

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
 Data File : VU025598.D
 Acq On : 23 Jul 2018 13:38
 Operator : MD/SY
 Sample : VLEB#02
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB#02

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	0.654	15	20	25	rBV3	301	368	0.03%	0.004%
2	0.712	35	38	42	rVB2	353	256	0.02%	0.003%
3	0.999	122	127	130	rBV2	291	254	0.02%	0.003%
4	1.089	130	155	174	rBV	230722	267114	25.23%	2.677%
5	1.400	245	252	265	rBV	105176	111574	10.54%	1.118%
6	1.683	332	340	354	rVB	90850	113889	10.76%	1.142%
7	2.275	514	524	534	rBV	206468	306274	28.92%	3.070%
8	2.442	568	576	589	rBV4	3214	6025	0.57%	0.060%
9	2.535	602	605	609	rVV2	444	448	0.04%	0.004%
10	2.619	624	631	640	rVB4	3596	6126	0.58%	0.061%
11	2.654	640	642	645	rVV3	458	250	0.02%	0.003%
12	2.703	645	657	669	rVV3	6741	12090	1.14%	0.121%
13	2.748	669	671	677	rVB2	328	295	0.03%	0.003%
14	2.812	688	691	692	rVV	447	265	0.03%	0.003%
15	2.844	692	701	713	rVB4	1804	4108	0.39%	0.041%
16	3.185	802	807	813	rBV5	577	748	0.07%	0.007%
17	3.410	871	877	889	rVB3	1392	2522	0.24%	0.025%
18	3.497	902	904	909	rVB3	392	293	0.03%	0.003%
19	3.526	909	913	916	rBV	517	453	0.04%	0.005%
20	3.593	931	934	941	rVB3	291	344	0.03%	0.003%
21	3.828	1004	1007	1011	rVV2	324	260	0.02%	0.003%
22	3.860	1013	1017	1022	rVB3	349	349	0.03%	0.003%
23	3.979	1052	1054	1060	rVV2	334	278	0.03%	0.003%
24	4.117	1093	1097	1099	rBV2	342	252	0.02%	0.003%
25	4.175	1099	1115	1137	rBV	96023	251618	23.76%	2.522%
26	4.542	1222	1229	1232	rBV3	267	318	0.03%	0.003%
27	4.651	1245	1263	1281	rBV	186734	435380	41.12%	4.364%
28	4.838	1319	1321	1326	rVB3	402	335	0.03%	0.003%
29	4.886	1326	1336	1345	rBV5	1136	2053	0.19%	0.021%
30	4.947	1352	1355	1358	rVB3	469	300	0.03%	0.003%
31	4.976	1358	1364	1367	rBV4	420	550	0.05%	0.006%
32	4.995	1367	1370	1374	rVB2	571	372	0.04%	0.004%
33	5.095	1397	1401	1405	rBV2	337	301	0.03%	0.003%
34	5.191	1428	1431	1436	rVB2	336	291	0.03%	0.003%

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35	5.342	1453	1478	1507	rBV2	352056	1058884	100.00%	10.614%
36	5.548	1527	1542	1561	rBV	95873	199649	18.85%	2.001%
37	5.793	1615	1618	1623	rVB3	522	468	0.04%	0.005%
38	5.889	1634	1648	1666	rBV	411783	799892	75.54%	8.018%
39	6.333	1772	1786	1806	rBV	246776	488540	46.14%	4.897%
40	6.529	1835	1847	1856	rBV2	3569	7746	0.73%	0.078%
41	6.577	1857	1862	1880	rVB2	5307	10053	0.95%	0.101%
42	6.709	1889	1903	1921	rBV	143072	258358	24.40%	2.590%
43	6.844	1938	1945	1947	rBV2	1906	1988	0.19%	0.020%
44	7.082	2017	2019	2024	rVB3	475	281	0.03%	0.003%
45	7.137	2034	2036	2039	rVB2	464	271	0.03%	0.003%
46	7.169	2044	2046	2049	rVB2	545	298	0.03%	0.003%
47	7.230	2053	2065	2096	rBV	148441	263732	24.91%	2.644%
48	7.423	2118	2125	2133	rBV3	5799	8687	0.82%	0.087%
49	7.458	2133	2136	2145	rVB6	1643	2352	0.22%	0.024%
50	7.567	2157	2170	2187	rBV	500710	874543	82.59%	8.766%
51	7.683	2204	2206	2209	rVB2	641	394	0.04%	0.004%
52	7.706	2209	2213	2218	rBV5	982	999	0.09%	0.010%
53	7.850	2247	2258	2276	rBV	108482	186971	17.66%	1.874%
54	8.024	2306	2312	2314	rBV3	596	478	0.05%	0.005%
55	8.069	2321	2326	2328	rBV	310	248	0.02%	0.002%
56	8.088	2328	2332	2334	rBV3	605	489	0.05%	0.005%
57	8.169	2345	2357	2358	rBV4	4714	6855	0.65%	0.069%
58	8.313	2392	2402	2425	rVB	322442	553112	52.24%	5.544%
59	8.419	2425	2435	2449	rVB	76494	120527	11.38%	1.208%
60	8.526	2460	2468	2483	rVB2	23525	36900	3.48%	0.370%
61	8.805	2552	2555	2560	rVB2	476	391	0.04%	0.004%
62	8.870	2572	2575	2576	rBV	569	356	0.03%	0.004%
63	8.908	2576	2587	2602	rVV	85610	136003	12.84%	1.363%
64	9.091	2626	2644	2665	rBV	587825	974596	92.04%	9.769%
65	9.230	2683	2687	2689	rBV	511	325	0.03%	0.003%
66	9.297	2706	2708	2715	rVV3	550	425	0.04%	0.004%
67	9.329	2715	2718	2722	rVV3	426	399	0.04%	0.004%
68	9.378	2730	2733	2740	rVB3	1227	1080	0.10%	0.011%
69	9.558	2784	2789	2791	rBV	418	338	0.03%	0.003%
70	9.583	2795	2797	2800	rVV	600	362	0.03%	0.004%
71	9.603	2800	2803	2808	rVV	407	360	0.03%	0.004%

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72	9.635	2810	2813	2817	rVB3	458	326	0.03%	0.003%
73	9.731	2838	2843	2846	rBV3	489	408	0.04%	0.004%
74	9.770	2846	2855	2868	rBV8	2233	4641	0.44%	0.047%
75	9.889	2888	2892	2895	rBV2	465	446	0.04%	0.004%
76	10.175	2977	2981	2984	rBV	482	450	0.04%	0.005%
77	10.297	3014	3019	3021	rBV2	570	488	0.05%	0.005%
78	10.435	3049	3062	3087	rVB	353790	562017	53.08%	5.633%
79	10.532	3089	3092	3098	rBV2	372	328	0.03%	0.003%
80	10.561	3098	3101	3105	rBV2	478	339	0.03%	0.003%
81	10.622	3110	3120	3133	rVB3	4688	9650	0.91%	0.097%
82	10.776	3159	3168	3176	rBV	3246	4725	0.45%	0.047%
83	10.808	3176	3178	3184	rVB2	335	273	0.03%	0.003%
84	10.892	3201	3204	3207	rBV2	336	320	0.03%	0.003%
85	11.149	3282	3284	3293	rBV4	653	634	0.06%	0.006%
86	11.226	3305	3308	3312	rBV2	334	280	0.03%	0.003%
87	11.487	3376	3389	3408	rBV	629825	988600	93.36%	9.909%
88	11.670	3443	3446	3448	rBV2	523	309	0.03%	0.003%
89	11.760	3471	3474	3481	rVB3	544	523	0.05%	0.005%
90	11.863	3493	3506	3523	rBV	540695	872774	82.42%	8.748%
91	11.940	3527	3530	3534	rVV3	551	394	0.04%	0.004%
92	12.101	3576	3580	3583	rBV2	470	524	0.05%	0.005%
93	12.345	3653	3656	3658	rBV2	454	233	0.02%	0.002%
94	12.400	3671	3673	3679	rVB4	357	284	0.03%	0.003%
95	12.574	3721	3727	3738	rVB6	1049	1706	0.16%	0.017%
96	12.889	3821	3825	3830	rBV3	808	915	0.09%	0.009%
97	13.117	3893	3896	3899	rBV	383	275	0.03%	0.003%
98	13.384	3977	3979	3982	rBV2	385	268	0.03%	0.003%
99	14.455	4309	4312	4313	rBV3	585	264	0.02%	0.003%
100	14.667	4375	4378	4381	rBV2	505	383	0.04%	0.004%

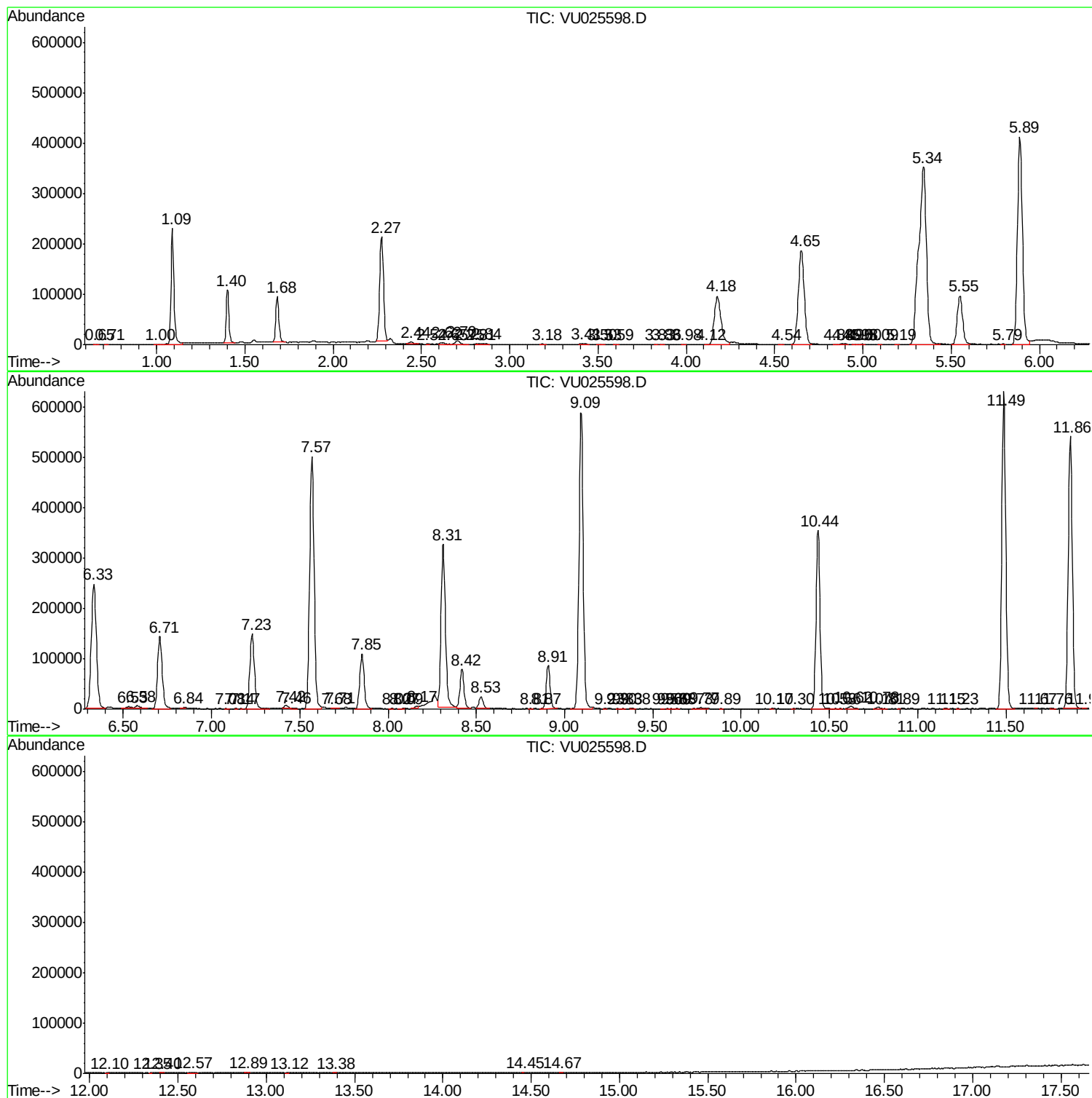
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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



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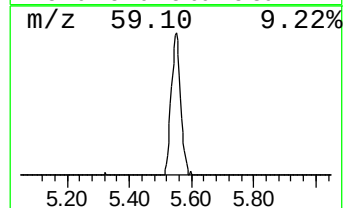
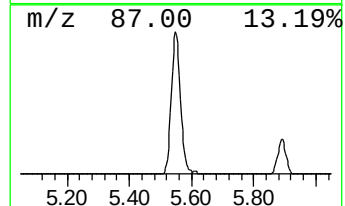
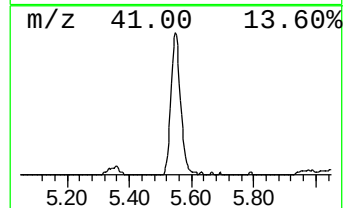
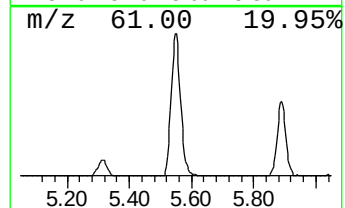
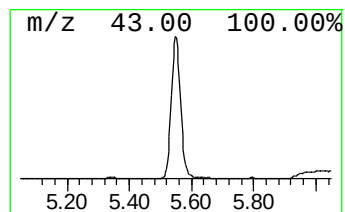
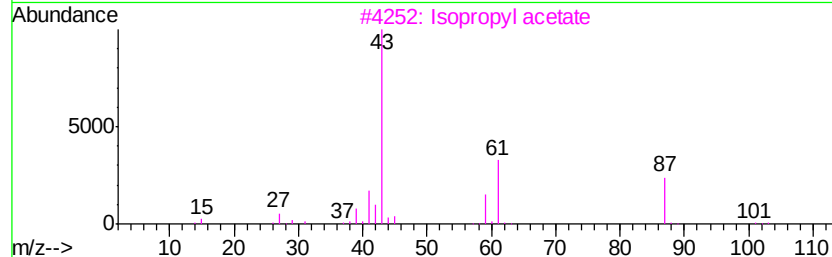
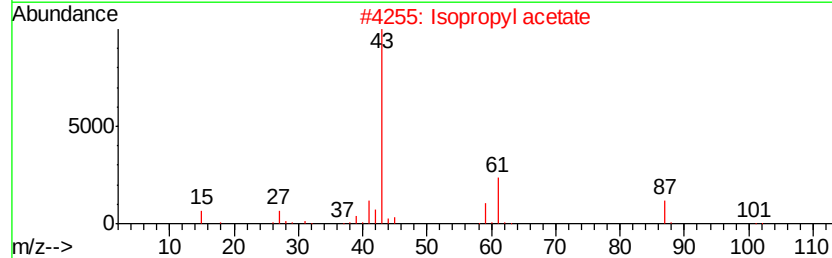
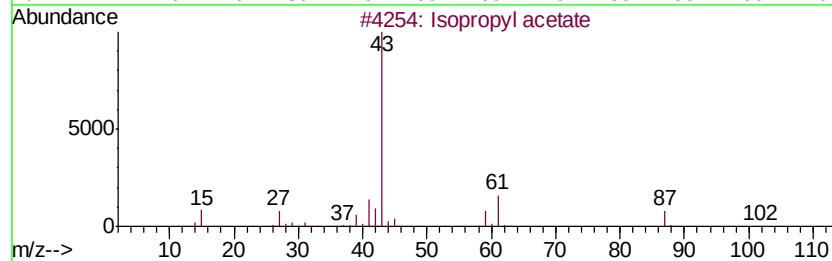
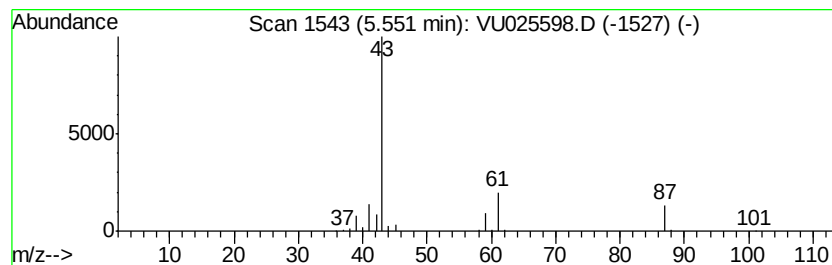
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.55	12.48 ug/L	199649	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl acetate	102	C5H10O2	000108-21-4	83
2		Isopropyl acetate	102	C5H10O2	000108-21-4	83
3		Isopropyl acetate	102	C5H10O2	000108-21-4	64
4		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	38
5		Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9



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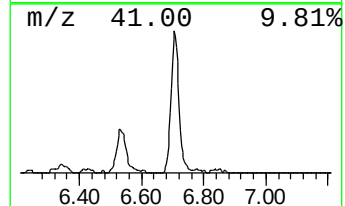
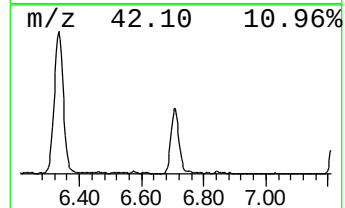
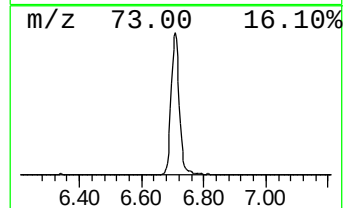
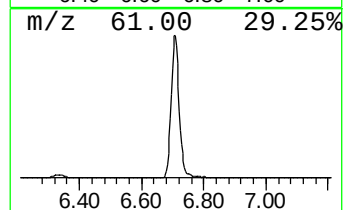
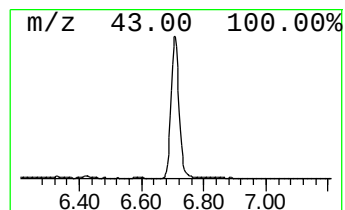
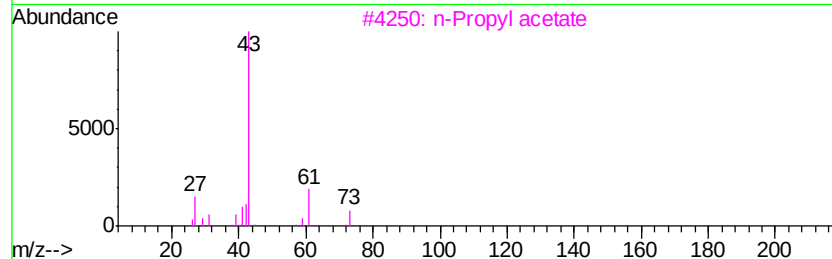
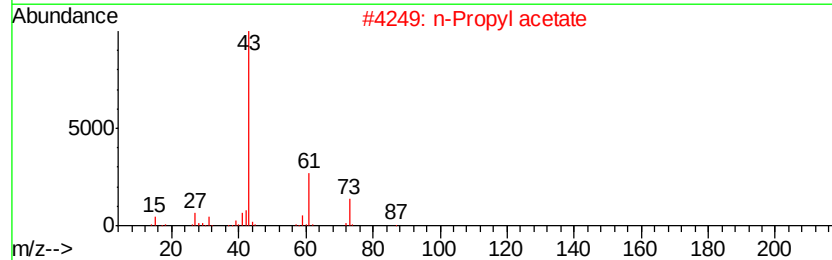
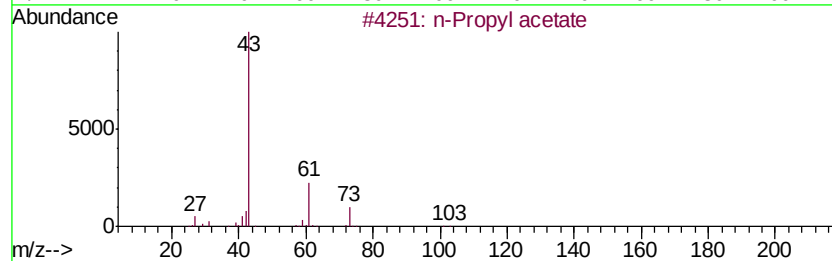
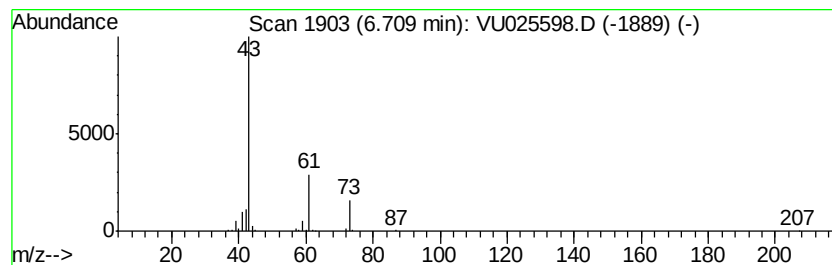
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	16.15 ug/L	258358	1,4-Difluorobenzene	5.89

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	50
4		Isopropyl acetate	102	C5H10O2	000108-21-4	36
5		Isopropyl acetate	102	C5H10O2	000108-21-4	9



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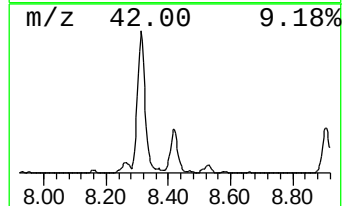
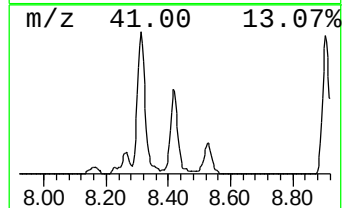
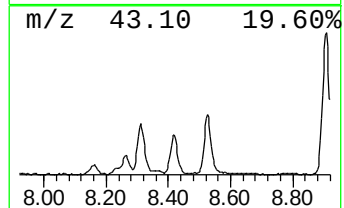
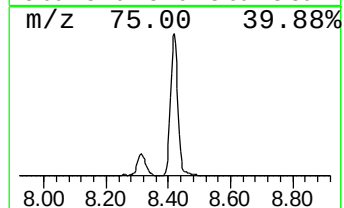
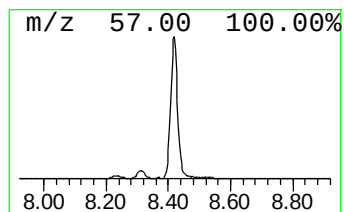
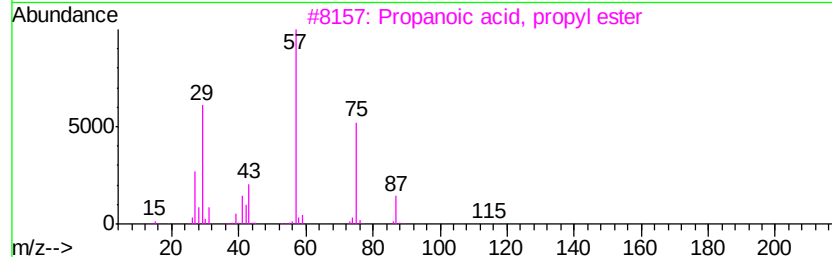
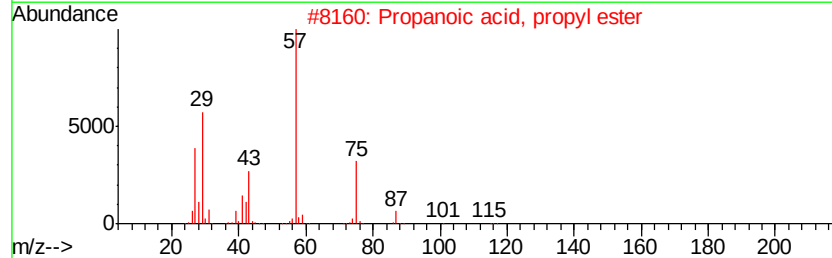
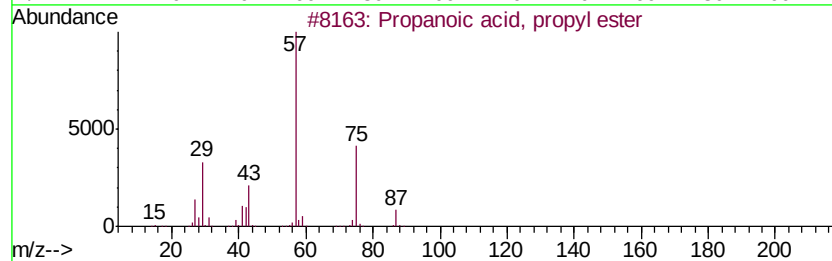
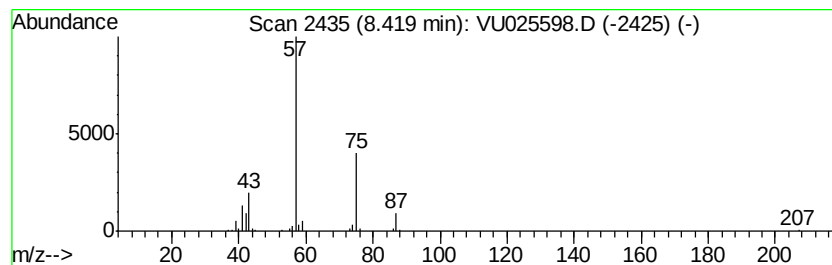
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Quant Title : VOC Analysis

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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	6.18 ug/L	120527	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	83
5		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39



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Sample : VLEB#02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
VLEB#02

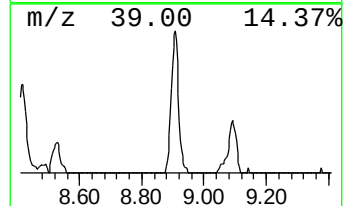
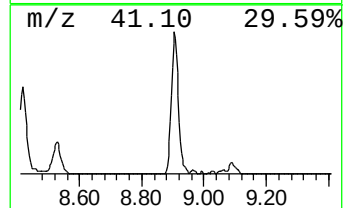
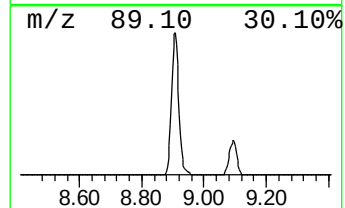
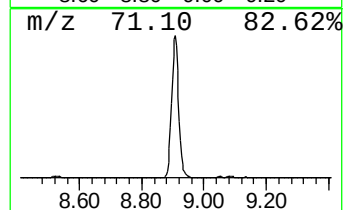
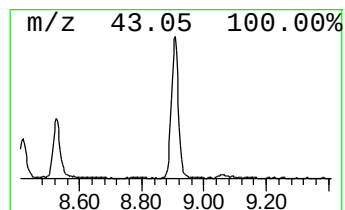
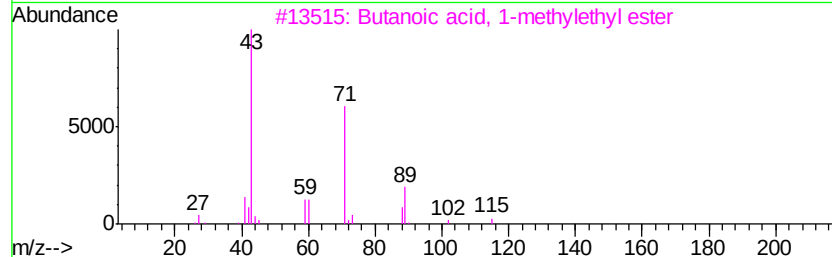
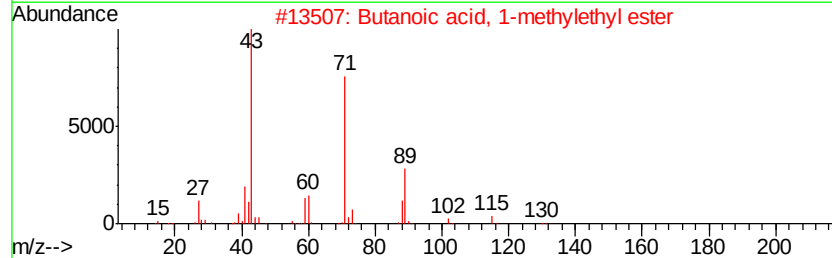
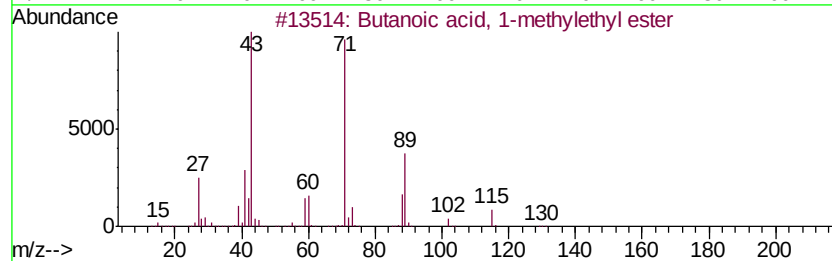
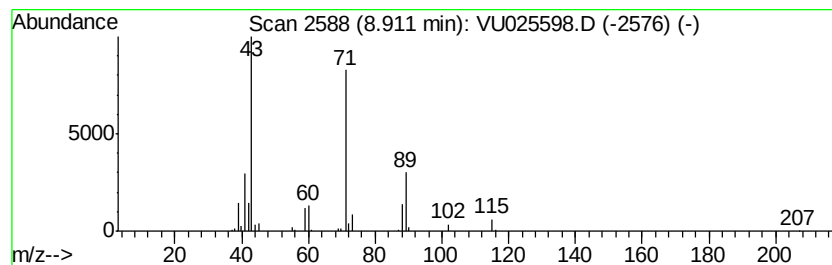
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Quant Title : VOC Analysis

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	6.98 ug/L	136003	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	78
4		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072318\
Data File : VU025598.D
Acq On : 23 Jul 2018 13:38
Operator : MD/SY
Sample : VLEB#02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB#02

Quant Method : Z:\VOASRV\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	12.5	ug/L	199649	1	5.89	799892	50.0
n-Propyl acetate	6.71	16.1	ug/L	258358	1	5.89	799892	50.0
Propanoic acid, p...	8.42	6.2	ug/L	120527	2	9.09	974596	50.0
Butanoic acid, 1-...	8.91	7.0	ug/L	136003	2	9.09	974596	50.0