

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
 Data File : VU025604.D
 Acq On : 23 Jul 2018 15:58
 Operator : MD/SY
 Sample : PB111343ZHE#10
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PB111343ZHE#10

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	0.632	10	13	16	rBV	297	224	0.002%	0.0002%
2	0.709	35	37	40	rVB2	291	180	0.002%	0.0002%
3	0.744	40	48	53	rBV3	409	675	0.007%	0.0007%
4	0.870	81	87	89	rBV2	314	346	0.003%	0.0004%
5	1.060	143	146	148	rBV2	790	605	0.006%	0.0006%
6	1.092	148	156	175	rVV	152130	174580	16.89%	1.807%
7	1.404	245	253	265	rBV	107826	112625	10.90%	1.166%
8	1.683	333	340	351	rVB	89168	111383	10.78%	1.153%
9	2.275	513	524	535	rBV	193767	294230	28.47%	3.046%
10	2.449	571	578	587	rVB2	3145	4692	0.45%	0.0049%
11	2.622	624	632	643	rVB2	3526	6285	0.61%	0.0065%
12	2.706	649	658	669	rVB2	8176	13381	1.29%	0.0139%
13	2.821	691	694	695	rBV	517	278	0.003%	0.0003%
14	2.831	695	697	698	rBV	657	285	0.003%	0.0003%
15	2.950	730	734	736	rBV	288	213	0.002%	0.0002%
16	2.989	741	746	750	rBV3	477	470	0.005%	0.0005%
17	3.053	764	766	771	rVB2	384	265	0.003%	0.0003%
18	3.082	771	775	776	rBV2	419	216	0.002%	0.0002%
19	3.172	801	803	805	rBV	517	247	0.002%	0.0003%
20	3.188	806	808	813	rVB2	371	325	0.003%	0.0003%
21	3.403	869	875	877	rBV3	1391	1468	0.14%	0.0015%
22	3.503	900	906	911	rBV3	430	607	0.006%	0.0006%
23	3.645	947	950	953	rVB2	330	177	0.002%	0.0002%
24	3.786	992	994	999	rVV2	329	261	0.003%	0.0003%
25	3.892	1022	1027	1029	rBV2	294	280	0.003%	0.0003%
26	3.908	1030	1032	1036	rVV	351	218	0.002%	0.0002%
27	3.937	1036	1041	1044	rVV2	285	270	0.003%	0.0003%
28	4.053	1074	1077	1082	rVB3	472	374	0.004%	0.0004%
29	4.082	1084	1086	1089	rVB	494	269	0.003%	0.0003%
30	4.098	1089	1091	1092	rBV	508	229	0.002%	0.0002%
31	4.178	1101	1116	1137	rBV	100004	257053	24.87%	2.661%
32	4.448	1194	1200	1203	rVB3	712	679	0.007%	0.0007%
33	4.471	1203	1207	1208	rBV	507	238	0.002%	0.0002%
34	4.516	1215	1221	1224	rBV2	545	525	0.005%	0.0005%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
 Data File : VU025604.D
 Acq On : 23 Jul 2018 15:58
 Operator : MD/SY
 Sample : PB111343ZHE#10
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PB111343ZHE#10

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

35	4.567	1234	1237	1239	rBV	314	189	0.02%	0.002%
36	4.654	1246	1264	1284	rBV	185497	433224	41.92%	4.484%
37	4.754	1292	1295	1299	rBV3	587	361	0.03%	0.004%
38	4.895	1337	1339	1342	rVB2	635	297	0.03%	0.003%
39	4.982	1361	1366	1369	rBV5	685	749	0.07%	0.008%
40	5.037	1376	1383	1384	rBV3	280	249	0.02%	0.003%
41	5.153	1415	1419	1421	rBV2	210	158	0.02%	0.002%
42	5.233	1442	1444	1449	rVB3	327	276	0.03%	0.003%
43	5.346	1454	1479	1498	rBV2	345463	1033559	100.00%	10.699%
44	5.551	1529	1543	1561	rVV	97468	200755	19.42%	2.078%
45	5.751	1599	1605	1608	rBV4	622	644	0.06%	0.007%
46	5.892	1624	1649	1666	rBV	399134	857223	82.94%	8.873%
47	6.336	1773	1787	1806	rVB	243096	479246	46.37%	4.961%
48	6.709	1891	1903	1929	rBV	147347	264493	25.59%	2.738%
49	7.230	2053	2065	2085	rVB	144115	251847	24.37%	2.607%
50	7.426	2117	2126	2133	rBV3	5972	9293	0.90%	0.096%
51	7.571	2157	2171	2200	rBV	483146	843511	81.61%	8.731%
52	7.853	2246	2259	2272	rBV	104329	177006	17.13%	1.832%
53	8.120	2339	2342	2344	rVB3	350	213	0.02%	0.002%
54	8.188	2344	2363	2370	rBV4	11780	30898	2.99%	0.320%
55	8.313	2392	2402	2424	rVB	338599	567886	54.94%	5.878%
56	8.419	2425	2435	2450	rVB	76080	120219	11.63%	1.244%
57	8.525	2459	2468	2482	rVB	24621	39141	3.79%	0.405%
58	8.908	2576	2587	2604	rBV	83843	134274	12.99%	1.390%
59	9.091	2627	2644	2667	rBV	543126	904615	87.52%	9.364%
60	9.291	2704	2706	2710	rBV2	462	314	0.03%	0.003%
61	9.358	2723	2727	2729	rBV2	476	383	0.04%	0.004%
62	9.413	2740	2744	2745	rBV2	440	332	0.03%	0.003%
63	9.561	2788	2790	2794	rVB	535	337	0.03%	0.003%
64	9.670	2822	2824	2829	rBV3	360	250	0.02%	0.003%
65	9.696	2830	2832	2837	rVB2	392	226	0.02%	0.002%
66	9.722	2837	2840	2842	rBV3	449	341	0.03%	0.004%
67	9.773	2848	2856	2863	rBV6	2129	3623	0.35%	0.038%
68	9.821	2869	2871	2875	rVB2	483	263	0.03%	0.003%
69	9.969	2914	2917	2921	rBV2	394	366	0.04%	0.004%
70	9.992	2922	2924	2926	rVB2	408	194	0.02%	0.002%
71	10.021	2930	2933	2935	rBV2	360	238	0.02%	0.002%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
 Data File : VU025604.D
 Acq On : 23 Jul 2018 15:58
 Operator : MD/SY
 Sample : PB111343ZHE#10
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PB111343ZHE#10

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

72	10.133	2965	2968	2969	rBV2	318	182	0.02%	0.002%
73	10.233	2995	2999	3000	rBV2	571	408	0.04%	0.004%
74	10.435	3050	3062	3082	rVB	352436	558796	54.07%	5.784%
75	10.535	3090	3093	3096	rBV2	434	324	0.03%	0.003%
76	10.612	3110	3117	3118	rBV5	2647	2460	0.24%	0.025%
77	10.776	3159	3168	3175	rBV5	3028	4784	0.46%	0.050%
78	10.882	3199	3201	3204	rBV	366	230	0.02%	0.002%
79	10.947	3219	3221	3224	rBV2	353	278	0.03%	0.003%
80	11.062	3255	3257	3259	rBV	449	256	0.02%	0.003%
81	11.114	3270	3273	3276	rVB2	392	266	0.03%	0.003%
82	11.143	3279	3282	3284	rBV2	520	343	0.03%	0.004%
83	11.406	3362	3364	3366	rBV3	545	313	0.03%	0.003%
84	11.487	3377	3389	3407	rBV	576711	903625	87.43%	9.354%
85	11.670	3442	3446	3447	rBV3	622	417	0.04%	0.004%
86	11.738	3465	3467	3469	rBV2	388	204	0.02%	0.002%
87	11.863	3493	3506	3527	rVB	528836	840633	81.33%	8.702%
88	12.027	3555	3557	3558	rBV	431	209	0.02%	0.002%
89	12.094	3575	3578	3581	rBV	313	220	0.02%	0.002%
90	12.172	3599	3602	3604	rBV2	727	505	0.05%	0.005%
91	12.194	3604	3609	3612	rVV4	533	579	0.06%	0.006%
92	12.233	3619	3621	3625	rBV2	327	156	0.02%	0.002%
93	12.307	3641	3644	3646	rBV	414	220	0.02%	0.002%
94	12.445	3684	3687	3692	rBV2	451	427	0.04%	0.004%
95	12.480	3692	3698	3707	rVV4	1119	1884	0.18%	0.020%
96	13.252	3936	3938	3941	rBV3	363	198	0.02%	0.002%
97	13.271	3941	3944	3946	rVV2	503	284	0.03%	0.003%
98	13.432	3992	3994	3997	rBV2	474	202	0.02%	0.002%
99	14.458	4310	4313	4314	rBV2	644	391	0.04%	0.004%
100	14.628	4362	4366	4369	rBV3	660	567	0.05%	0.006%

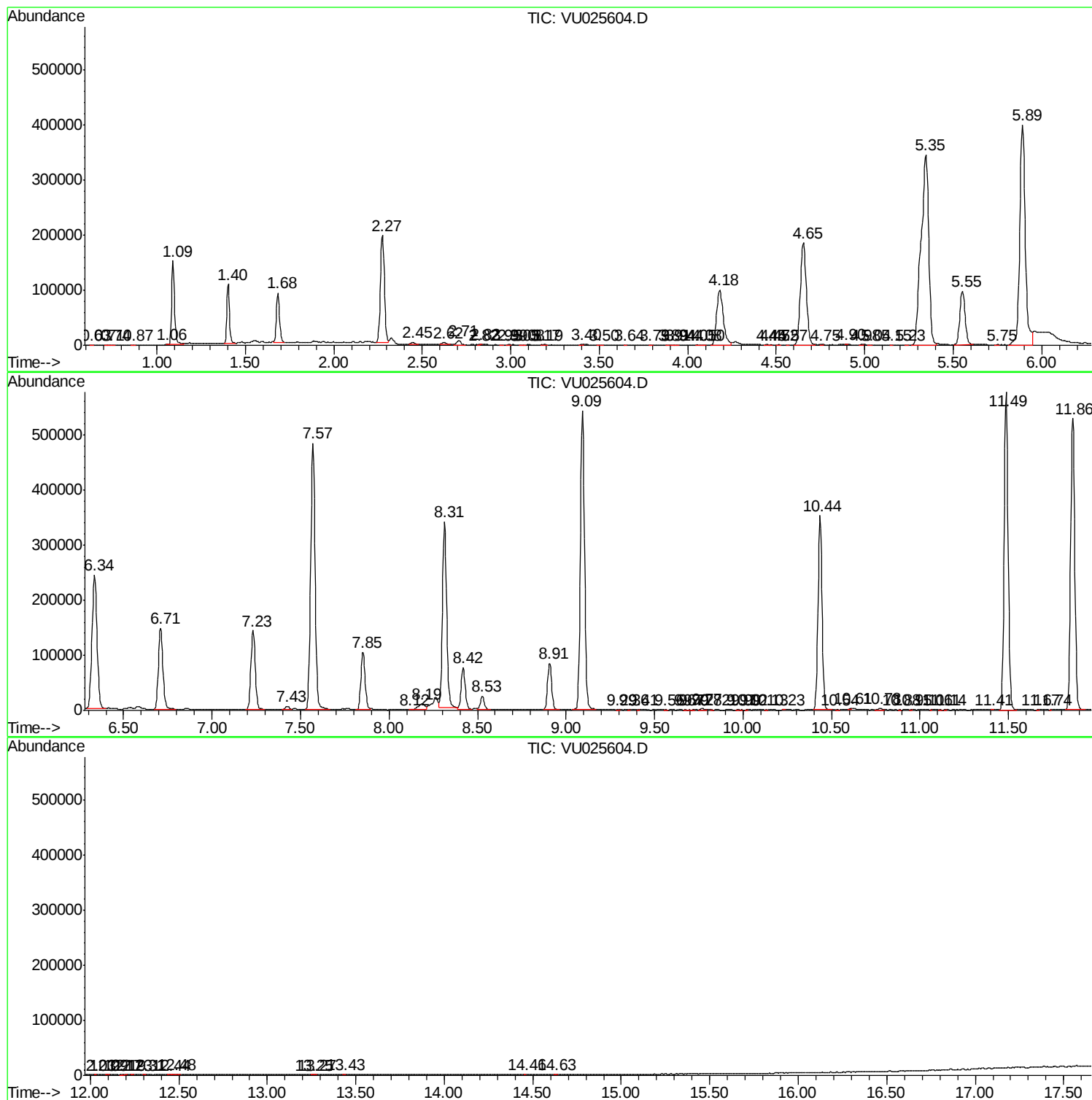
Sum of corrected areas: 9660707

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025604.D
Acq On : 23 Jul 2018 15:58
Operator : MD/SY
Sample : PB111343ZHE#10
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#10

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025604.D
Acq On : 23 Jul 2018 15:58
Operator : MD/SY
Sample : PB111343ZHE#10
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 10 Sample Multiplier: 1

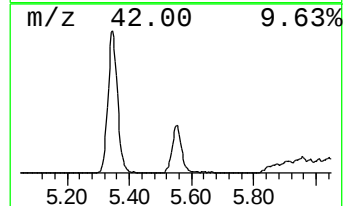
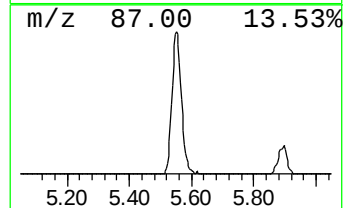
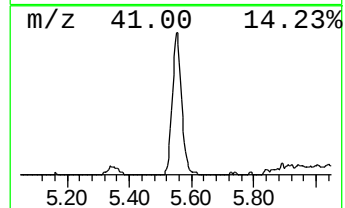
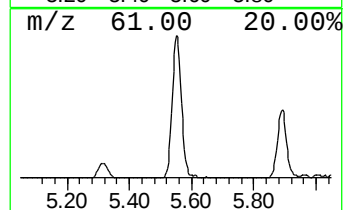
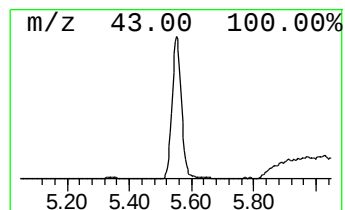
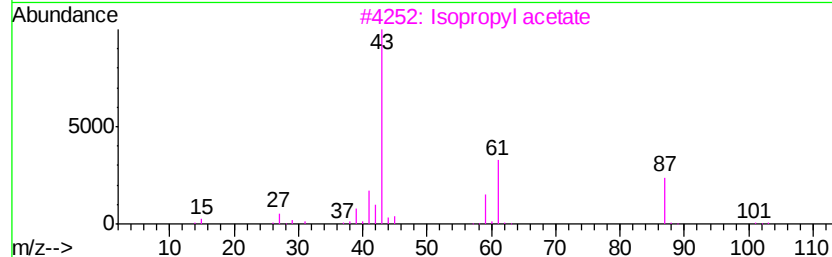
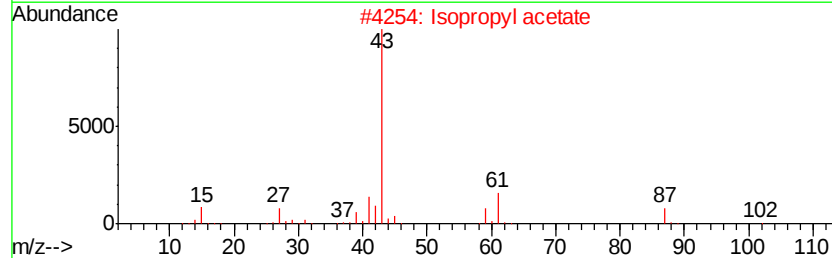
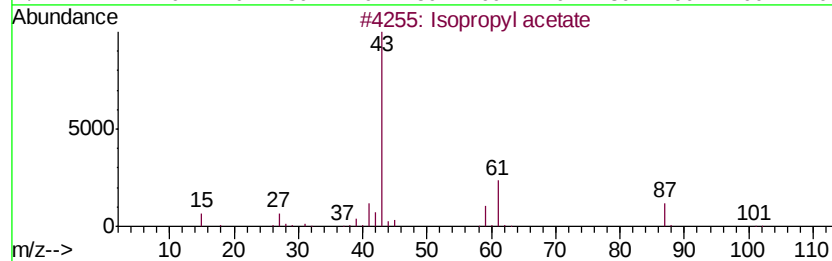
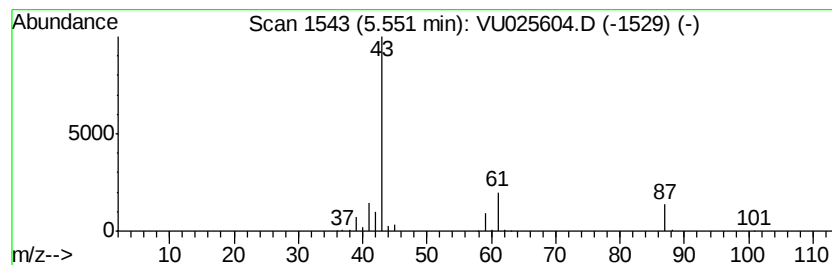
Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#10

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	11.71 ug/L	200755	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	Propane, 1-(1-methylethoxy)-		102	C6H14O	000627-08-7	38
5	Propane, 1-(1-methylethoxy)-		102	C6H14O	000627-08-7	28



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025604.D
Acq On : 23 Jul 2018 15:58
Operator : MD/SY
Sample : PB111343ZHE#10
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#10

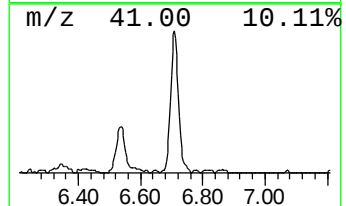
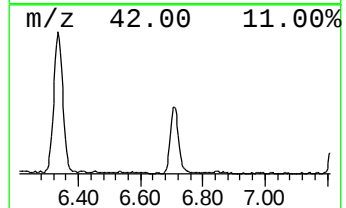
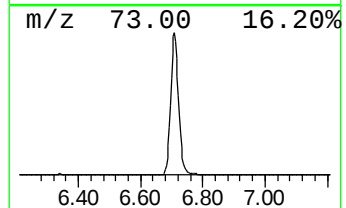
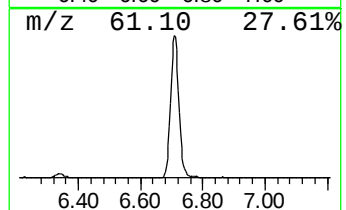
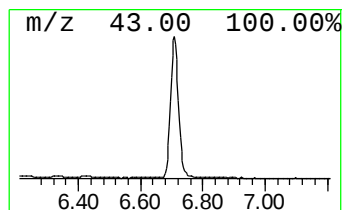
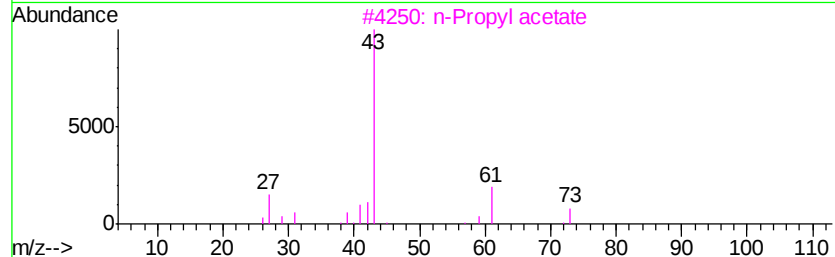
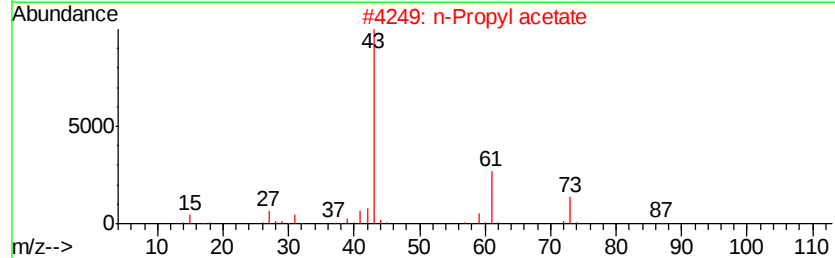
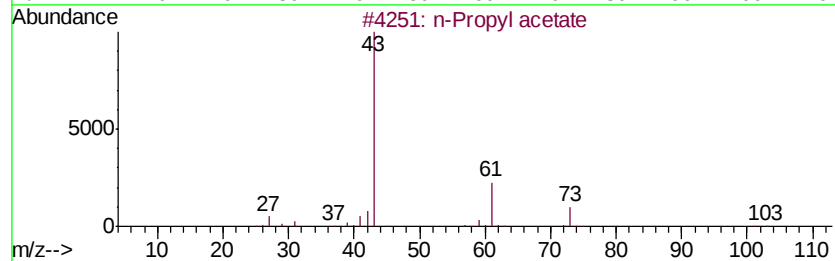
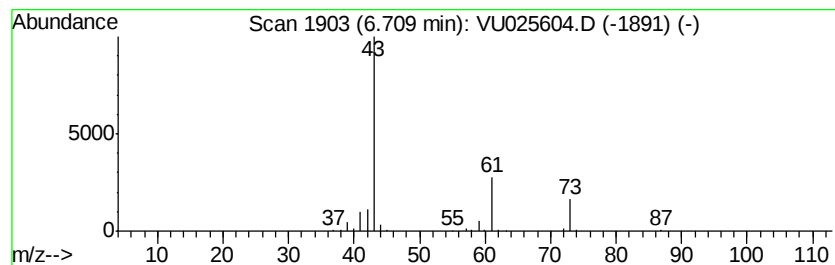
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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	15.43 ug/L	264493	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		Isopropyl acetate	102	C5H10O2	000108-21-4	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025604.D
Acq On : 23 Jul 2018 15:58
Operator : MD/SY
Sample : PB111343ZHE#10
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 10 Sample Multiplier: 1

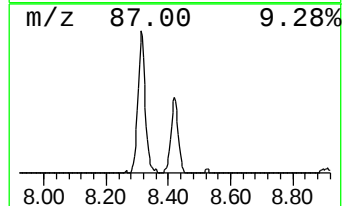
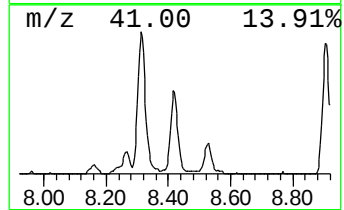
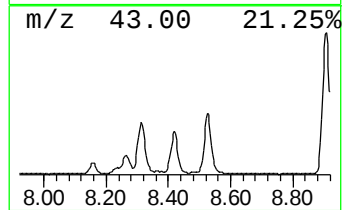
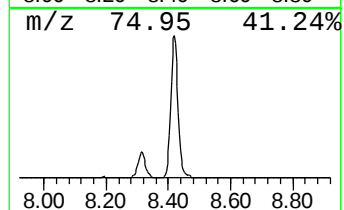
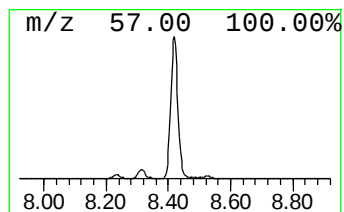
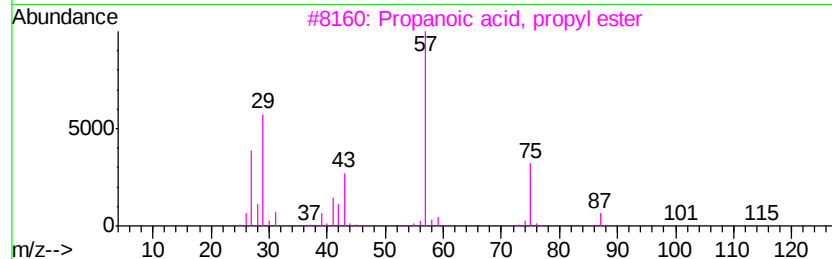
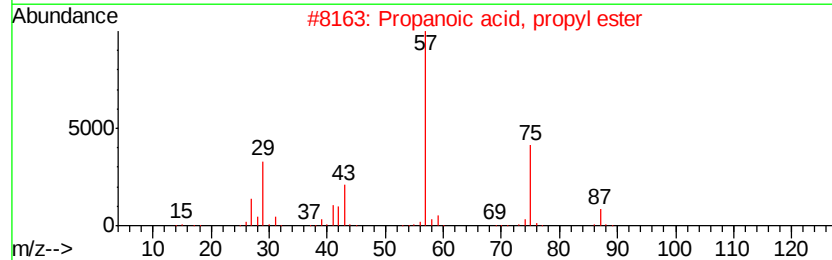
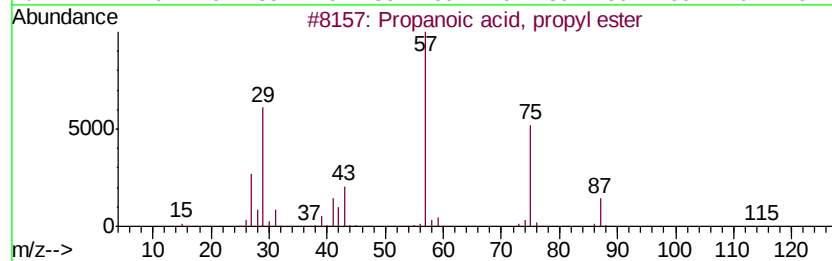
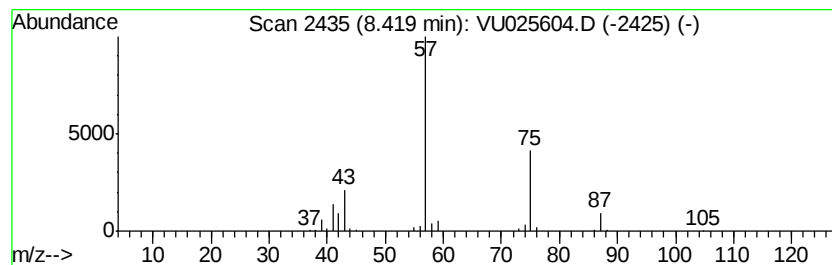
Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#10

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 5 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.42	6.64 ug/L	120219	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	78	
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025604.D
Acq On : 23 Jul 2018 15:58
Operator : MD/SY
Sample : PB111343ZHE#10
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#10

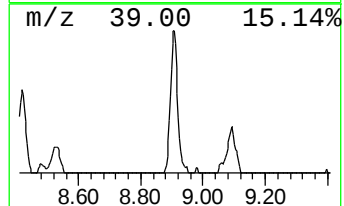
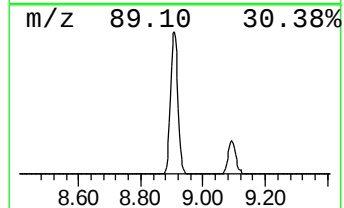
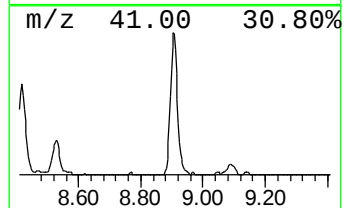
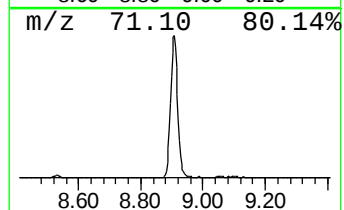
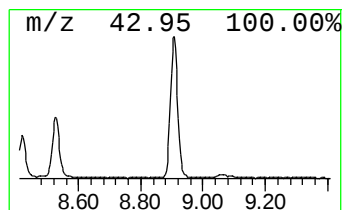
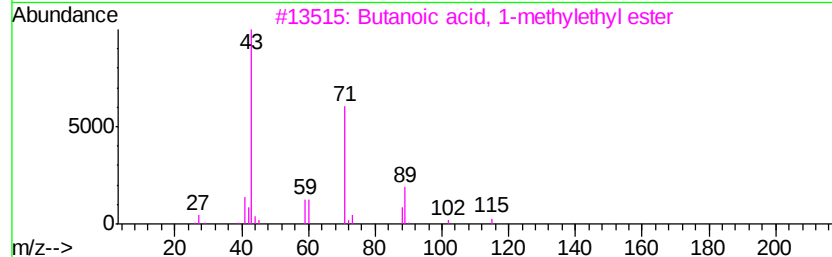
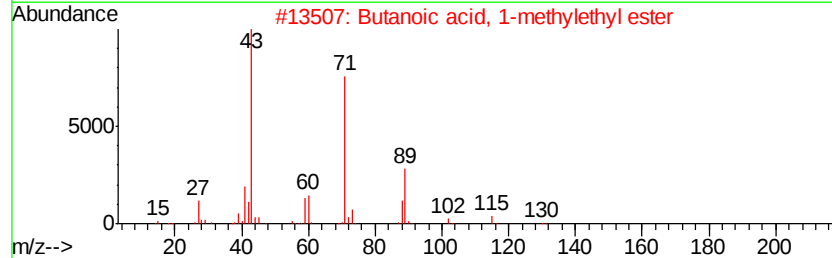
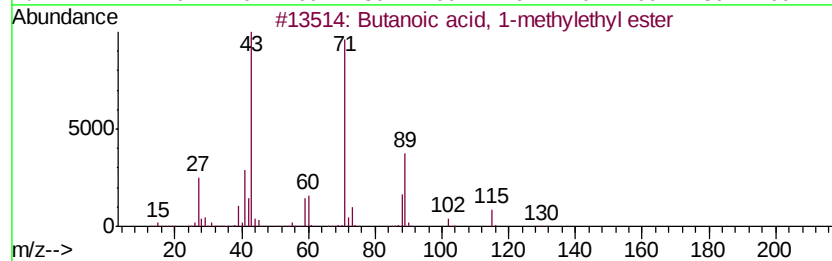
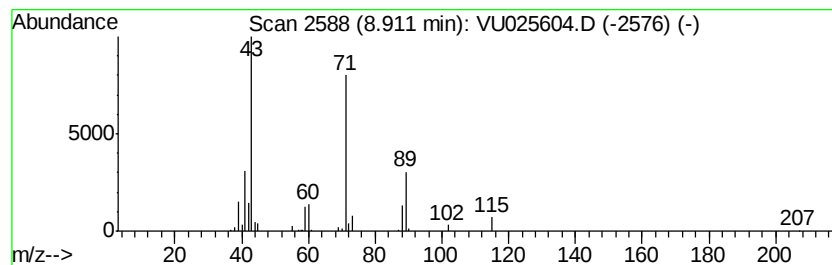
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.91	7.42 ug/L	134274	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-, propyl...	130	C7H14O2	000644-49-5	72
5		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU072318\
Data File : VU025604.D
Acq On : 23 Jul 2018 15:58
Operator : MD/SY
Sample : PB111343ZHE#10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PB111343ZHE#10

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	11.7	ug/L	200755	1	5.89	857223	50.0
n-Propyl acetate	6.71	15.4	ug/L	264493	1	5.89	857223	50.0
Propanoic acid, p...	8.42	6.6	ug/L	120219	2	9.09	904615	50.0
Butanoic acid, 1-...	8.91	7.4	ug/L	134274	2	9.09	904615	50.0