

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
 Data File : VU025602.D
 Acq On : 23 Jul 2018 15:11
 Operator : MD/SY
 Sample : PB111343ZHE#08
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PB111343ZHE#08

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	0.619	5	9	11	rBV3	365	270	0.03%	0.003%
2	0.770	51	56	59	rVB3	307	279	0.03%	0.003%
3	0.834	72	76	80	rBV3	225	226	0.02%	0.002%
4	0.860	80	84	88	rVV	346	316	0.03%	0.003%
5	1.092	142	156	171	rBV	145934	167969	15.97%	1.705%
6	1.400	246	252	263	rBV	104711	110297	10.49%	1.119%
7	1.683	332	340	353	rVB	90671	114413	10.88%	1.161%
8	2.275	513	524	534	rBV	204227	306440	29.14%	3.110%
9	2.445	569	577	591	rBV2	3566	7143	0.68%	0.072%
10	2.555	608	611	614	rVB3	549	303	0.03%	0.003%
11	2.590	619	622	624	rVV	707	383	0.04%	0.004%
12	2.619	624	631	640	rVV3	3613	5970	0.57%	0.061%
13	2.706	649	658	674	rVB2	7661	13369	1.27%	0.136%
14	2.777	676	680	681	rBV3	372	297	0.03%	0.003%
15	2.822	688	694	695	rBV4	918	719	0.07%	0.007%
16	2.963	734	738	740	rBV2	318	278	0.03%	0.003%
17	2.986	740	745	748	rVV2	425	375	0.04%	0.004%
18	3.005	748	751	757	rVB3	377	373	0.04%	0.004%
19	3.133	789	791	796	rVB3	349	252	0.02%	0.003%
20	3.249	823	827	829	rVV3	233	218	0.02%	0.002%
21	3.346	854	857	860	rBV	308	240	0.02%	0.002%
22	3.407	868	876	879	rBV6	982	1418	0.13%	0.014%
23	3.526	909	913	916	rBV3	328	298	0.03%	0.003%
24	3.580	922	930	934	rBV3	476	531	0.05%	0.005%
25	3.606	934	938	942	rBV4	251	232	0.02%	0.002%
26	3.709	968	970	974	rBV	269	211	0.02%	0.002%
27	4.178	1097	1116	1138	rBV2	101956	262549	24.97%	2.664%
28	4.474	1203	1208	1211	rBV3	457	493	0.05%	0.005%
29	4.535	1223	1227	1234	rBV3	593	808	0.08%	0.008%
30	4.654	1247	1264	1283	rBV	189156	440400	41.88%	4.469%
31	4.889	1330	1337	1343	rVB4	967	1386	0.13%	0.014%
32	4.956	1354	1358	1360	rBV3	455	322	0.03%	0.003%
33	4.982	1362	1366	1368	rBV3	441	347	0.03%	0.004%
34	5.050	1381	1387	1389	rBV2	296	319	0.03%	0.003%

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Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
 Title : VOC Analysis

35	5.133	1410	1413	1417	rBV2	386	316	0.03%	0.003%
36	5.159	1417	1421	1424	rVV2	319	236	0.02%	0.002%
37	5.239	1441	1446	1451	rVB3	386	420	0.04%	0.004%
38	5.346	1451	1479	1508	rBV2	349594	1051652	100.00%	10.673%
39	5.551	1529	1543	1568	rBV	96973	200135	19.03%	2.031%
40	5.741	1597	1602	1606	rBV3	645	726	0.07%	0.007%
41	5.892	1624	1649	1665	rBV	411552	880710	83.75%	8.938%
42	6.336	1773	1787	1808	rVB	247558	488467	46.45%	4.957%
43	6.535	1843	1849	1856	rBV2	2374	4018	0.38%	0.041%
44	6.709	1891	1903	1922	rBV	145832	257050	24.44%	2.609%
45	7.088	2019	2021	2023	rBV	402	211	0.02%	0.002%
46	7.140	2032	2037	2043	rBV4	560	725	0.07%	0.007%
47	7.169	2043	2046	2051	rVV3	423	347	0.03%	0.004%
48	7.233	2053	2066	2090	rVV2	146403	260496	24.77%	2.644%
49	7.423	2117	2125	2134	rBV2	5570	8969	0.85%	0.091%
50	7.571	2158	2171	2193	rBV	493110	861361	81.91%	8.742%
51	7.760	2220	2230	2243	rVB7	2925	7063	0.67%	0.072%
52	7.853	2247	2259	2272	rBV	107029	181680	17.28%	1.844%
53	8.185	2347	2362	2369	rBV4	10282	26163	2.49%	0.266%
54	8.313	2392	2402	2424	rVB	341183	577867	54.95%	5.864%
55	8.419	2425	2435	2449	rVB	76399	120832	11.49%	1.226%
56	8.525	2460	2468	2484	rVB2	23601	38113	3.62%	0.387%
57	8.632	2499	2501	2504	rVB2	509	263	0.03%	0.003%
58	8.770	2540	2544	2546	rBV2	424	300	0.03%	0.003%
59	8.908	2575	2587	2603	rBV	85423	134474	12.79%	1.365%
60	9.091	2627	2644	2671	rVV	553320	924824	87.94%	9.386%
61	9.323	2711	2716	2719	rBV4	598	584	0.06%	0.006%
62	9.368	2728	2730	2733	rVV2	539	356	0.03%	0.004%
63	9.390	2733	2737	2743	rVB5	704	773	0.07%	0.008%
64	9.429	2743	2749	2752	rBV3	413	479	0.05%	0.005%
65	9.583	2793	2797	2801	rBV3	419	507	0.05%	0.005%
66	9.651	2816	2818	2821	rVB	385	213	0.02%	0.002%
67	9.767	2847	2854	2866	rBV9	2560	4377	0.42%	0.044%
68	9.860	2880	2883	2884	rBV	404	245	0.02%	0.002%
69	9.889	2889	2892	2899	rVV4	421	411	0.04%	0.004%
70	10.123	2962	2965	2969	rBV3	521	385	0.04%	0.004%
71	10.168	2972	2979	2984	rBV3	496	670	0.06%	0.007%

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72	10.233	2996	2999	3002	rBV2	746	535	0.05%	0.005%
73	10.249	3002	3004	3006	rVB	823	378	0.04%	0.004%
74	10.297	3016	3019	3021	rBV2	404	220	0.02%	0.002%
75	10.316	3022	3025	3030	rVB3	556	376	0.04%	0.004%
76	10.435	3049	3062	3082	rBV	358750	566038	53.82%	5.744%
77	10.567	3100	3103	3107	rVB3	479	337	0.03%	0.003%
78	10.615	3107	3118	3133	rBV4	3071	6050	0.58%	0.061%
79	10.776	3160	3168	3175	rVV3	3167	4287	0.41%	0.044%
80	11.281	3322	3325	3329	rBV	291	247	0.02%	0.003%
81	11.310	3330	3334	3337	rBV2	413	361	0.03%	0.004%
82	11.365	3349	3351	3356	rVB3	503	394	0.04%	0.004%
83	11.390	3356	3359	3360	rBV3	542	299	0.03%	0.003%
84	11.487	3376	3389	3405	rBV	596943	930089	88.44%	9.439%
85	11.644	3432	3438	3442	rVB3	590	653	0.06%	0.007%
86	11.715	3457	3460	3462	rBV2	527	299	0.03%	0.003%
87	11.799	3484	3486	3493	rVB3	367	343	0.03%	0.003%
88	11.863	3493	3506	3525	rBV	538016	861629	81.93%	8.744%
89	12.021	3552	3555	3558	rBV2	459	358	0.03%	0.004%
90	12.483	3696	3699	3701	rBV2	594	379	0.04%	0.004%
91	12.574	3725	3727	3730	rBV3	395	257	0.02%	0.003%
92	12.631	3740	3745	3746	rBV4	638	554	0.05%	0.006%
93	12.895	3823	3827	3830	rBV4	705	666	0.06%	0.007%
94	13.085	3883	3886	3888	rVB	555	280	0.03%	0.003%
95	13.101	3888	3891	3896	rBV2	454	457	0.04%	0.005%
96	13.239	3931	3934	3935	rBV	448	233	0.02%	0.002%
97	13.564	4033	4035	4037	rBV2	444	241	0.02%	0.002%
98	14.168	4216	4223	4227	rBV4	835	1028	0.10%	0.010%
99	14.448	4307	4310	4314	rBV3	582	483	0.05%	0.005%
100	15.040	4492	4494	4496	rBV	654	349	0.03%	0.004%

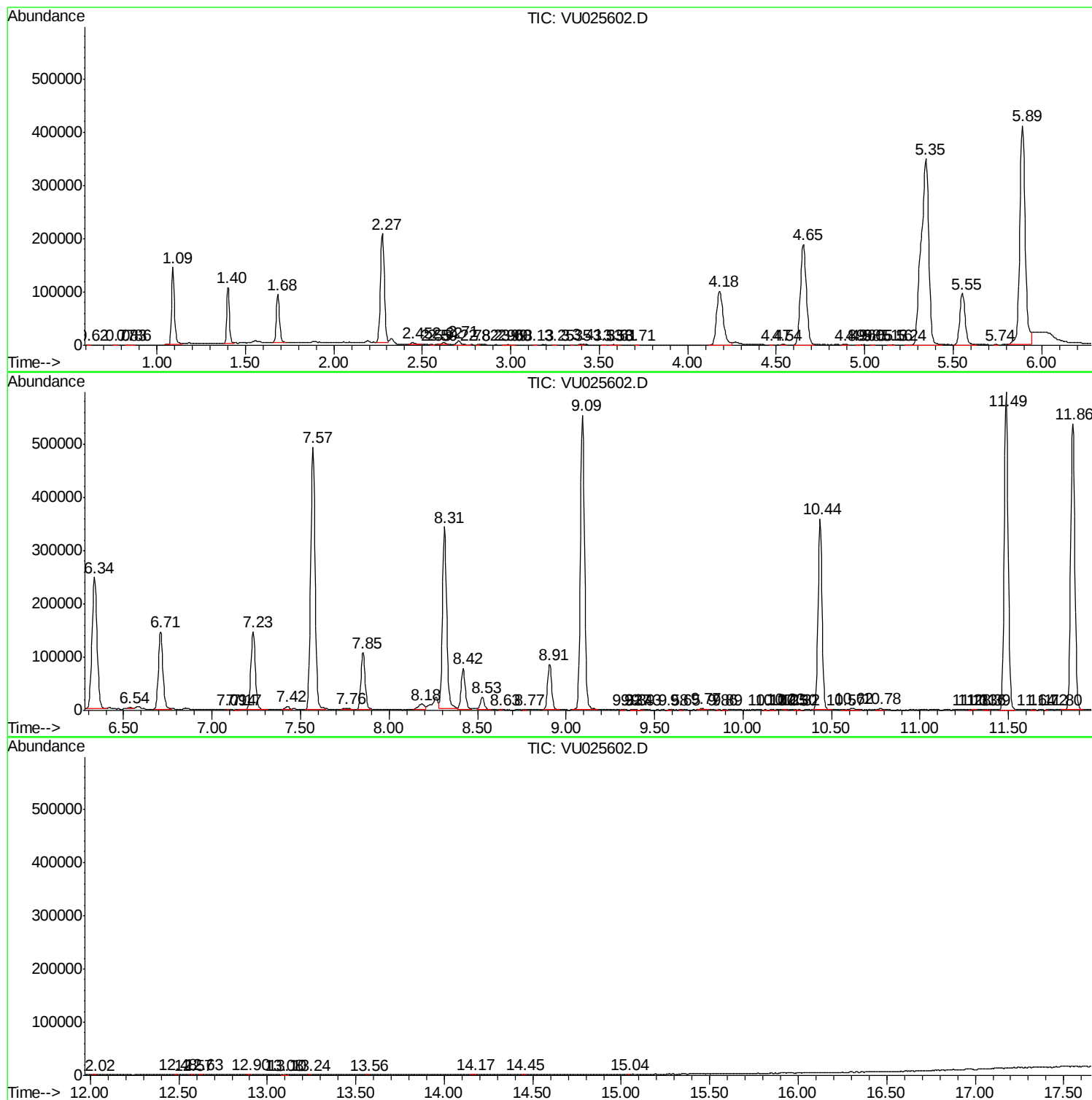
Sum of corrected areas: 9853682

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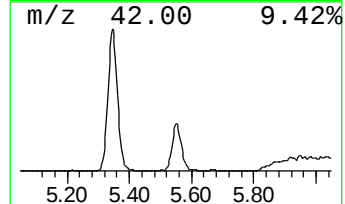
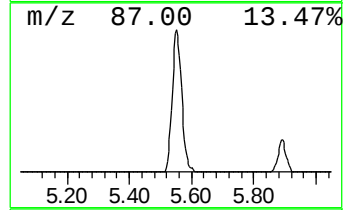
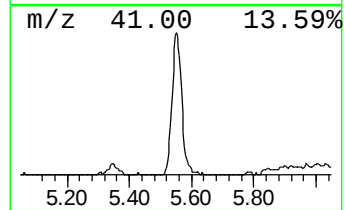
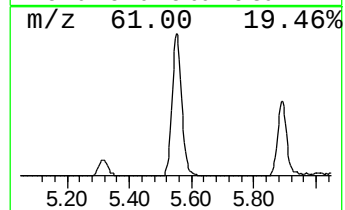
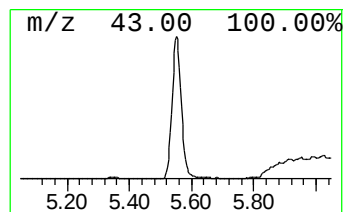
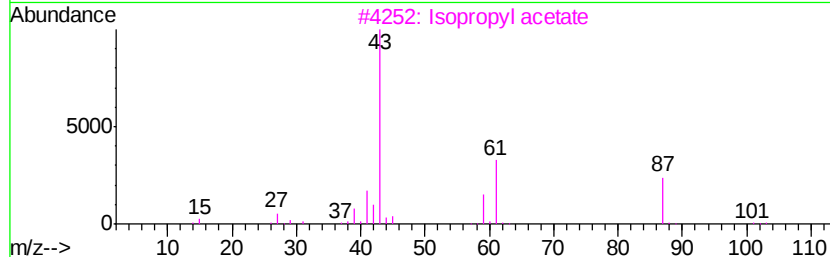
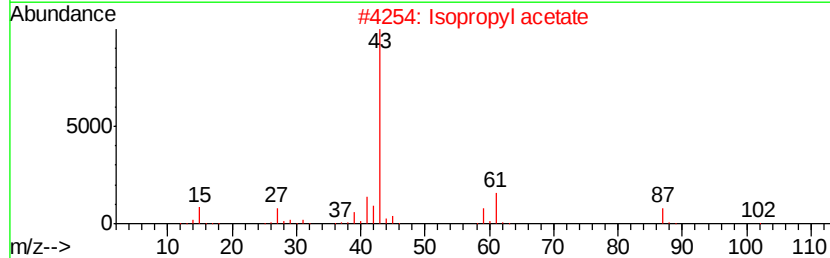
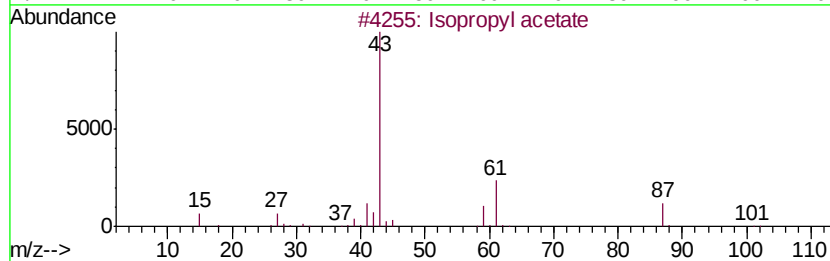
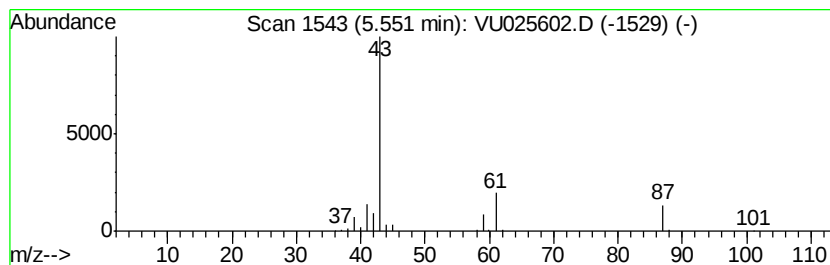
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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	11.36 ug/L	200135	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	64
3	Isopropyl	acetate	102	C5H10O2	000108-21-4	64
4	1,1-Ethanediol,	diacetate	146	C6H10O4	000542-10-9	9
5	sec-Butyl	acetate	116	C6H12O2	000105-46-4	9



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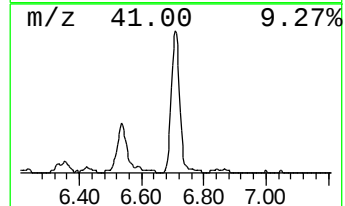
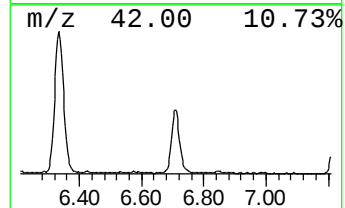
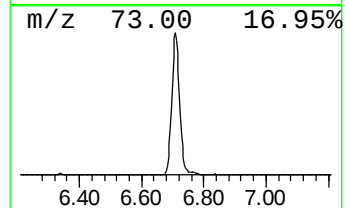
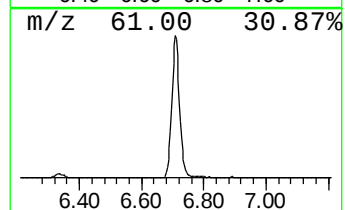
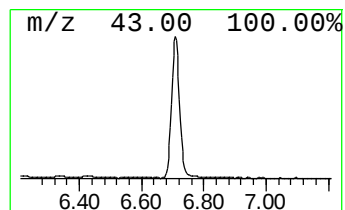
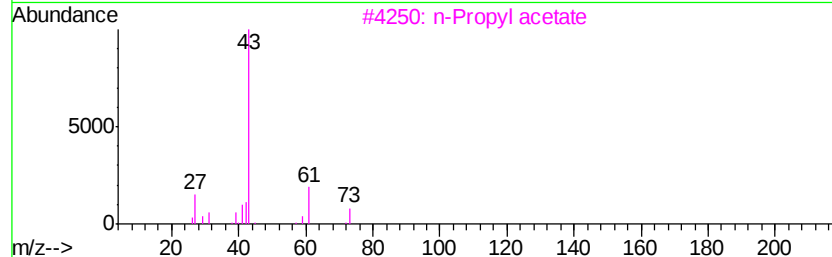
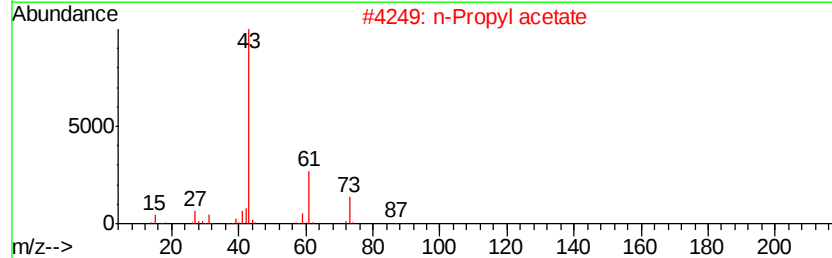
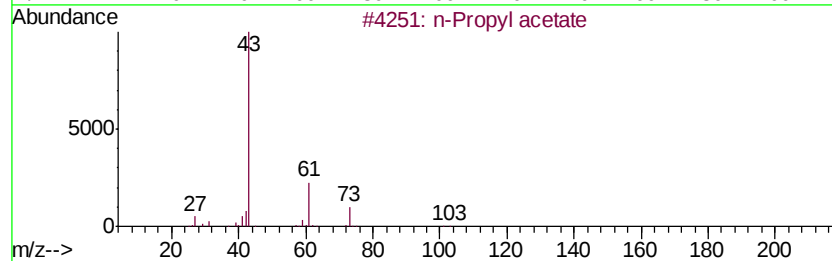
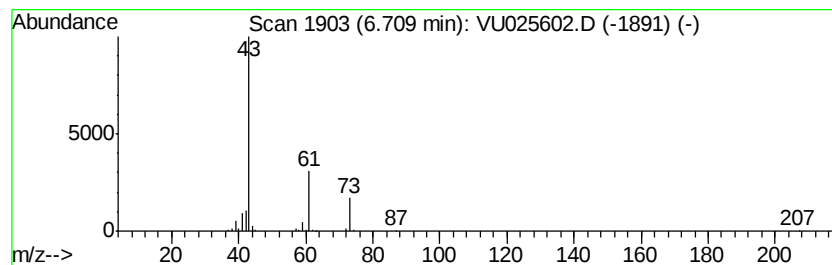
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Quant Title : VOC Analysis

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

Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	14.59 ug/L	257050	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	83
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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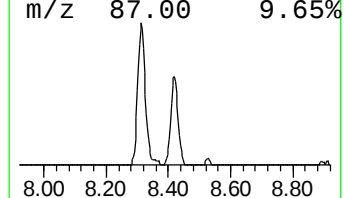
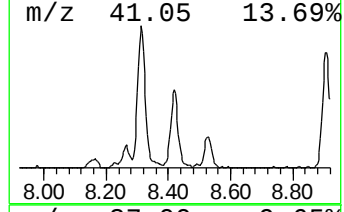
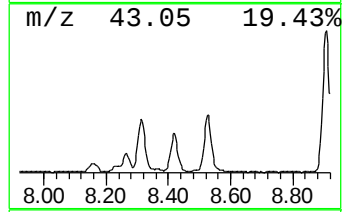
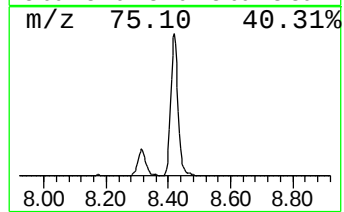
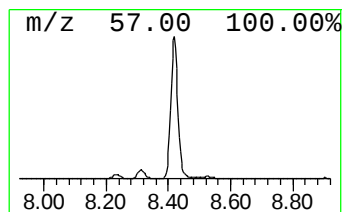
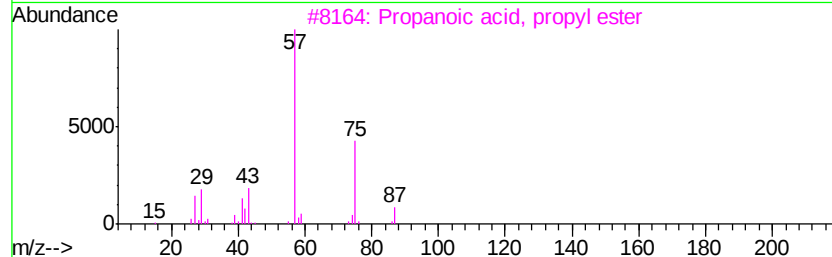
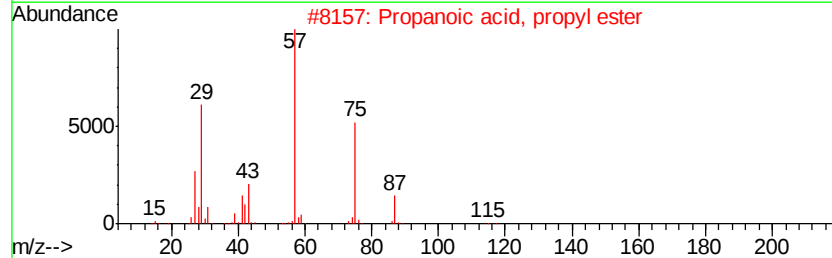
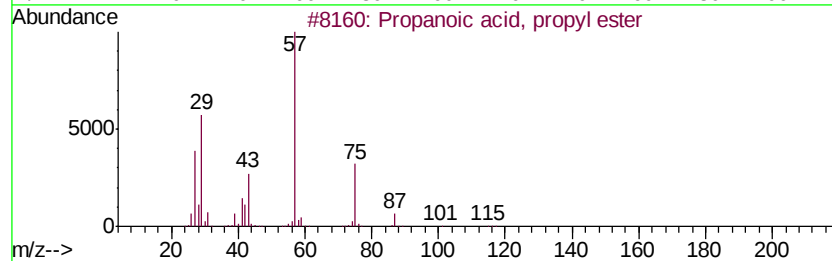
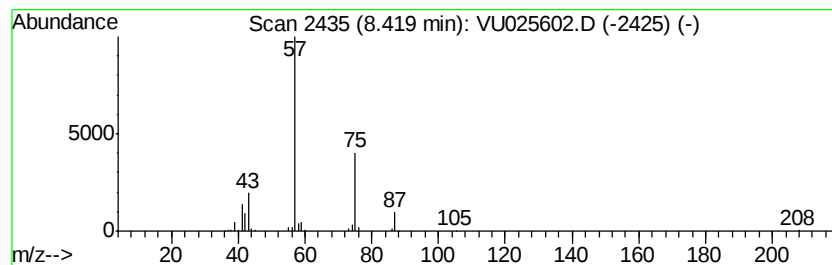
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Quant Title : VOC Analysis

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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	6.53 ug/L	120832	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 : VU025602.D
Acq On : 23 Jul 2018 15:11
Operator : MD/SY
Sample : PB111343ZHE#08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#08

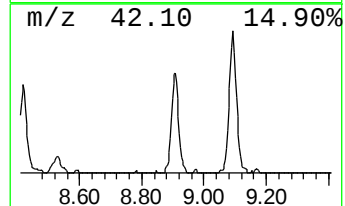
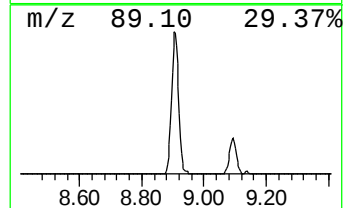
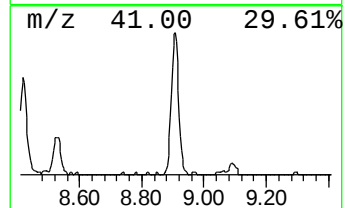
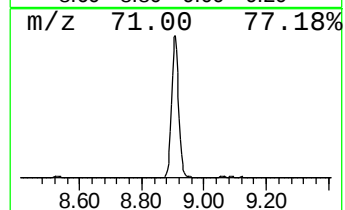
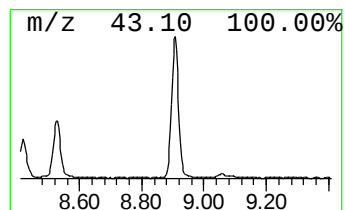
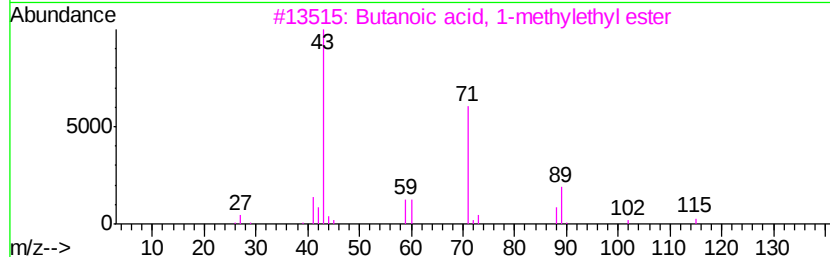
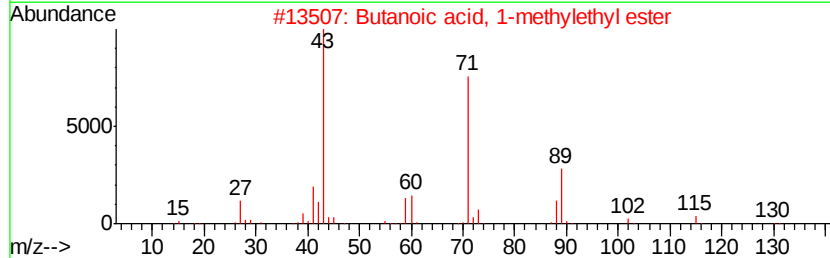
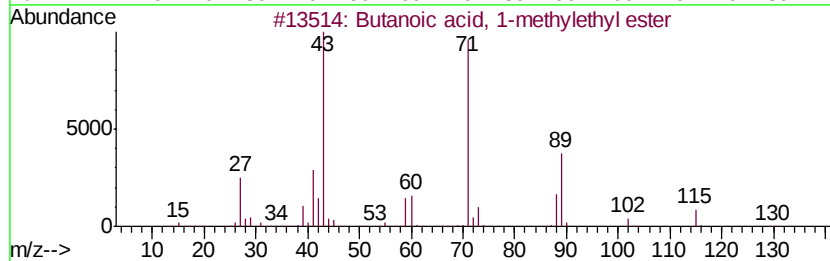
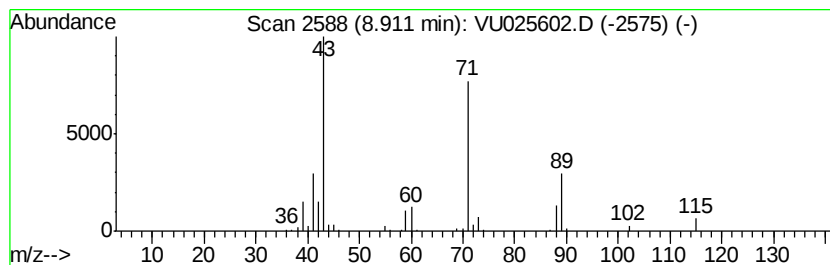
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Quant Title : VOC Analysis

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	7.27 ug/L	134474	Chlorobenzene-d5	9.09

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



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ClientSampleId :
PB111343ZHE#08

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	11.4	ug/L	200135	1	5.89	880710	50.0
n-Propyl acetate	6.71	14.6	ug/L	257050	1	5.89	880710	50.0
Propanoic acid, p...	8.42	6.5	ug/L	120832	2	9.09	924824	50.0
Butanoic acid, 1-...	8.91	7.3	ug/L	134474	2	9.09	924824	50.0