

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
 Data File : VU025605.D
 Acq On : 23 Jul 2018 16:21
 Operator : MD/SY
 Sample : PB111343ZHE#11
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PB111343ZHE#11

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	0.677	23	27	33	rVV3	237	268	0.03%	0.003%
2	0.754	48	51	60	rVB3	346	461	0.04%	0.005%
3	1.056	138	145	146	rBV2	963	759	0.07%	0.008%
4	1.092	148	156	171	rBV	155726	175081	16.92%	1.793%
5	1.404	246	253	262	rBV	100710	103961	10.05%	1.065%
6	1.683	333	340	355	rVB	90398	114386	11.06%	1.171%
7	2.275	514	524	535	rBV	201009	299383	28.94%	3.066%
8	2.384	556	558	562	rVB2	831	453	0.04%	0.005%
9	2.407	562	565	569	rVV3	679	414	0.04%	0.004%
10	2.448	569	578	594	rVB	4378	7893	0.76%	0.081%
11	2.551	606	610	611	rBV	464	320	0.03%	0.003%
12	2.622	623	632	640	rBV	4074	6982	0.67%	0.071%
13	2.706	649	658	671	rVB3	6576	12411	1.20%	0.127%
14	2.841	690	700	702	rBV3	2009	2860	0.28%	0.029%
15	2.966	738	739	746	rVB3	451	325	0.03%	0.003%
16	3.002	746	750	754	rBV4	315	301	0.03%	0.003%
17	3.137	787	792	795	rBV3	471	417	0.04%	0.004%
18	3.256	824	829	833	rVB2	346	330	0.03%	0.003%
19	3.323	847	850	854	rVB2	717	519	0.05%	0.005%
20	3.416	865	879	891	rVB6	1629	3400	0.33%	0.035%
21	3.719	967	973	977	rBV3	317	395	0.04%	0.004%
22	3.767	983	988	990	rBV3	289	311	0.03%	0.003%
23	3.831	999	1008	1009	rBV	496	598	0.06%	0.006%
24	3.905	1028	1031	1034	rVV3	403	282	0.03%	0.003%
25	4.182	1101	1117	1136	rBV	100040	262603	25.38%	2.689%
26	4.654	1244	1264	1292	rBV	186126	436689	42.21%	4.472%
27	4.831	1316	1319	1322	rVB	533	270	0.03%	0.003%
28	4.863	1322	1329	1331	rBV3	519	545	0.05%	0.006%
29	4.985	1361	1367	1368	rBV	495	456	0.04%	0.005%
30	5.345	1450	1479	1502	rBV2	344090	1034498	100.00%	10.594%
31	5.551	1530	1543	1563	rBV	99649	202943	19.62%	2.078%
32	5.802	1618	1621	1624	rVB3	385	254	0.02%	0.003%
33	5.892	1624	1649	1670	rBV	407621	887544	85.79%	9.089%
34	6.336	1773	1787	1805	rVB	243198	478972	46.30%	4.905%

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

35	6.709	1891	1903	1932	rVB	150519	269395	26.04%	2.759%
36	7.233	2052	2066	2087	rBV2	141277	254846	24.63%	2.610%
37	7.361	2102	2106	2107	rBV3	746	591	0.06%	0.006%
38	7.423	2118	2125	2134	rBV3	5801	8802	0.85%	0.090%
39	7.570	2157	2171	2199	rBV	489616	849244	82.09%	8.697%
40	7.738	2219	2223	2224	rBV2	1174	806	0.08%	0.008%
41	7.853	2246	2259	2275	rBV	105418	175322	16.95%	1.795%
42	8.008	2302	2307	2311	rBV3	677	741	0.07%	0.008%
43	8.181	2346	2361	2371	rBV4	11414	30536	2.95%	0.313%
44	8.313	2392	2402	2424	rVB	337753	567208	54.83%	5.808%
45	8.419	2425	2435	2450	rVB	76081	120878	11.68%	1.238%
46	8.525	2460	2468	2482	rVB	23886	38247	3.70%	0.392%
47	8.580	2482	2485	2488	rVB2	672	390	0.04%	0.004%
48	8.779	2544	2547	2551	rBV2	372	285	0.03%	0.003%
49	8.908	2576	2587	2606	rBV	87519	136861	13.23%	1.402%
50	8.995	2611	2614	2617	rBV2	341	283	0.03%	0.003%
51	9.091	2627	2644	2664	rBV	552333	913145	88.27%	9.351%
52	9.242	2687	2691	2692	rBV3	545	360	0.03%	0.004%
53	9.294	2705	2707	2711	rVB3	392	293	0.03%	0.003%
54	9.355	2723	2726	2729	rBV3	449	321	0.03%	0.003%
55	9.384	2731	2735	2739	rBV3	600	575	0.06%	0.006%
56	9.451	2753	2756	2759	rBV2	440	462	0.04%	0.005%
57	9.545	2782	2785	2787	rBV2	746	439	0.04%	0.004%
58	9.612	2802	2806	2809	rBV3	510	372	0.04%	0.004%
59	9.770	2849	2855	2865	rVB7	2376	3545	0.34%	0.036%
60	9.976	2916	2919	2923	rBV2	345	270	0.03%	0.003%
61	10.075	2945	2950	2953	rBV2	501	420	0.04%	0.004%
62	10.197	2985	2988	2994	rVB3	513	422	0.04%	0.004%
63	10.233	2994	2999	3001	rBV4	875	724	0.07%	0.007%
64	10.303	3017	3021	3023	rBV	672	565	0.05%	0.006%
65	10.368	3038	3041	3045	rBV3	512	477	0.05%	0.005%
66	10.435	3050	3062	3082	rVV	353496	564057	54.52%	5.776%
67	10.548	3094	3097	3102	rBV4	554	529	0.05%	0.005%
68	10.612	3108	3117	3118	rBV4	3103	3059	0.30%	0.031%
69	10.693	3138	3142	3145	rBV3	594	499	0.05%	0.005%
70	10.776	3161	3168	3174	rBV4	3301	4169	0.40%	0.043%
71	10.937	3214	3218	3221	rBV2	436	351	0.03%	0.004%

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 Title : VOC Analysis

72	11.172	3286	3291	3294	rBV2	546	518	0.05%	0.005%
73	11.377	3353	3355	3360	rVB2	731	514	0.05%	0.005%
74	11.419	3363	3368	3372	rVV3	528	480	0.05%	0.005%
75	11.487	3377	3389	3410	rBV	578808	918508	88.79%	9.406%
76	11.766	3473	3476	3483	rVB4	532	546	0.05%	0.006%
77	11.863	3492	3506	3527	rBV	523444	848188	81.99%	8.686%
78	12.040	3559	3561	3566	rBV2	438	314	0.03%	0.003%
79	12.127	3583	3588	3591	rBV4	336	354	0.03%	0.004%
80	12.184	3604	3606	3611	rBV2	418	345	0.03%	0.004%
81	12.339	3651	3654	3660	rVB2	536	425	0.04%	0.004%
82	12.413	3675	3677	3679	rBV2	462	256	0.02%	0.003%
83	12.483	3693	3699	3700	rBV2	867	785	0.08%	0.008%
84	12.577	3721	3728	3731	rBV4	920	1061	0.10%	0.011%
85	12.618	3738	3741	3743	rBV	407	278	0.03%	0.003%
86	12.667	3752	3756	3758	rBV2	356	254	0.02%	0.003%
87	12.702	3765	3767	3770	rBV2	349	273	0.03%	0.003%
88	12.815	3799	3802	3807	rVB3	629	559	0.05%	0.006%
89	12.895	3824	3827	3829	rBV2	447	341	0.03%	0.003%
90	12.943	3839	3842	3846	rBV	358	267	0.03%	0.003%
91	13.011	3859	3863	3866	rBV3	794	609	0.06%	0.006%
92	13.107	3890	3893	3897	rBV2	517	473	0.05%	0.005%
93	13.162	3908	3910	3913	rVB2	634	339	0.03%	0.003%
94	13.364	3970	3973	3976	rBV2	347	308	0.03%	0.003%
95	13.747	4087	4092	4096	rBV2	642	650	0.06%	0.007%
96	13.792	4104	4106	4112	rBV	619	431	0.04%	0.004%
97	13.831	4116	4118	4122	rBV2	519	297	0.03%	0.003%
98	13.879	4130	4133	4137	rVB	586	351	0.03%	0.004%
99	14.181	4224	4227	4234	rBV4	486	505	0.05%	0.005%
100	14.371	4284	4286	4289	rBV2	491	270	0.03%	0.003%

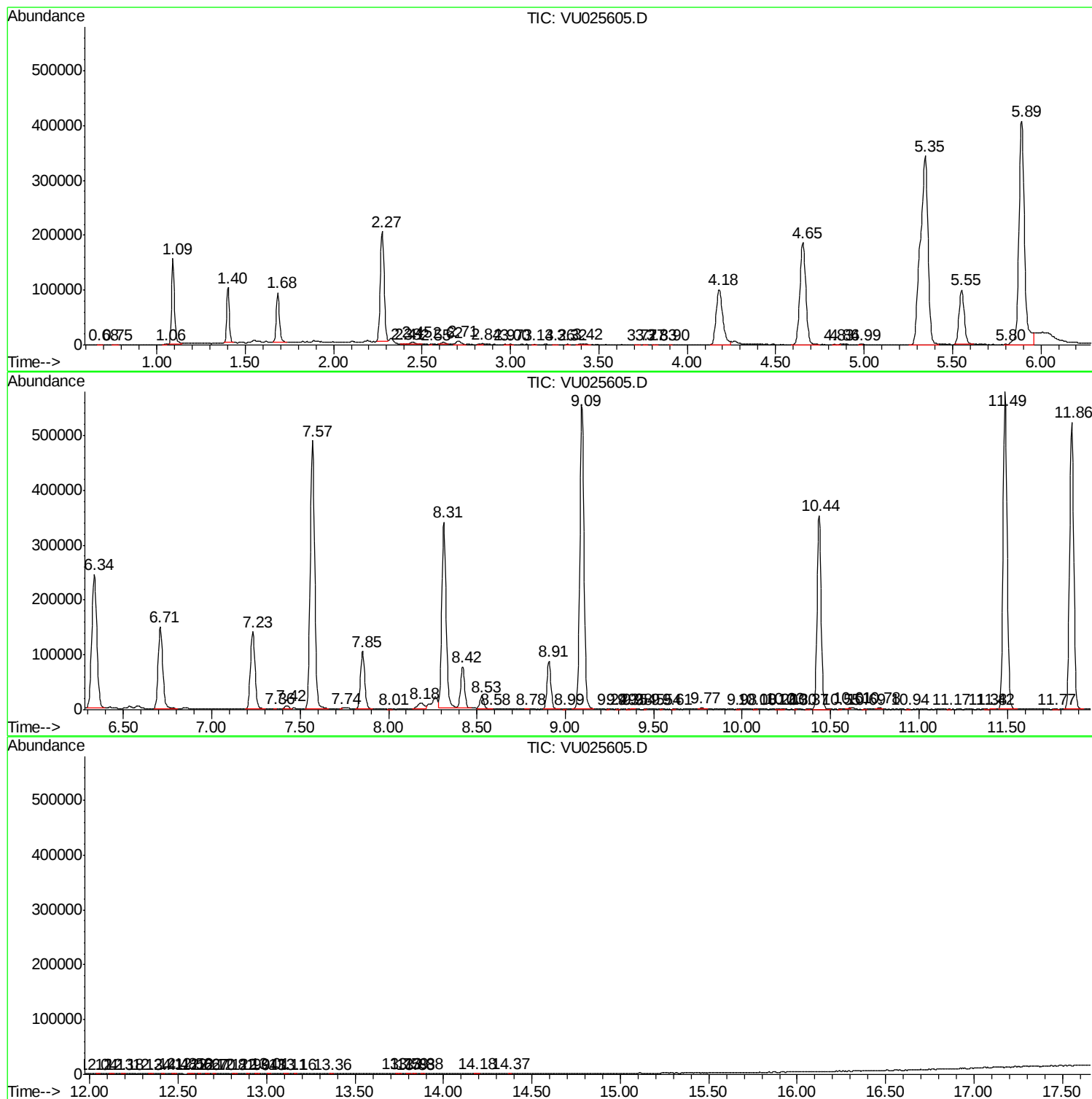
Sum of corrected areas: 9765272

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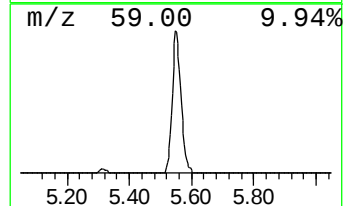
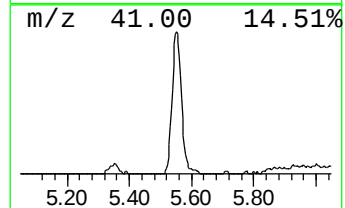
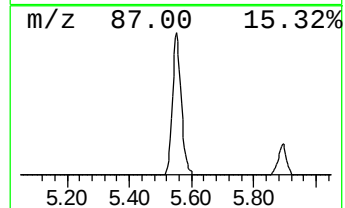
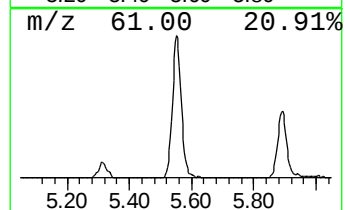
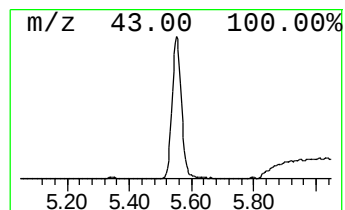
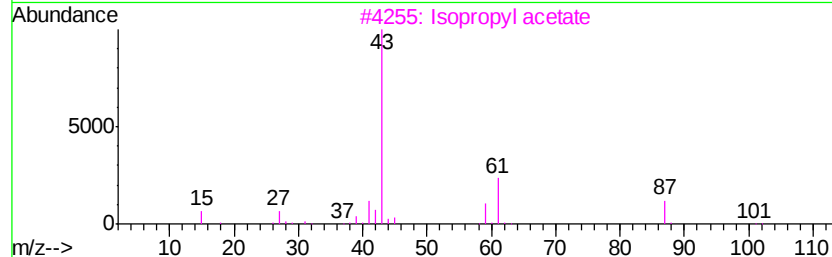
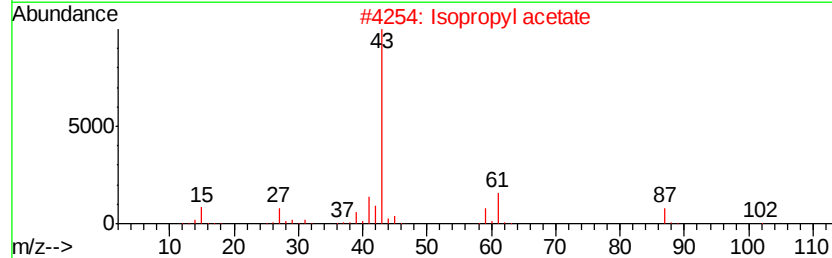
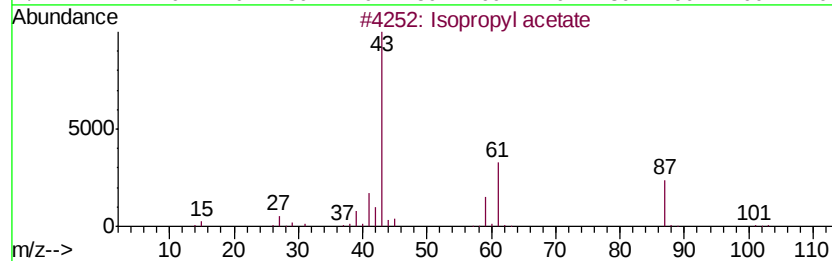
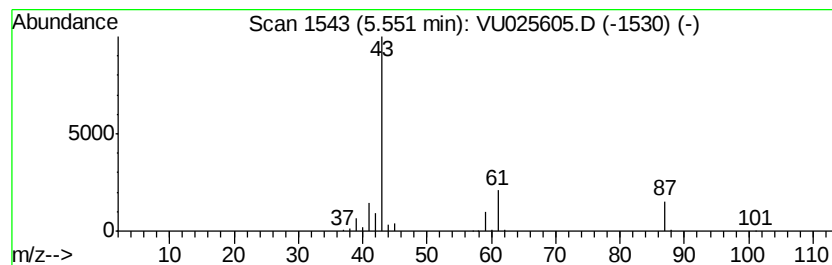
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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	11.43 ug/L	202943	1,4-Difluorobenzene	5.89		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl acetate		102	C5H10O2	000108-21-4	64
2	Isopropyl acetate		102	C5H10O2	000108-21-4	56
3	Isopropyl acetate		102	C5H10O2	000108-21-4	42
4	Propane, 1-(1-methylethoxy)-		102	C6H14O	000627-08-7	38
5	Acetaldehyde, O-ethyloxime-		87	C4H9NO	1000288-34-6	9



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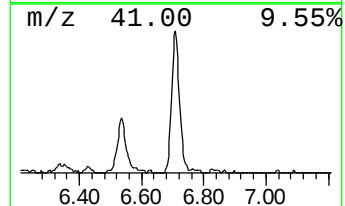
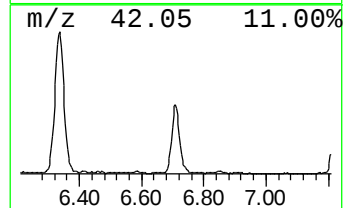
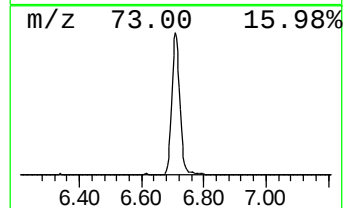
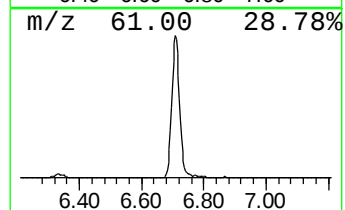
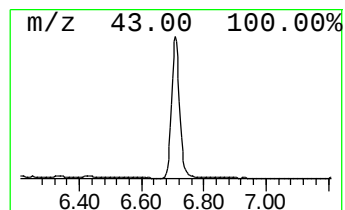
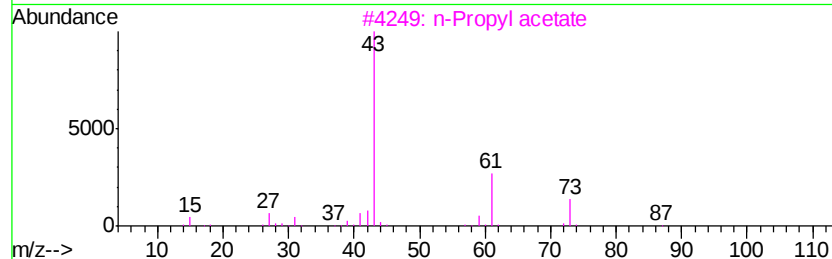
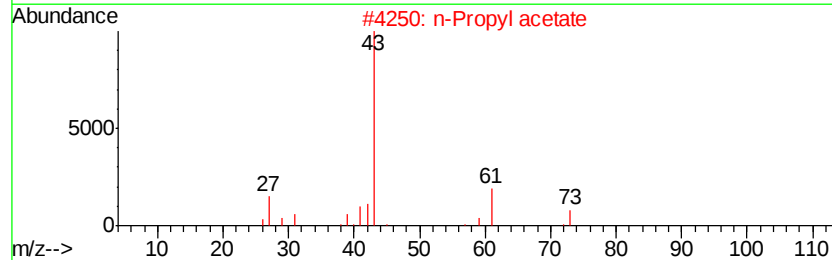
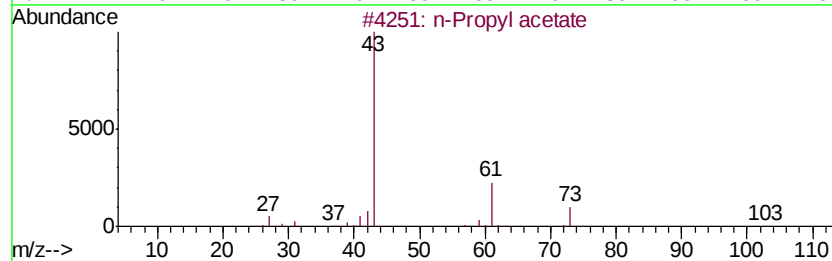
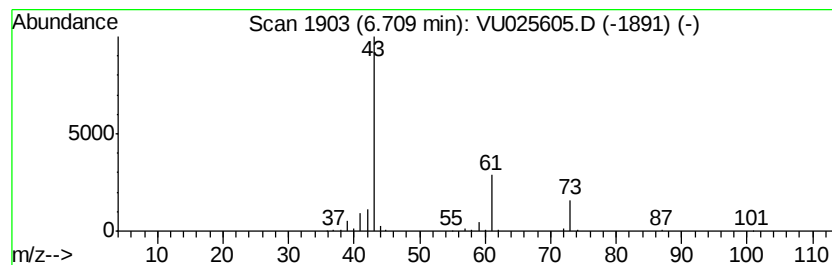
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	15.18 ug/L	269395	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	9
5		Isobutyl acetate	116	C6H12O2	000110-19-0	9



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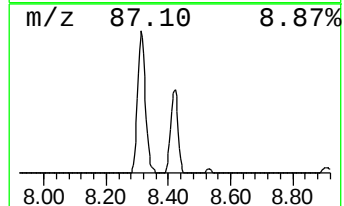
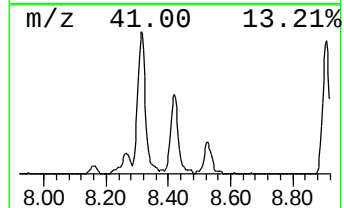
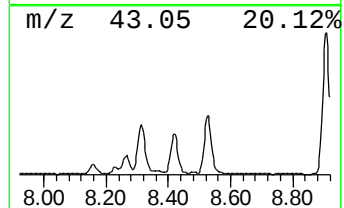
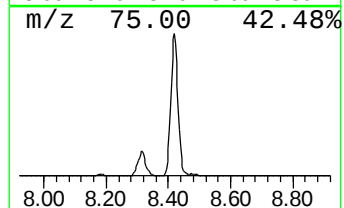
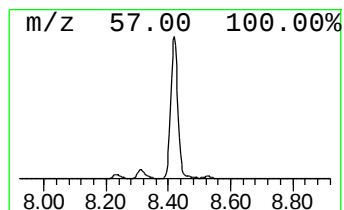
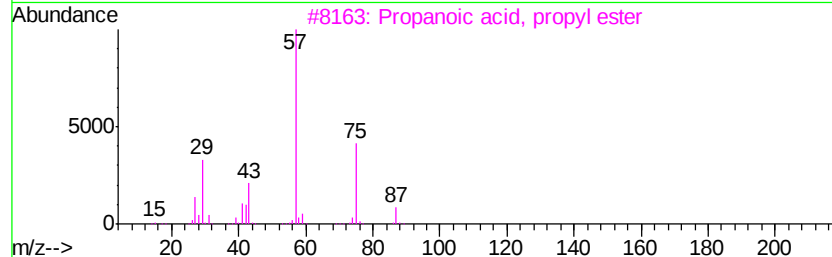
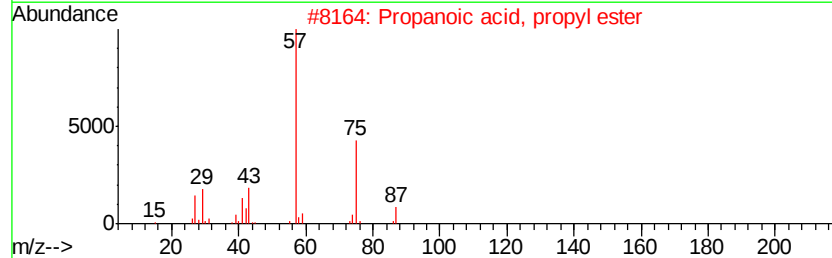
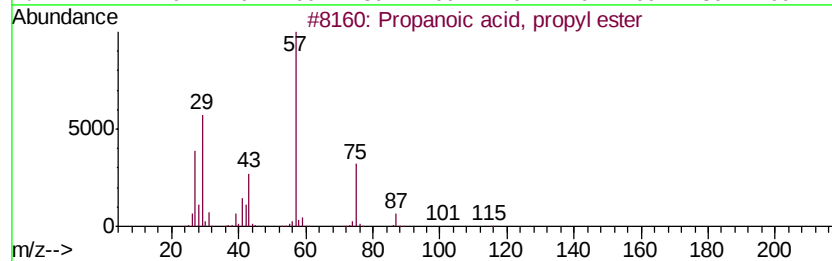
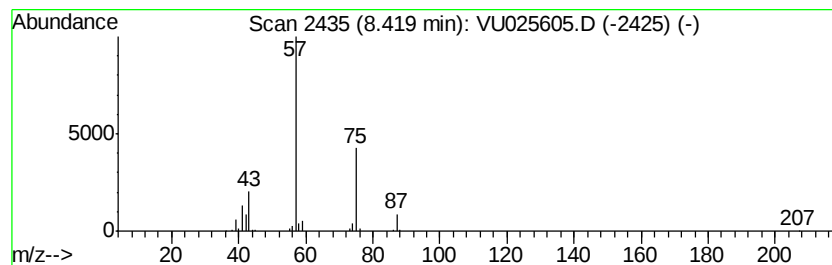
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Quant Title : VOC Analysis

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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	6.62 ug/L	120878	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	56



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025605.D
Acq On : 23 Jul 2018 16:21
Operator : MD/SY
Sample : PB111343ZHE#11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#11

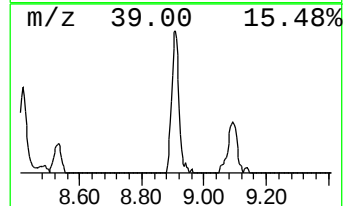
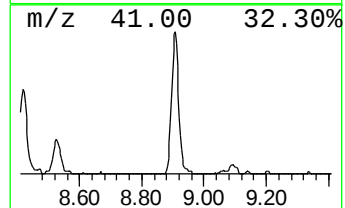
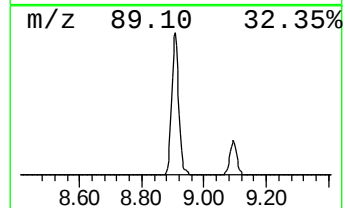
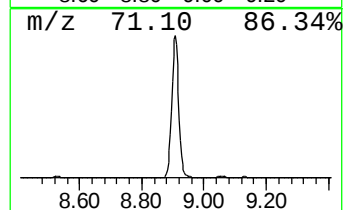
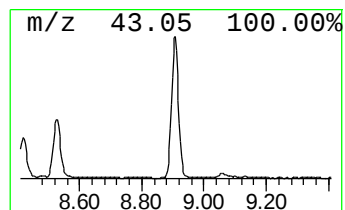
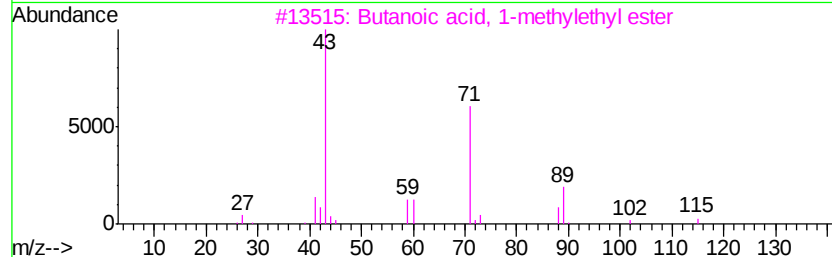
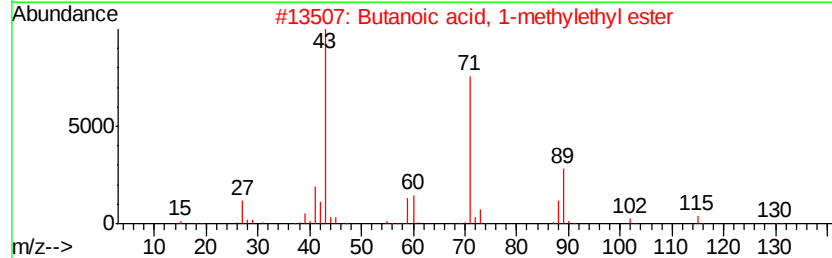
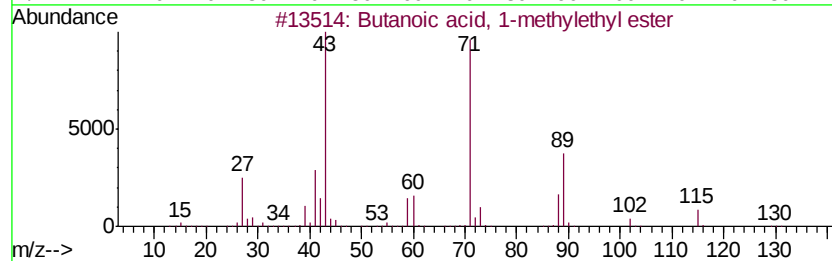
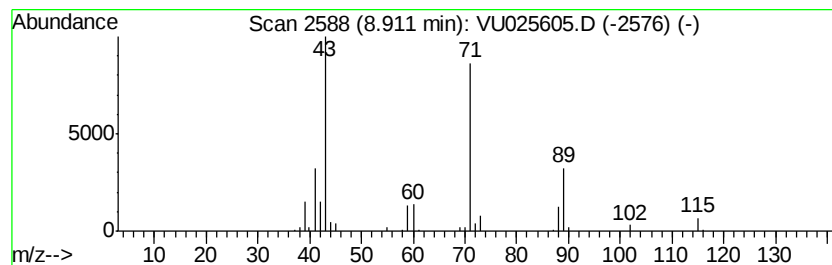
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Quant Title : VOC Analysis

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	7.49 ug/L	136861	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	78
4		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5		Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU072318\
Data File : VU025605.D
Acq On : 23 Jul 2018 16:21
Operator : MD/SY
Sample : PB111343ZHE#11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#11

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	11.4	ug/L	202943	1	5.89	887544	50.0
n-Propyl acetate	6.71	15.2	ug/L	269395	1	5.89	887544	50.0
Propanoic acid, p...	8.42	6.6	ug/L	120878	2	9.09	913145	50.0
Butanoic acid, 1-...	8.91	7.5	ug/L	136861	2	9.09	913145	50.0