

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
 Data File : VU025606.D
 Acq On : 23 Jul 2018 16:45
 Operator : MD/SY
 Sample : PB111343ZHE#12
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PB111343ZHE#12

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	0.628	5	12	15	RBV3	193	241	0.02%	0.002%
2	1.063	137	147	148	RBV2	1068	1320	0.13%	0.013%
3	1.091	148	156	169	RBV	166469	183886	17.69%	1.880%
4	1.403	246	253	266	rVB	104903	109228	10.51%	1.117%
5	1.683	333	340	357	rVB	89239	114578	11.02%	1.171%
6	2.275	514	524	535	RBV	204026	310507	29.87%	3.174%
7	2.323	535	539	552	rVB4	11086	17461	1.68%	0.178%
8	2.448	567	578	585	RBV2	3883	6828	0.66%	0.070%
9	2.619	624	631	642	rVB	4554	7827	0.75%	0.080%
10	2.709	650	659	668	rVB2	6774	11129	1.07%	0.114%
11	2.792	681	685	688	RBV3	368	254	0.02%	0.003%
12	2.834	693	698	699	RBV2	734	641	0.06%	0.007%
13	3.181	799	806	809	RBV2	598	720	0.07%	0.007%
14	3.320	843	849	852	rVV3	325	363	0.03%	0.004%
15	3.397	867	873	874	RBV2	828	592	0.06%	0.006%
16	3.525	910	913	918	RBV2	320	295	0.03%	0.003%
17	3.799	994	998	1001	rVB2	316	278	0.03%	0.003%
18	3.898	1026	1029	1035	RBV2	303	362	0.03%	0.004%
19	4.056	1075	1078	1082	RBV3	330	231	0.02%	0.002%
20	4.123	1093	1099	1100	RBV3	364	334	0.03%	0.003%
21	4.181	1102	1117	1138	RBV	98738	256875	24.71%	2.626%
22	4.493	1211	1214	1217	rVV3	377	309	0.03%	0.003%
23	4.519	1218	1222	1225	rVV3	603	452	0.04%	0.005%
24	4.541	1226	1229	1233	rVV2	390	270	0.03%	0.003%
25	4.654	1246	1264	1294	RBV	182415	432414	41.60%	4.420%
26	4.815	1310	1314	1315	RBV2	330	294	0.03%	0.003%
27	4.879	1330	1334	1336	RBV3	674	599	0.06%	0.006%
28	4.940	1350	1353	1361	rVB3	479	493	0.05%	0.005%
29	4.988	1361	1368	1375	RBV4	667	1038	0.10%	0.011%
30	5.062	1387	1391	1394	rVV3	332	238	0.02%	0.002%
31	5.246	1445	1448	1450	RBV3	315	244	0.02%	0.002%
32	5.345	1453	1479	1501	RBV2	345577	1039441	100.00%	10.626%
33	5.551	1529	1543	1562	RBV	99194	204803	19.70%	2.094%
34	5.664	1575	1578	1580	RBV	295	248	0.02%	0.003%

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 Title : VOC Analysis

35	5.750	1598	1605	1607	rBV2	518	714	0.07%	0.007%
36	5.892	1623	1649	1665	rBV	404501	861707	82.90%	8.809%
37	6.336	1773	1787	1807	rVB	242710	478998	46.08%	4.897%
38	6.709	1891	1903	1925	rBV	150674	267680	25.75%	2.736%
39	7.162	2040	2044	2048	rBV5	500	480	0.05%	0.005%
40	7.181	2048	2050	2052	rBV2	451	247	0.02%	0.003%
41	7.233	2053	2066	2082	rBV2	142392	250773	24.13%	2.564%
42	7.426	2117	2126	2132	rBV4	5821	9103	0.88%	0.093%
43	7.570	2157	2171	2189	rBV	489683	846025	81.39%	8.648%
44	7.754	2219	2228	2229	rBV4	2333	2851	0.27%	0.029%
45	7.853	2245	2259	2279	rBV	105758	178028	17.13%	1.820%
46	8.117	2338	2341	2344	rBV2	397	324	0.03%	0.003%
47	8.184	2346	2362	2371	rBV4	12509	32307	3.11%	0.330%
48	8.313	2392	2402	2425	rVB	345901	573335	55.16%	5.861%
49	8.419	2426	2435	2449	rVB	78528	123604	11.89%	1.264%
50	8.474	2449	2452	2454	rBV3	1315	1040	0.10%	0.011%
51	8.525	2460	2468	2481	rVB	22801	36382	3.50%	0.372%
52	8.596	2488	2490	2496	rVB4	475	352	0.03%	0.004%
53	8.667	2509	2512	2515	rVB3	441	318	0.03%	0.003%
54	8.709	2523	2525	2529	rVB4	641	325	0.03%	0.003%
55	8.744	2532	2536	2539	rVV3	636	444	0.04%	0.005%
56	8.908	2575	2587	2603	rBV	89173	141041	13.57%	1.442%
57	9.094	2626	2645	2665	rBV	551859	916515	88.17%	9.369%
58	9.233	2687	2688	2691	rBV2	382	225	0.02%	0.002%
59	9.516	2774	2776	2778	rBV2	532	343	0.03%	0.004%
60	9.596	2798	2801	2804	rBV2	420	285	0.03%	0.003%
61	9.680	2821	2827	2830	rBV2	547	555	0.05%	0.006%
62	9.770	2849	2855	2868	rVV5	2289	3773	0.36%	0.039%
63	9.975	2914	2919	2923	rBV2	712	627	0.06%	0.006%
64	10.316	3021	3025	3027	rBV2	390	255	0.02%	0.003%
65	10.332	3027	3030	3036	rVB3	479	476	0.05%	0.005%
66	10.435	3048	3062	3078	rBV	360850	567650	54.61%	5.803%
67	10.561	3098	3101	3103	rVB	442	264	0.03%	0.003%
68	10.622	3109	3120	3128	rBV6	3399	6684	0.64%	0.068%
69	10.776	3161	3168	3177	rVB4	3075	4373	0.42%	0.045%
70	10.882	3198	3201	3204	rBV3	413	361	0.03%	0.004%
71	10.972	3227	3229	3235	rVB3	854	633	0.06%	0.006%

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72	11.004	3235	3239	3242	rBV2	560	497	0.05%	0.005%
73	11.152	3281	3285	3288	rVB3	566	375	0.04%	0.004%
74	11.168	3288	3290	3294	rBV2	340	226	0.02%	0.002%
75	11.265	3313	3320	3332	rBV4	713	1197	0.12%	0.012%
76	11.384	3354	3357	3362	rVB3	456	445	0.04%	0.005%
77	11.487	3376	3389	3407	rBV	573537	907125	87.27%	9.273%
78	11.651	3437	3440	3442	rBV3	572	356	0.03%	0.004%
79	11.773	3476	3478	3482	rVB2	486	302	0.03%	0.003%
80	11.805	3486	3488	3491	rVB	495	235	0.02%	0.002%
81	11.863	3491	3506	3521	rBV	528795	849713	81.75%	8.686%
82	12.104	3578	3581	3583	rBV2	467	289	0.03%	0.003%
83	12.467	3692	3694	3695	rBV	473	232	0.02%	0.002%
84	12.638	3742	3747	3753	rBV6	1025	1182	0.11%	0.012%
85	12.766	3783	3787	3789	rBV2	504	361	0.03%	0.004%
86	12.888	3822	3825	3826	rBV3	722	408	0.04%	0.004%
87	12.975	3849	3852	3854	rBV2	586	367	0.04%	0.004%
88	13.223	3926	3929	3931	rBV	382	290	0.03%	0.003%
89	13.303	3951	3954	3959	rBV3	420	337	0.03%	0.003%
90	13.512	4017	4019	4023	rVB2	648	328	0.03%	0.003%
91	13.605	4046	4048	4051	rVB2	485	229	0.02%	0.002%
92	13.712	4078	4081	4086	rVB3	696	481	0.05%	0.005%
93	13.869	4126	4130	4136	rBV3	644	766	0.07%	0.008%
94	13.975	4159	4163	4167	rBV2	419	434	0.04%	0.004%
95	14.043	4182	4184	4187	rBV3	505	299	0.03%	0.003%
96	14.162	4218	4221	4224	rBV2	602	363	0.03%	0.004%
97	14.261	4250	4252	4254	rBV2	456	283	0.03%	0.003%
98	14.908	4450	4453	4459	rVB4	678	493	0.05%	0.005%
99	14.998	4479	4481	4484	rBV2	519	274	0.03%	0.003%
100	15.020	4484	4488	4492	rVV3	781	661	0.06%	0.007%

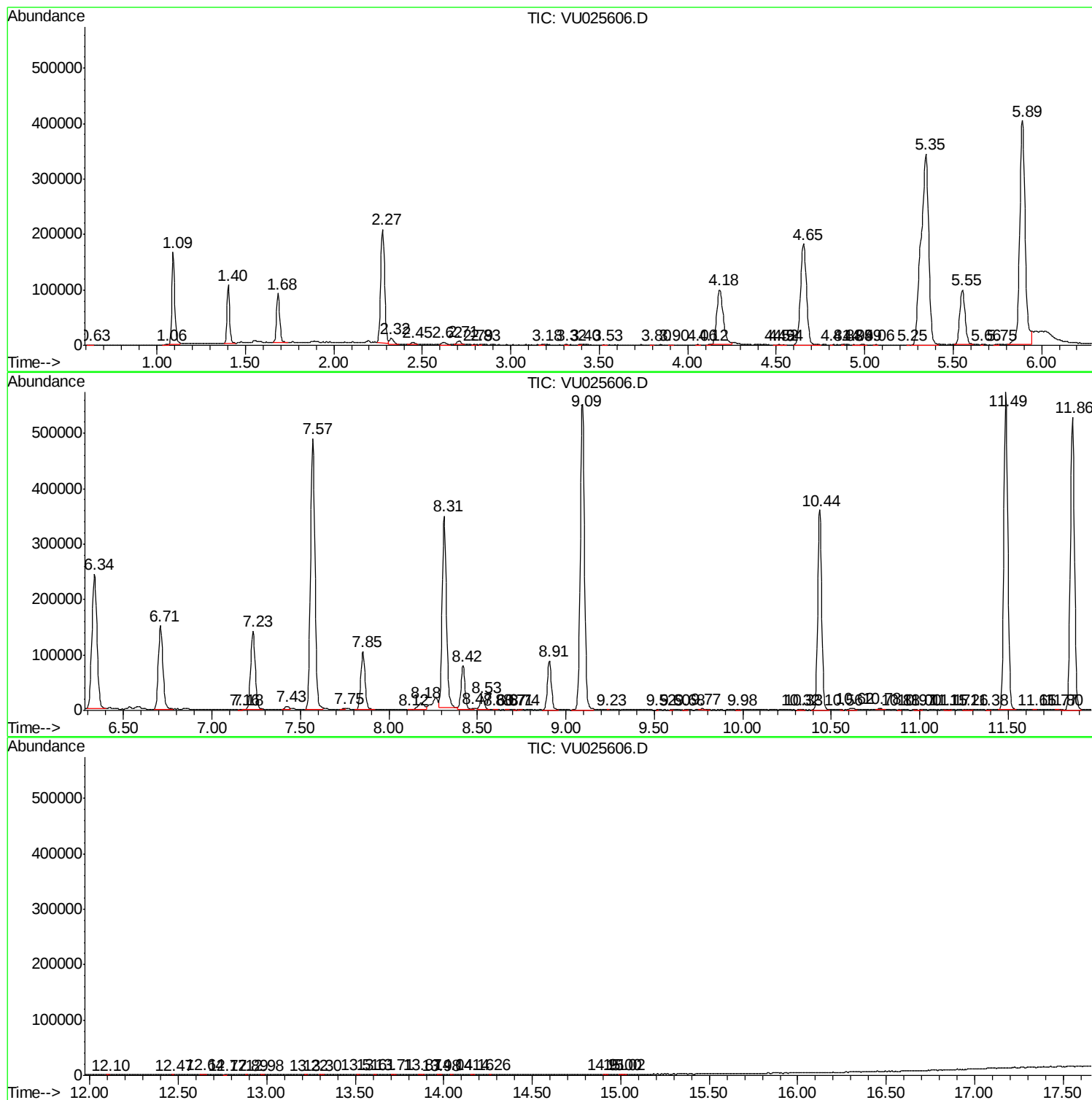
Sum of corrected areas: 9782438

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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



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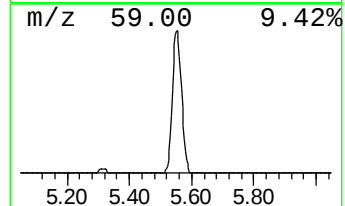
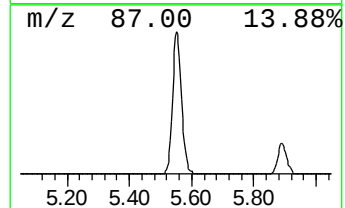
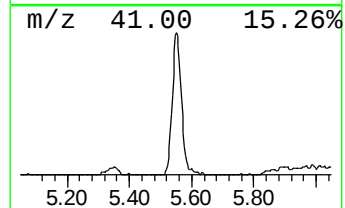
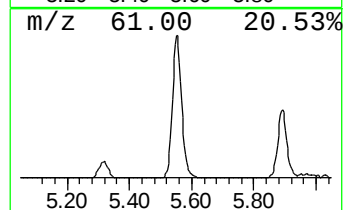
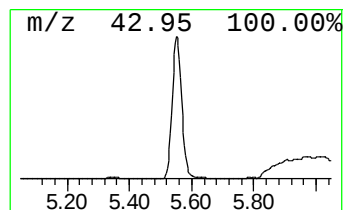
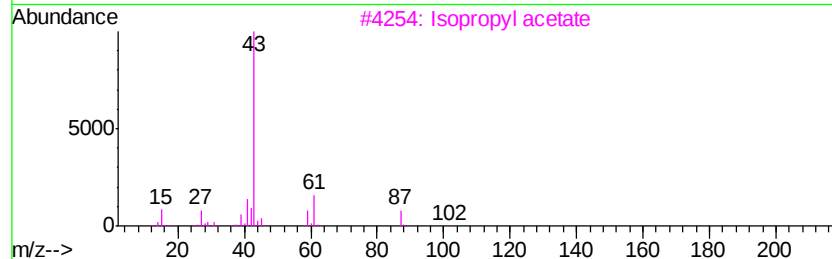
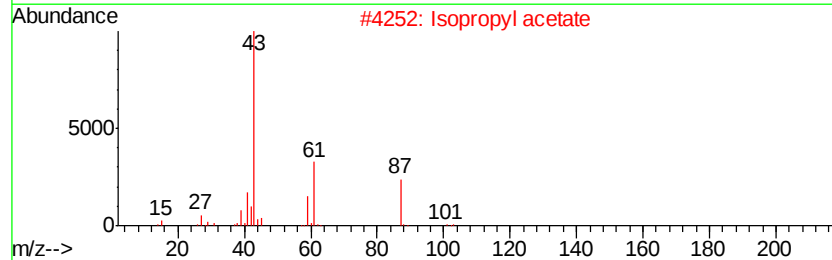
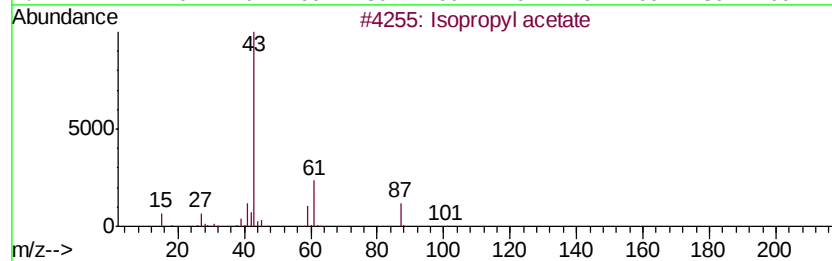
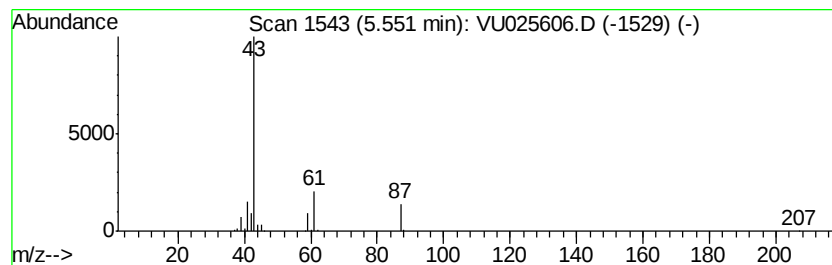
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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	11.88 ug/L	204803	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	78
3		Isopropyl acetate	102	C5H10O2	000108-21-4	56
4		Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9
5		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	9



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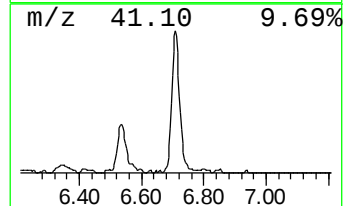
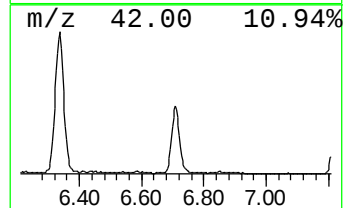
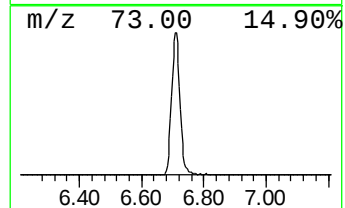
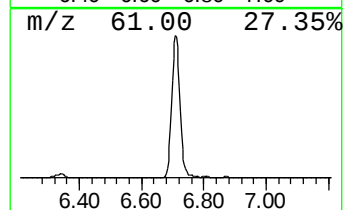
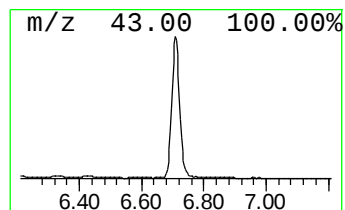
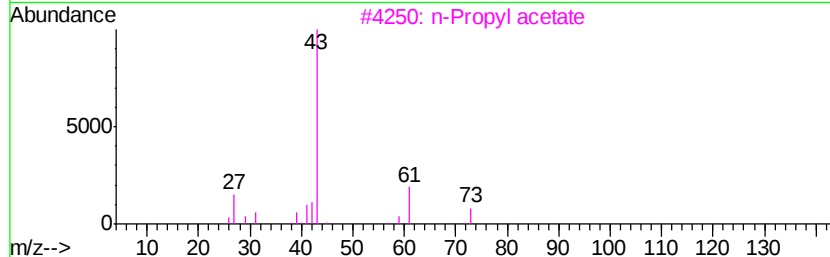
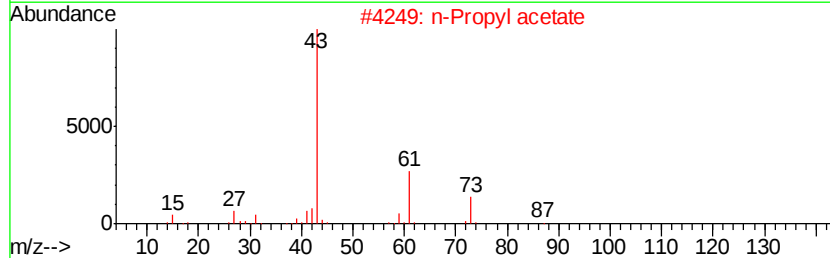
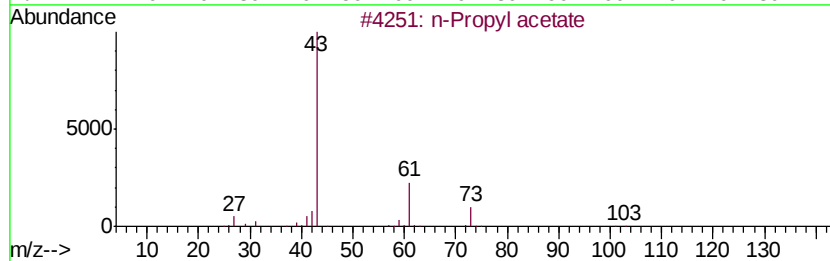
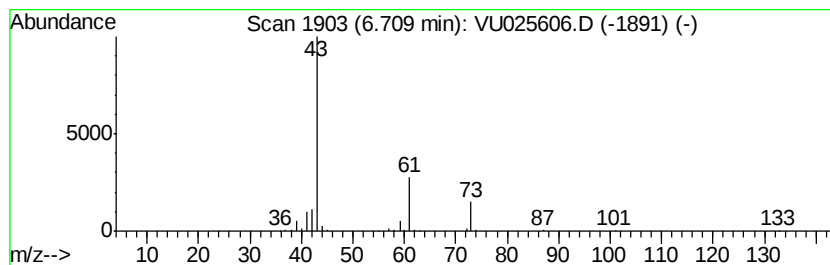
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Quant Title : VOC Analysis

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

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	15.53 ug/L	267680	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	78
4		Isopropyl acetate	102	C5H10O2	000108-21-4	36
5		Isobutylamine	73	C4H11N	000078-81-9	9



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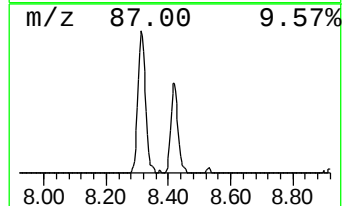
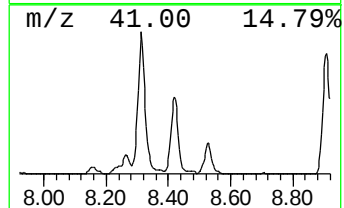
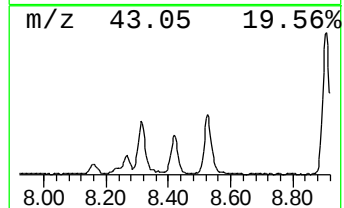
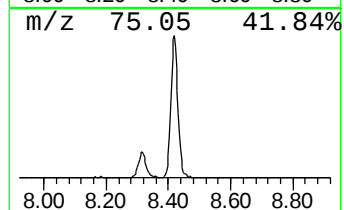
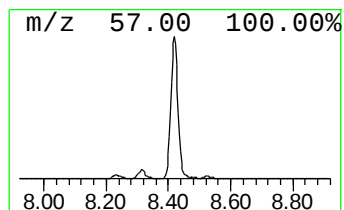
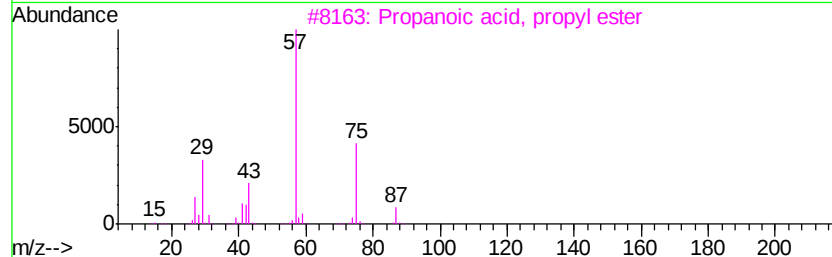
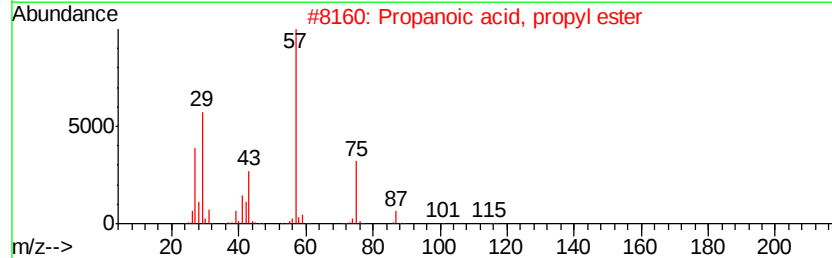
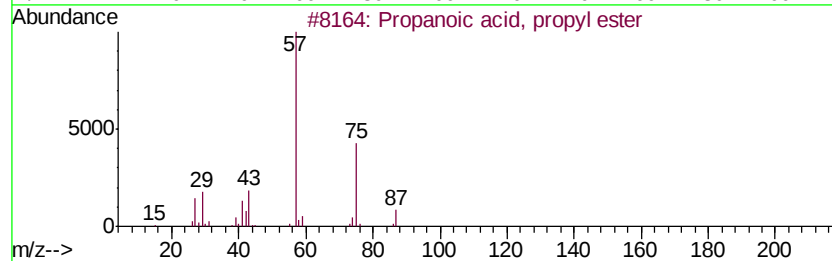
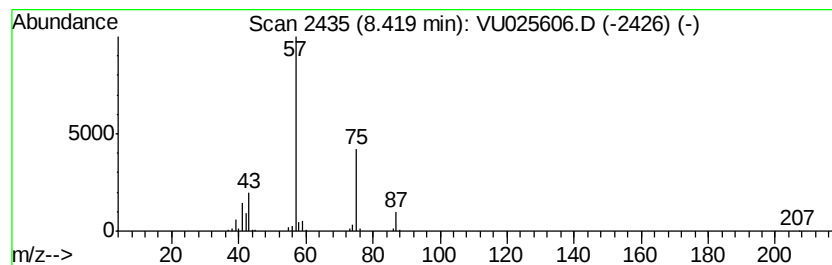
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Peak Number 5 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	6.74 ug/L	123604	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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025606.D
Acq On : 23 Jul 2018 16:45
Operator : MD/SY
Sample : PB111343ZHE#12
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#12

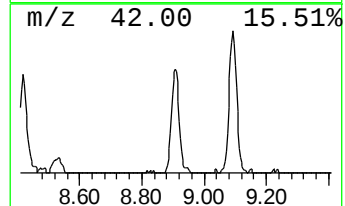
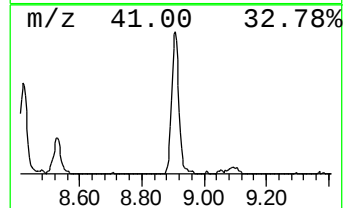
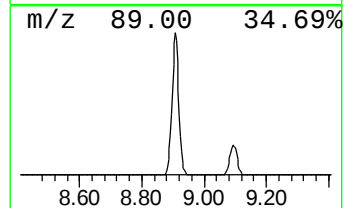
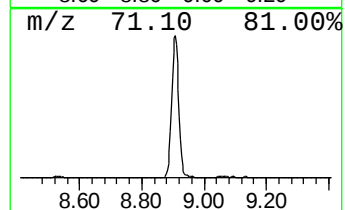
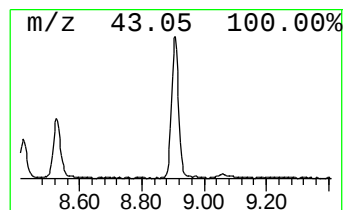
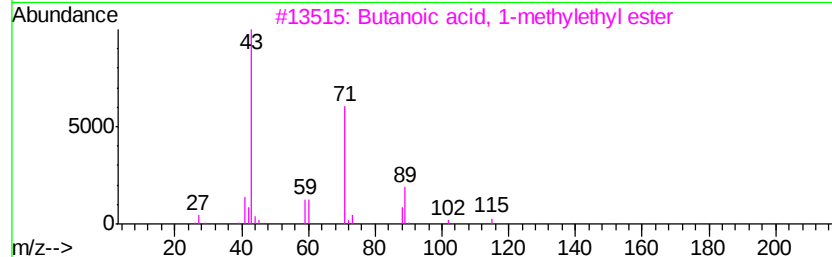
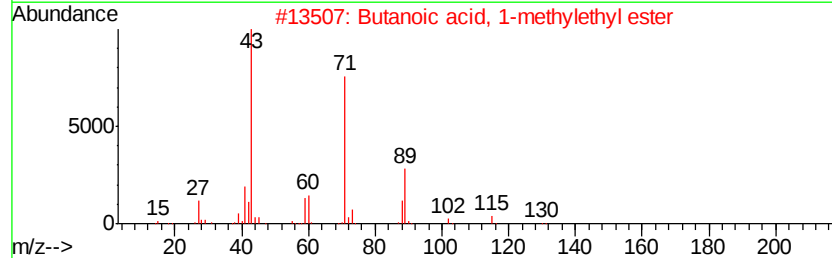
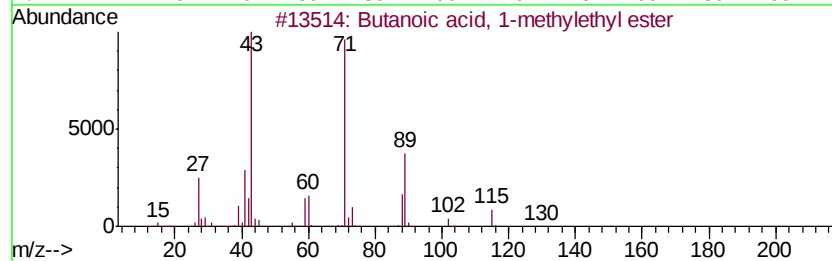
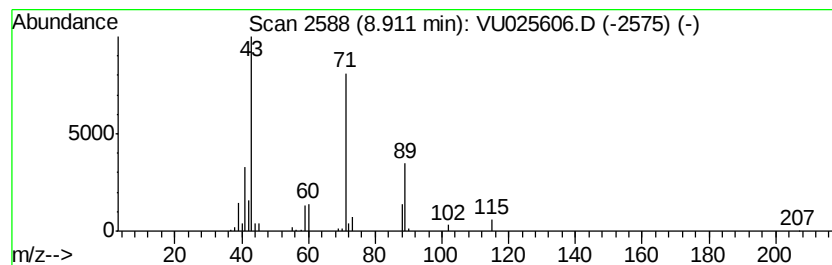
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Quant Title : VOC Analysis

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	7.69 ug/L	141041	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		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	72
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU072318\
Data File : VU025606.D
Acq On : 23 Jul 2018 16:45
Operator : MD/SY
Sample : PB111343ZHE#12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#12

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	11.9	ug/L	204803	1	5.89	861707	50.0
n-Propyl acetate	6.71	15.5	ug/L	267680	1	5.89	861707	50.0
Propanoic acid, p...	8.42	6.7	ug/L	123604	2	9.09	916515	50.0
Butanoic acid, 1-...	8.91	7.7	ug/L	141041	2	9.09	916515	50.0