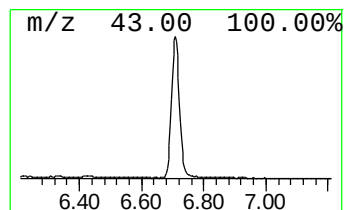
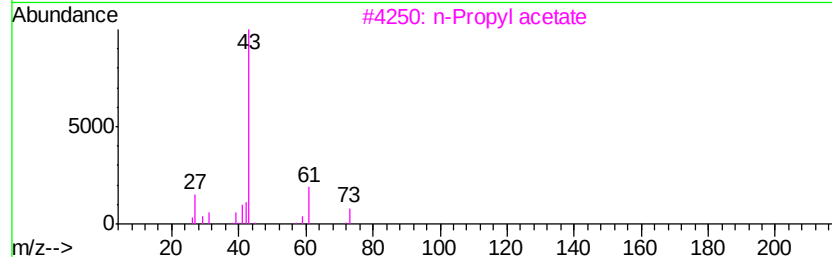
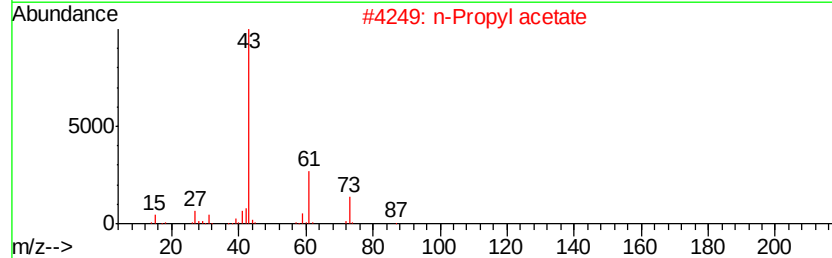
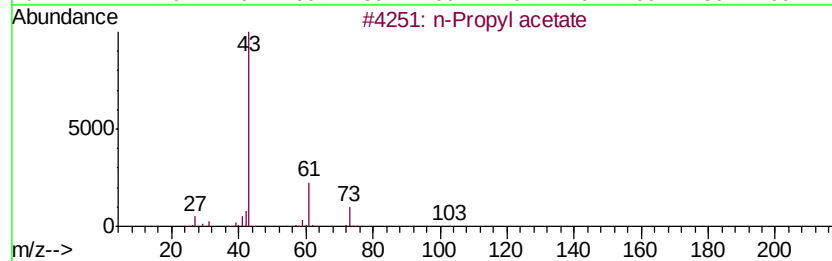
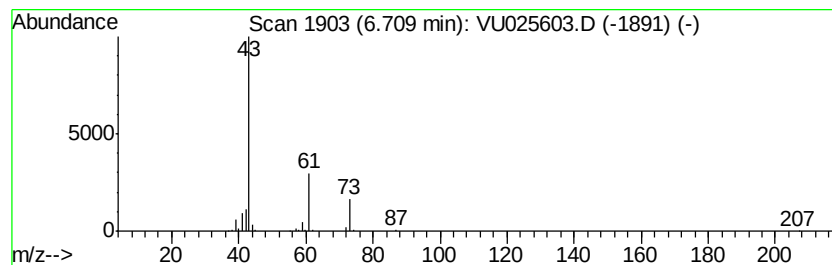
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	15.30 ug/L	262720	1,4-Difluorobenzene	5.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	36	
5	Isopropyl acetate	102	C5H10O2	000108-21-4	33	



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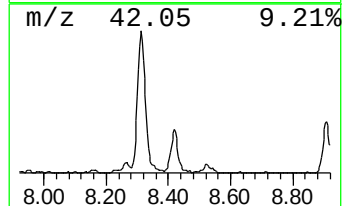
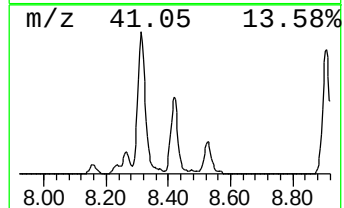
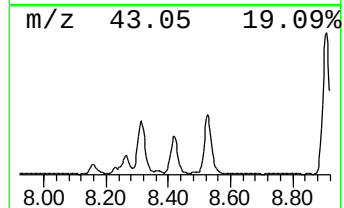
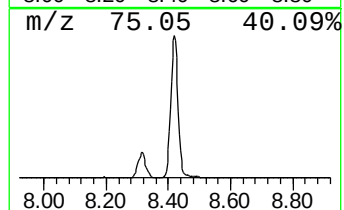
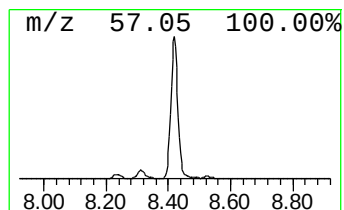
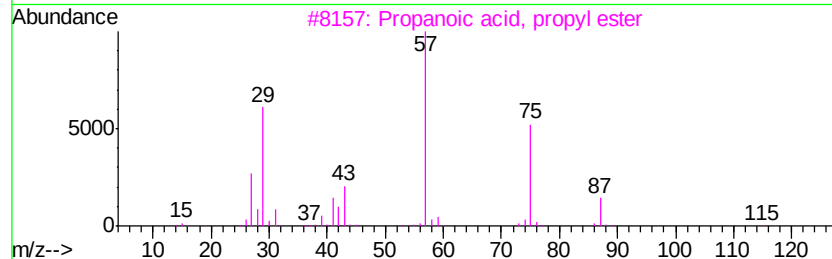
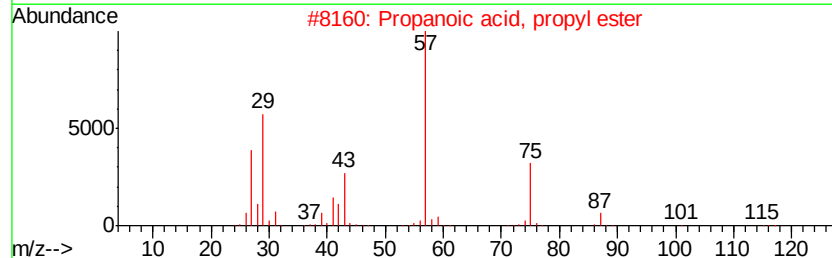
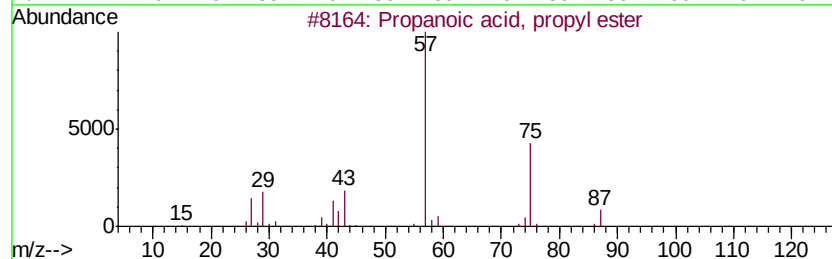
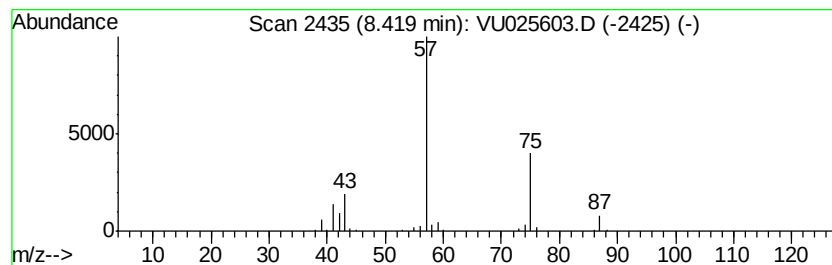
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	6.51 ug/L	115955	Chlorobenzene-d5	9.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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	36



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Acq On : 23 Jul 2018 15:35
Operator : MD/SY
Sample : PB111343ZHE#09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#09

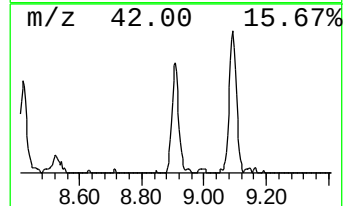
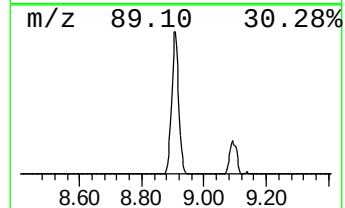
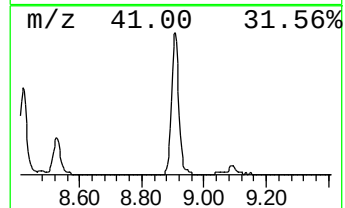
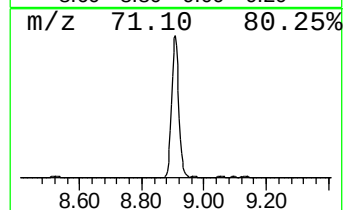
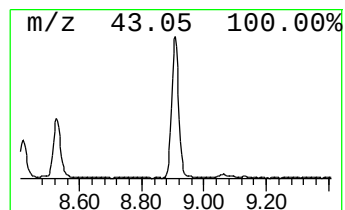
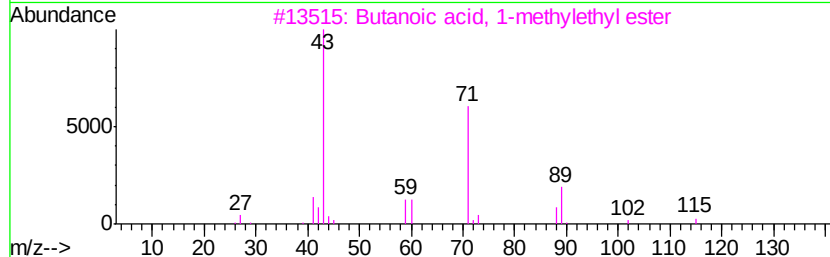
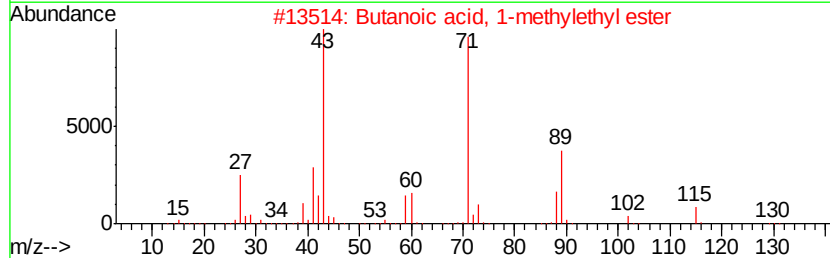
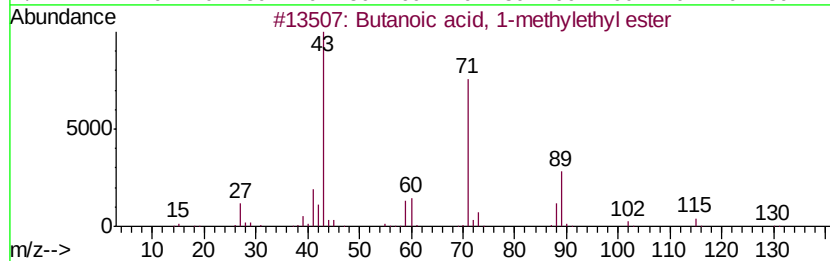
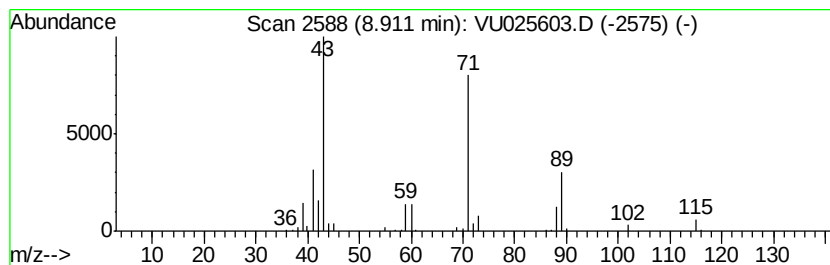
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Quant Title : VOC Analysis

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

Peak Number 6 Butanoic acid, 1-methylethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.91	7.64 ug/L	136051	Chlorobenzene-d5	9.09

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		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU072318\
Data File : VU025603.D
Acq On : 23 Jul 2018 15:35
Operator : MD/SY
Sample : PB111343ZHE#09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#09

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.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	5.55	11.8	ug/L	202588	1	5.89	858658	50.0
n-Propyl acetate	6.71	15.3	ug/L	262720	1	5.89	858658	50.0
Propanoic acid, p...	8.42	6.5	ug/L	115955	2	9.09	890489	50.0
Butanoic acid, 1-...	8.91	7.6	ug/L	136051	2	9.09	890489	50.0