

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092519\
 Data File : VU034811.D
 Acq On : 25 Sep 2019 18:47
 Operator : JC/SP
 Sample : PB123366TB
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB03

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\SOMULM091919WMA.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	1.177	24	27	32	rBV2	7244	5718	0.03%	0.013%
2	1.392	87	94	107	rBV	314996	329165	1.80%	0.738%
3	1.672	173	181	195	rVB	267903	342082	1.87%	0.767%
4	2.257	354	363	375	rVB	464162	696926	3.81%	1.562%
5	2.604	464	471	480	rBV4	4891	8683	0.05%	0.019%
6	2.682	480	495	534	rBV	10160716	18301854	100.00%	41.014%
7	3.540	760	762	764	rBV2	982	593	0.00%	0.001%
8	3.604	779	782	787	rVB6	2140	1694	0.01%	0.004%
9	3.627	787	789	792	rBV3	1008	563	0.00%	0.001%
10	3.669	799	802	806	rVV5	692	528	0.00%	0.001%
11	3.755	825	829	831	rVB2	843	544	0.00%	0.001%
12	3.784	835	838	839	rBV2	1070	567	0.00%	0.001%
13	3.881	865	868	872	rBV5	1793	1010	0.01%	0.002%
14	3.945	882	888	890	rBV4	1126	866	0.00%	0.002%
15	3.984	897	900	905	rVB5	791	707	0.00%	0.002%
16	4.038	914	917	922	rVB5	894	903	0.00%	0.002%
17	4.064	922	925	928	rBV3	1720	1248	0.01%	0.003%
18	4.096	932	935	938	rVB2	1230	768	0.00%	0.002%
19	4.148	938	951	982	rBV2	223512	613204	3.35%	1.374%
20	4.453	1044	1046	1049	rVB4	1377	712	0.00%	0.002%
21	4.485	1051	1056	1057	rBV3	1208	1074	0.01%	0.002%
22	4.534	1062	1071	1078	rVV9	5332	9828	0.05%	0.022%
23	4.620	1082	1098	1125	rVV	351704	841761	4.60%	1.886%
24	4.743	1134	1136	1139	rBV4	1720	947	0.01%	0.002%
25	4.964	1197	1205	1207	rBV6	5081	6149	0.03%	0.014%
26	5.042	1226	1229	1236	rBV6	1598	1724	0.01%	0.004%
27	5.083	1236	1242	1245	rBV6	2268	2573	0.01%	0.006%
28	5.183	1271	1273	1275	rBV3	1179	623	0.00%	0.001%
29	5.315	1291	1314	1345	rVV2	755237	2246021	12.27%	5.033%
30	5.530	1369	1381	1401	rBV2	90614	198032	1.08%	0.444%
31	5.733	1442	1444	1446	rBV3	1392	655	0.00%	0.001%
32	5.865	1472	1485	1507	rBV	598825	1289982	7.05%	2.891%
33	6.308	1610	1623	1642	rVB2	512503	1030691	5.63%	2.310%
34	6.562	1696	1702	1705	rBV2	12774	17037	0.09%	0.038%

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 Title : VOC Analysis

35	6.681	1727	1739	1772	rBV	2161571	3896894	21.29%	8.733%
36	7.205	1890	1902	1923	rBV	298896	567003	3.10%	1.271%
37	7.398	1951	1962	1989	rBV	258857	468646	2.56%	1.050%
38	7.543	1994	2007	2025	rBV	1048544	1885688	10.30%	4.226%
39	7.826	2085	2095	2121	rBV2	280228	505889	2.76%	1.134%
40	8.051	2158	2165	2171	rBV10	4295	5713	0.03%	0.013%
41	8.135	2178	2191	2206	rBV	511950	858925	4.69%	1.925%
42	8.215	2207	2216	2218	rBV4	25062	35802	0.20%	0.080%
43	8.289	2230	2239	2262	rVV	843971	1467554	8.02%	3.289%
44	8.395	2262	2272	2299	rVB	805651	1307128	7.14%	2.929%
45	8.508	2301	2307	2327	rVB2	40712	68433	0.37%	0.153%
46	8.884	2411	2424	2444	rBV	1064375	1708267	9.33%	3.828%
47	9.067	2462	2481	2508	rBV	852166	1501004	8.20%	3.364%
48	9.231	2526	2532	2543	rVB7	6905	11658	0.06%	0.026%
49	9.324	2555	2561	2563	rBV6	2948	3737	0.02%	0.008%
50	9.424	2589	2592	2597	rBV6	1851	1249	0.01%	0.003%
51	9.553	2629	2632	2634	rBV3	1592	979	0.01%	0.002%
52	9.588	2634	2643	2659	rVV2	22032	40742	0.22%	0.091%
53	9.746	2682	2692	2716	rBV2	142110	263119	1.44%	0.590%
54	10.148	2809	2817	2828	rVB2	8038	12129	0.07%	0.027%
55	10.189	2828	2830	2835	rVV5	1134	759	0.00%	0.002%
56	10.212	2835	2837	2844	rVB7	1944	1594	0.01%	0.004%
57	10.305	2864	2866	2868	rVB2	1391	600	0.00%	0.001%
58	10.331	2868	2874	2879	rBV7	2361	2114	0.01%	0.005%
59	10.408	2882	2898	2916	rBV	678689	1139715	6.23%	2.554%
60	10.540	2936	2939	2940	rBV3	1723	938	0.01%	0.002%
61	10.665	2972	2978	2982	rBV7	2056	2371	0.01%	0.005%
62	10.752	2996	3005	3018	rVB2	29483	47219	0.26%	0.106%
63	10.836	3027	3031	3034	rVB5	1481	958	0.01%	0.002%
64	10.922	3055	3058	3061	rVB2	964	529	0.00%	0.001%
65	10.971	3071	3073	3077	rVB2	1258	794	0.00%	0.002%
66	11.003	3077	3083	3085	rBV4	1711	1700	0.01%	0.004%
67	11.038	3091	3094	3096	rVB3	1989	957	0.01%	0.002%
68	11.067	3096	3103	3109	rBV7	2121	3412	0.02%	0.008%
69	11.131	3116	3123	3131	rBV4	6317	9106	0.05%	0.020%
70	11.395	3201	3205	3213	rBV7	5605	6711	0.04%	0.015%
71	11.459	3214	3225	3255	rVV	755201	1272727	6.95%	2.852%

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 Title : VOC Analysis

72	11.742	3310	3313	3320	rVB6	2127	1588	0.01%	0.004%
73	11.836	3330	3342	3367	rBV	914970	1534253	8.38%	3.438%
74	12.218	3457	3461	3466	rVB7	1373	1343	0.01%	0.003%
75	12.318	3489	3492	3496	rVB5	1044	685	0.00%	0.002%
76	12.463	3535	3537	3542	rVB4	1587	892	0.00%	0.002%
77	12.543	3558	3562	3567	rVB7	1368	1232	0.01%	0.003%
78	12.610	3581	3583	3586	rVB4	1078	751	0.00%	0.002%
79	12.678	3603	3604	3608	rVB3	1258	764	0.00%	0.002%
80	12.700	3608	3611	3614	rBV3	1596	1187	0.01%	0.003%
81	12.720	3614	3617	3619	rBV3	1202	817	0.00%	0.002%
82	12.755	3624	3628	3629	rBV2	1100	782	0.00%	0.002%
83	12.836	3650	3653	3657	rVB5	1613	1289	0.01%	0.003%
84	12.877	3657	3666	3668	rBV8	2541	2958	0.02%	0.007%
85	13.093	3730	3733	3735	rBV3	1124	628	0.00%	0.001%
86	13.131	3743	3745	3748	rVB2	940	582	0.00%	0.001%
87	13.151	3748	3751	3755	rVB4	1196	901	0.00%	0.002%
88	13.170	3755	3757	3760	rBV4	1025	754	0.00%	0.002%
89	13.228	3771	3775	3776	rBV3	1680	1103	0.01%	0.002%
90	13.401	3823	3829	3833	rBV7	1865	2453	0.01%	0.005%
91	13.459	3845	3847	3850	rVB4	1345	613	0.00%	0.001%
92	13.482	3851	3854	3859	rVB5	1488	1220	0.01%	0.003%
93	13.524	3865	3867	3869	rBV3	1453	584	0.00%	0.001%
94	13.713	3923	3926	3927	rBV3	1024	532	0.00%	0.001%
95	13.749	3935	3937	3940	rBV2	1308	842	0.00%	0.002%
96	13.932	3991	3994	3996	rBV3	1512	991	0.01%	0.002%
97	14.707	4233	4235	4239	rVB5	1821	865	0.00%	0.002%
98	14.890	4290	4292	4294	rBV3	1492	736	0.00%	0.002%
99	14.961	4312	4314	4317	rBV3	1901	1216	0.01%	0.003%
100	15.466	4468	4471	4476	rBV5	2582	2752	0.02%	0.006%

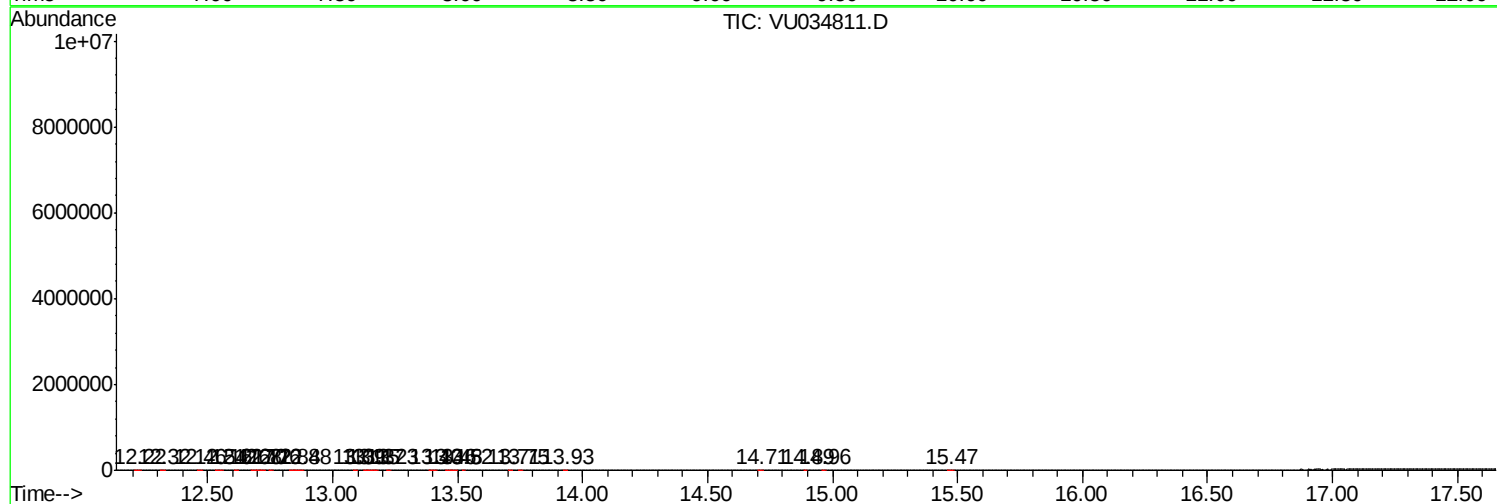
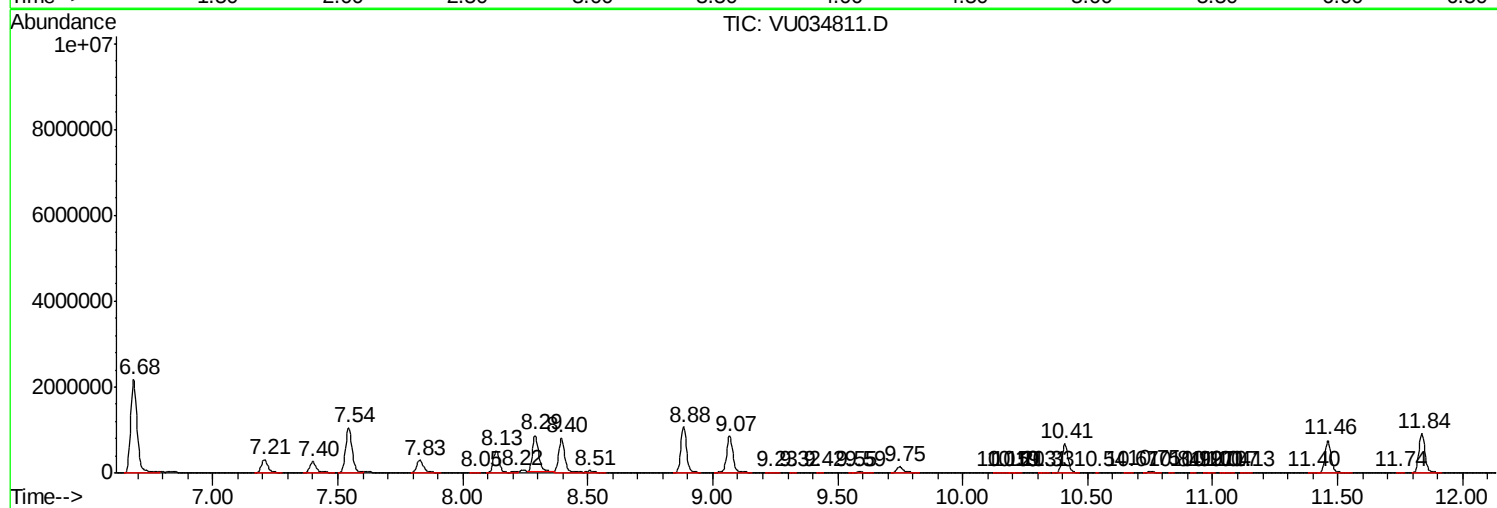
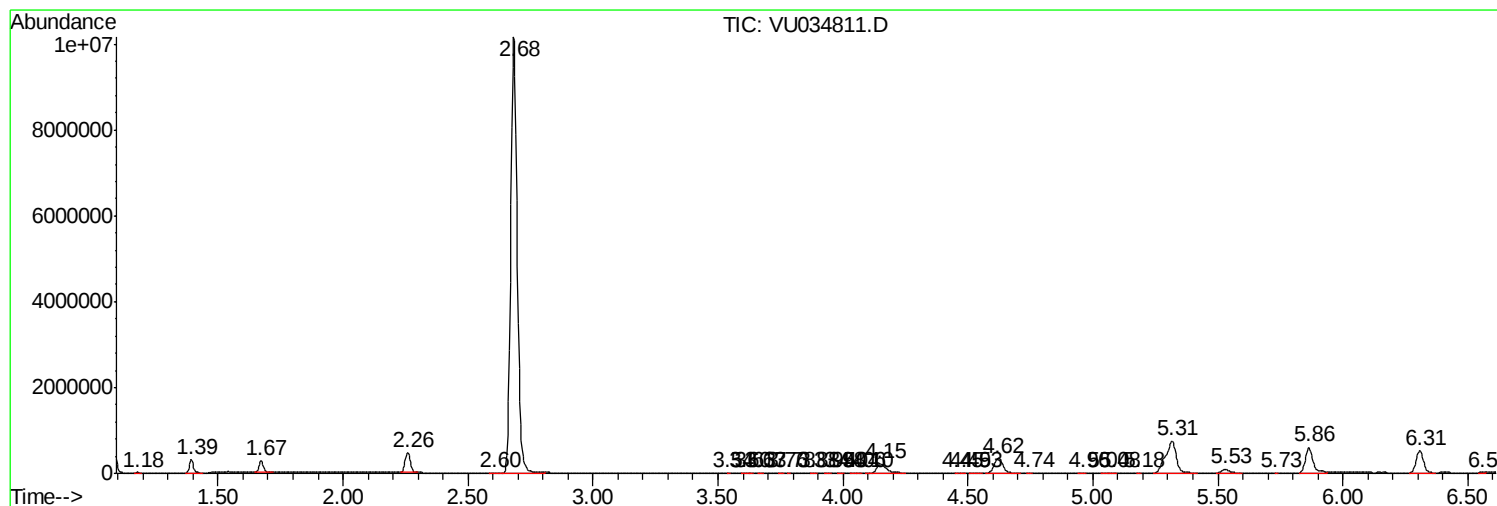
Sum of corrected areas: 44623508

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Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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



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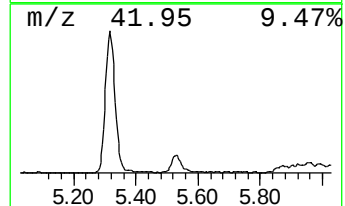
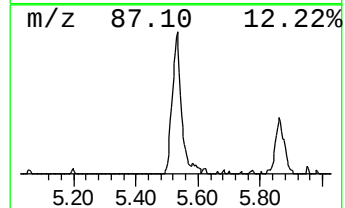
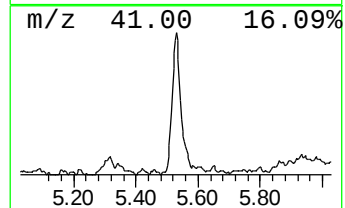
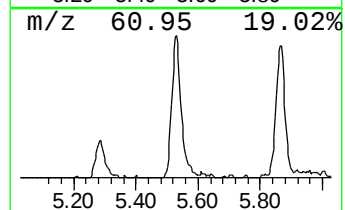
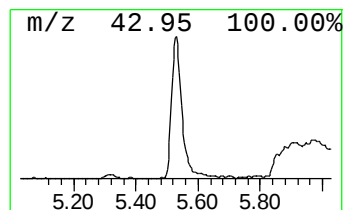
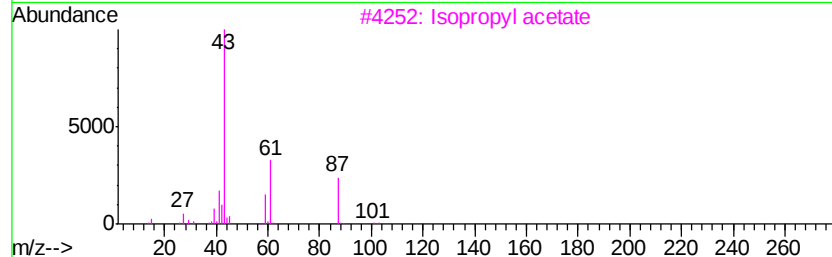
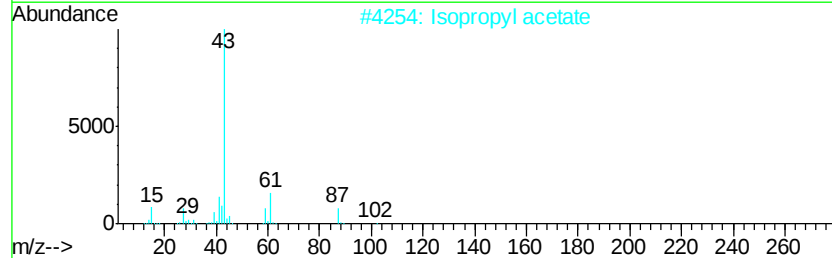
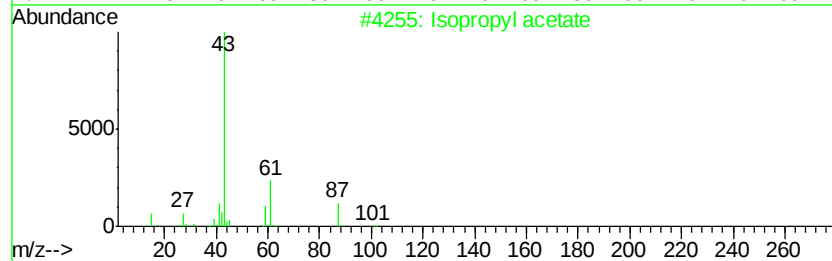
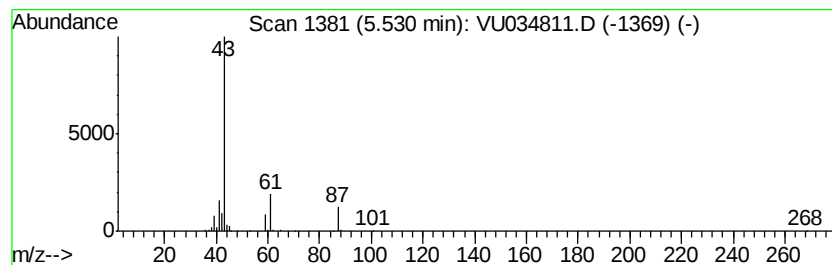
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.53	7.68 ug/L	198032	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl acetate	102	C5H10O2	000108-21-4	78
2		Isopropyl acetate	102	C5H10O2	000108-21-4	56
3		Isopropyl acetate	102	C5H10O2	000108-21-4	56
4		Isopropyl acetate	102	C5H10O2	000108-21-4	50
5		Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9



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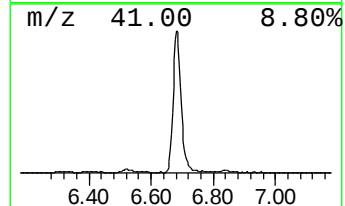
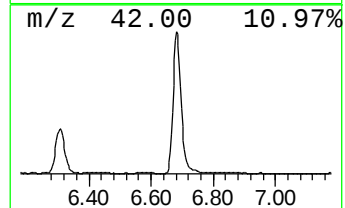
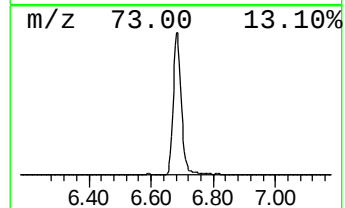
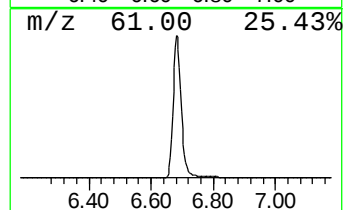
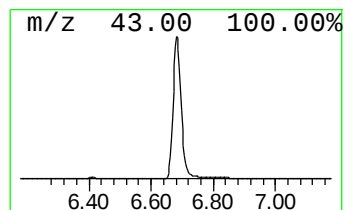
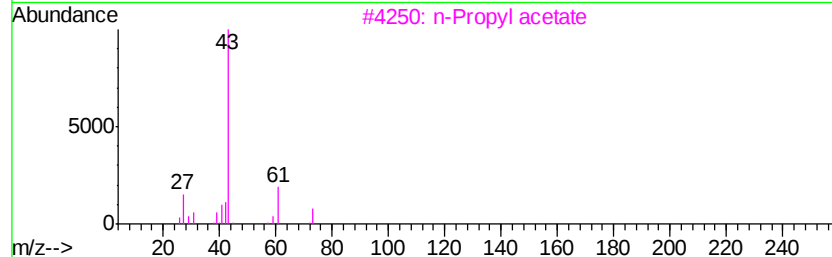
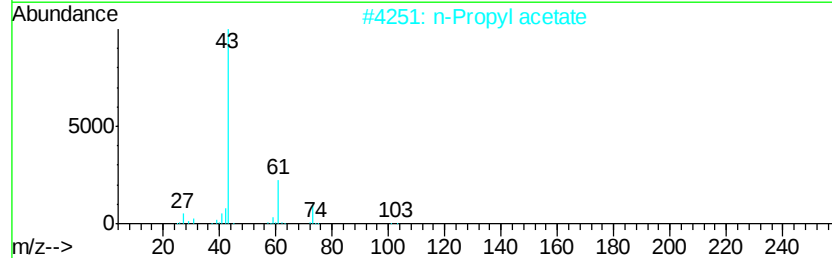
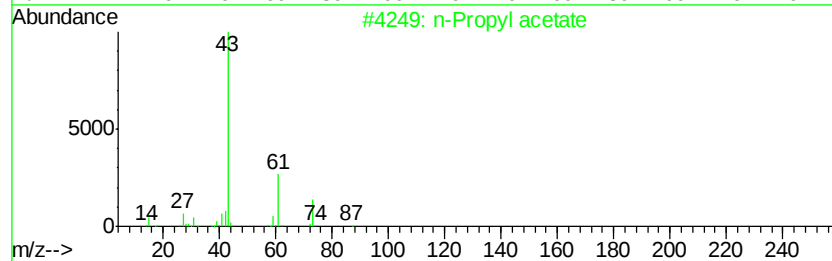
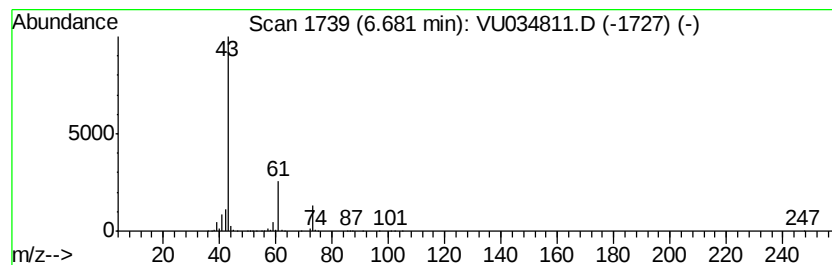
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Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	151.05 ug/L	3896890	1,4-Difluorobenzene	5.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	78
4	Isopropyl	acetate	102	C5H10O2	000108-21-4	36
5	Isopropyl	acetate	102	C5H10O2	000108-21-4	9



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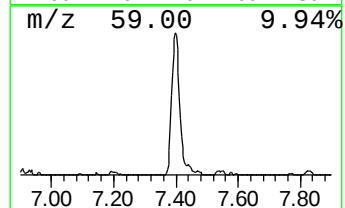
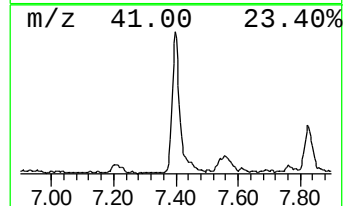
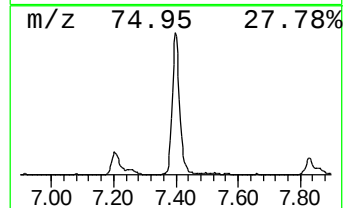
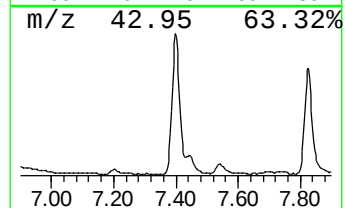
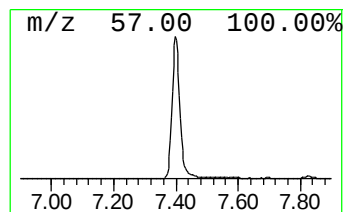
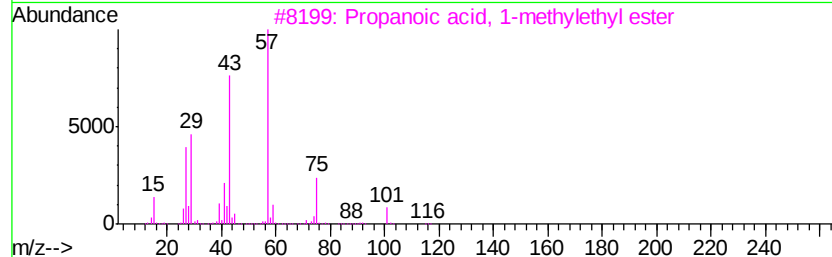
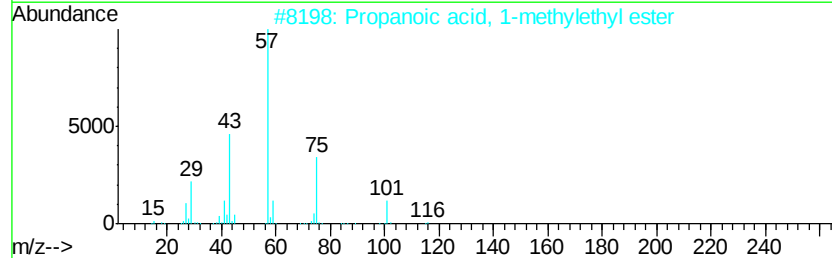
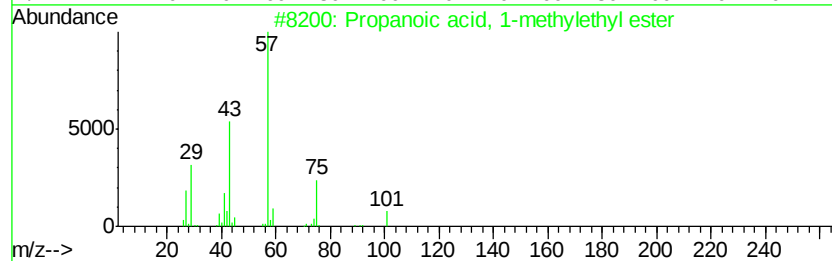
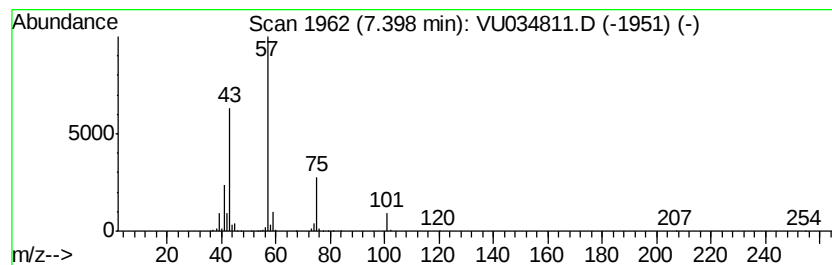
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	18.16 ug/L	468646	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45
5		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
Data File : VU034811.D
Acq On : 25 Sep 2019 18:47
Operator : JC/SP
Sample : PB123366TB
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB03

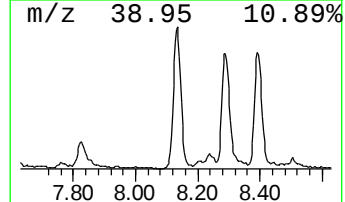
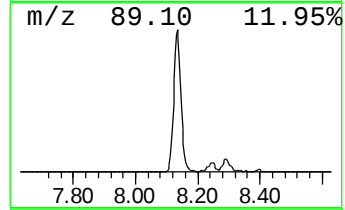
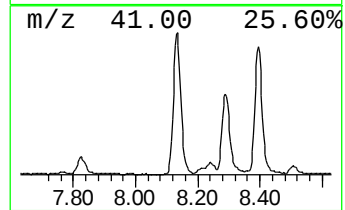
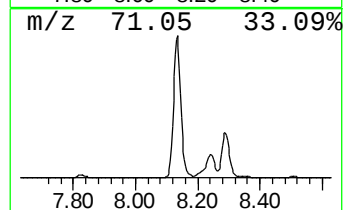
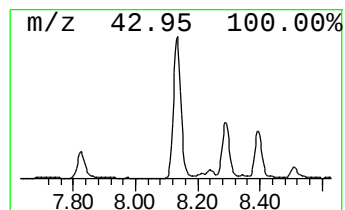
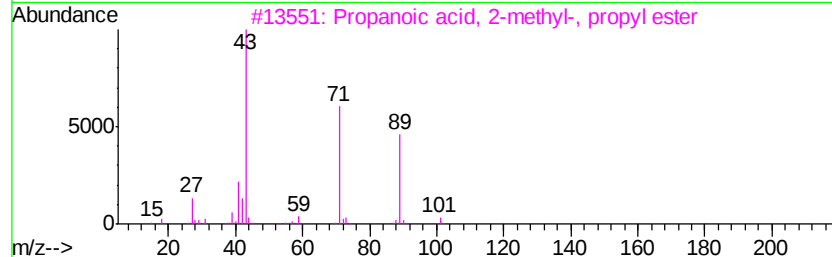
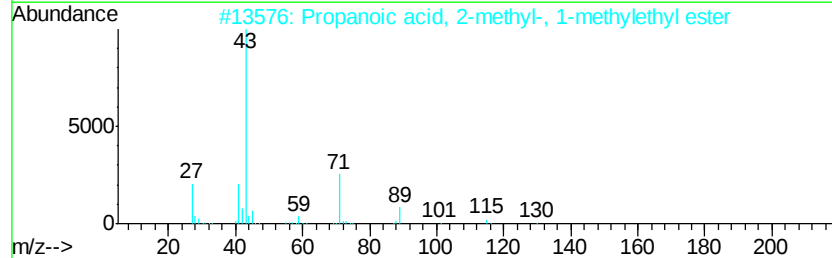
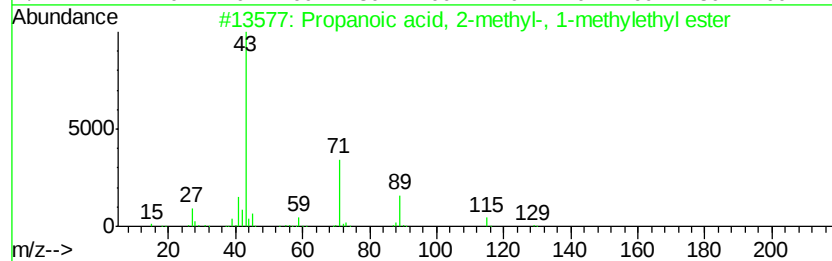
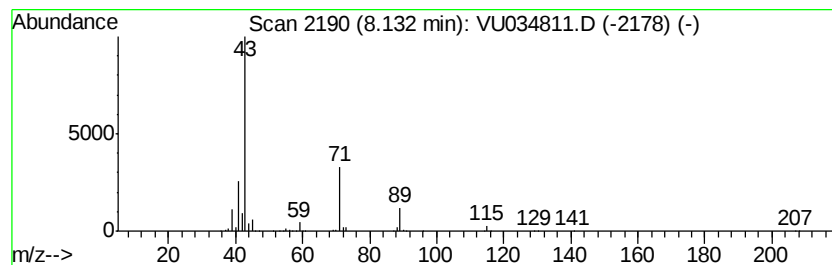
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.13	28.61 ug/L	858925	Chlorobenzene-d5	9.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83	
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83	
3	Propanoic acid, 2-methyl-, propv...	130	C7H14O2	000644-49-5	78	
4	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72	
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
Data File : VU034811.D
Acq On : 25 Sep 2019 18:47
Operator : JC/SP
Sample : PB123366TB
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 22 Sample Multiplier: 1

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ClientSampleId :
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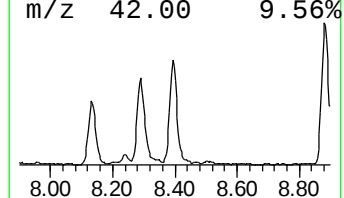
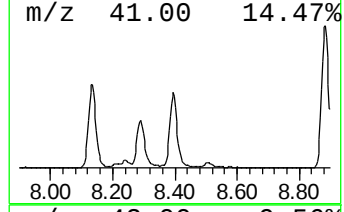
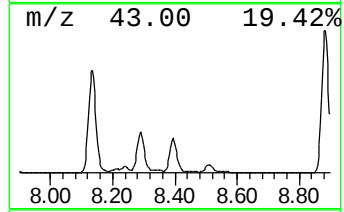
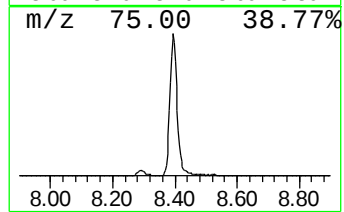
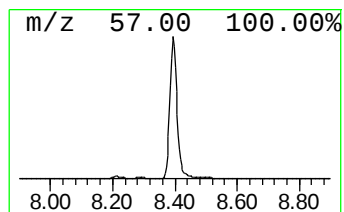
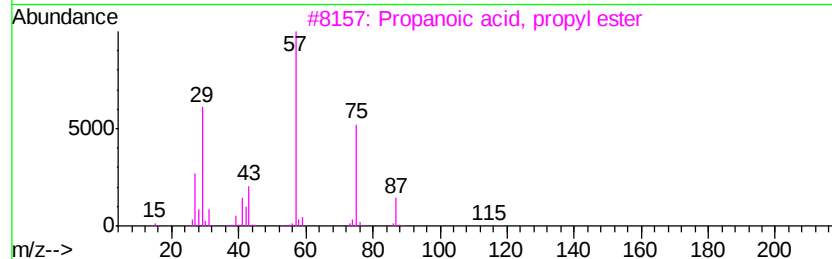
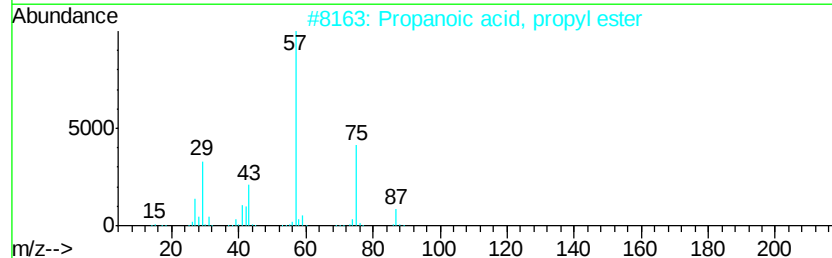
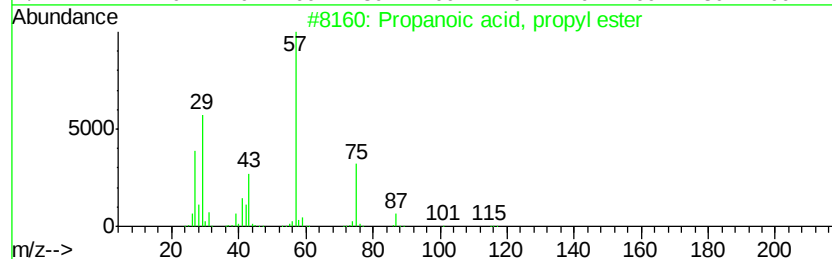
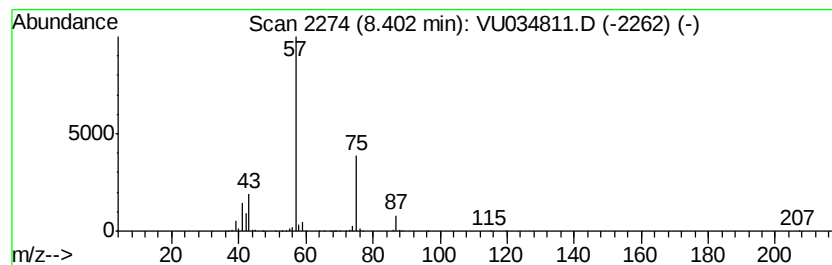
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Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	43.54 ug/L	1307130	Chlorobenzene-d5	9.07

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	78
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5		1-Pentanamine	87	C5H13N	000110-58-7	10



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
Data File : VU034811.D
Acq On : 25 Sep 2019 18:47
Operator : JC/SP
Sample : PB123366TB
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 22 Sample Multiplier: 1

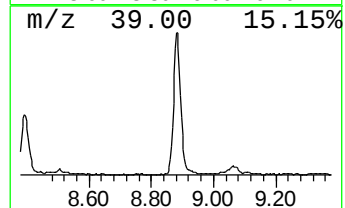
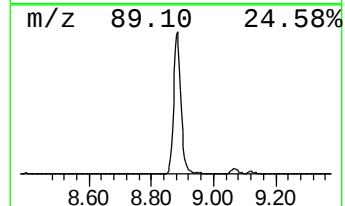
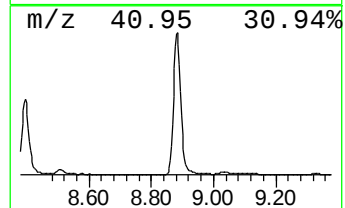
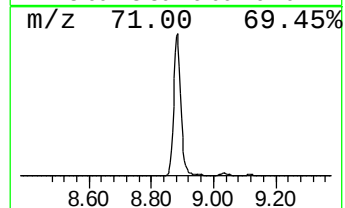
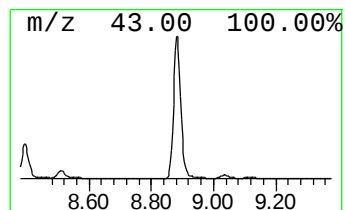
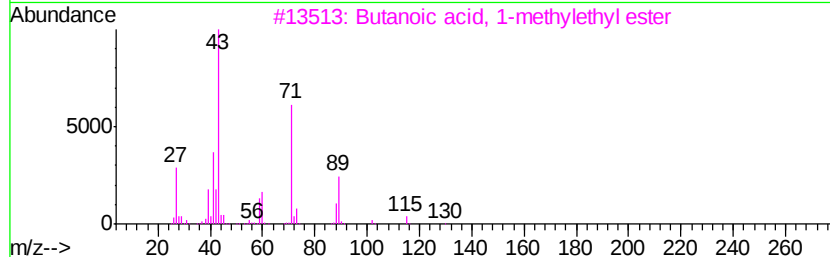
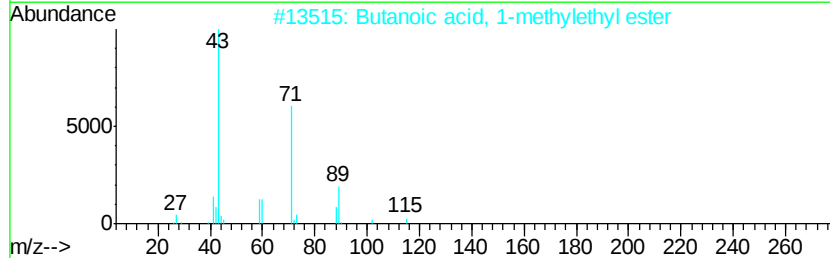
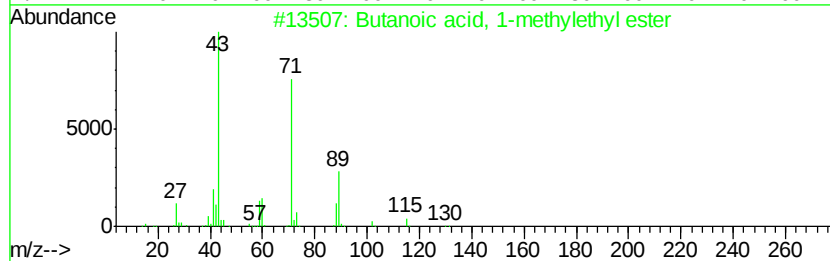
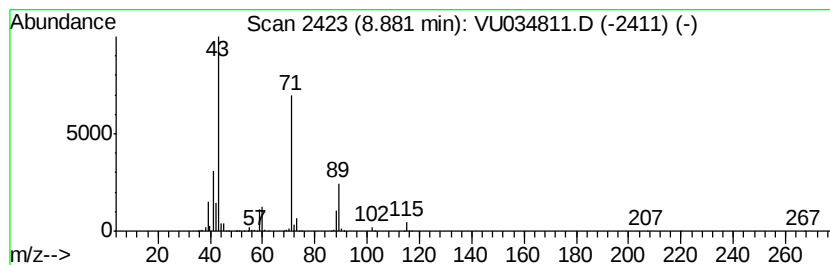
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.88	56.90 ug/L	1708270	Chlorobenzene-d5	9.07		
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	90	
4	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	86	
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
Data File : VU034811.D
Acq On : 25 Sep 2019 18:47
Operator : JC/SP
Sample : PB123366TB
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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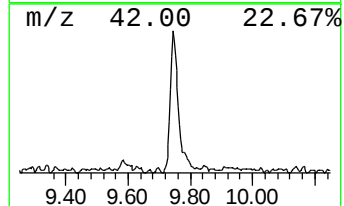
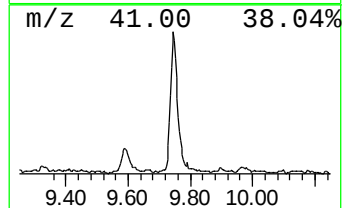
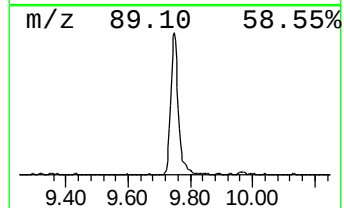
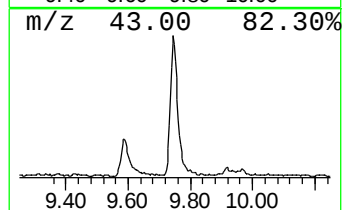
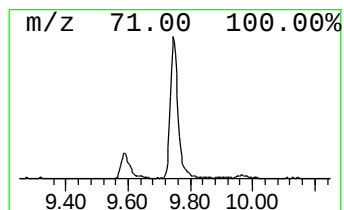
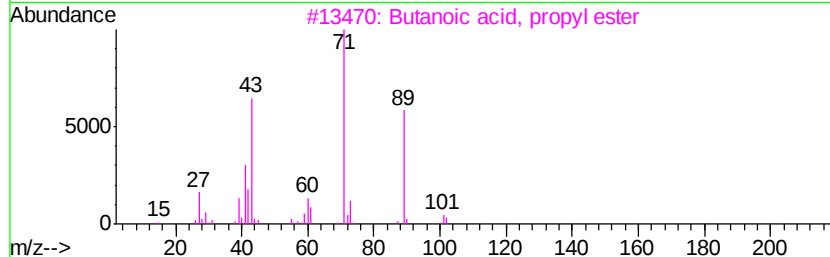
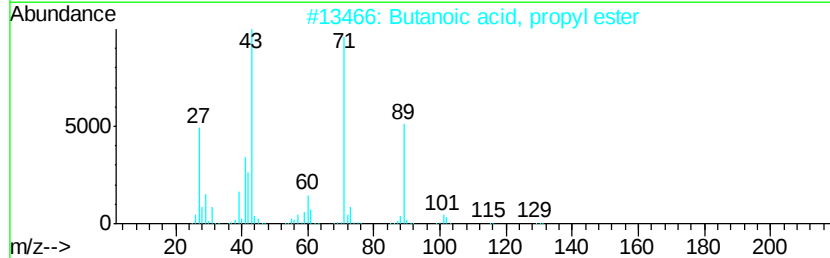
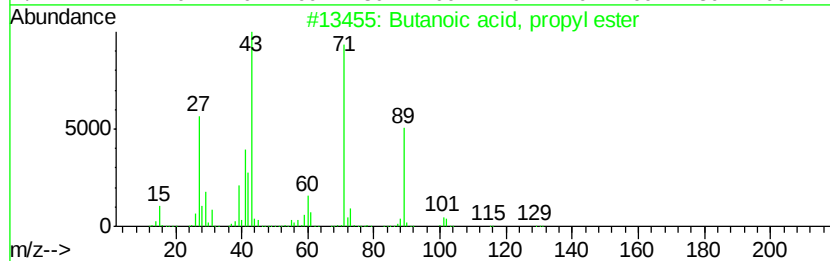
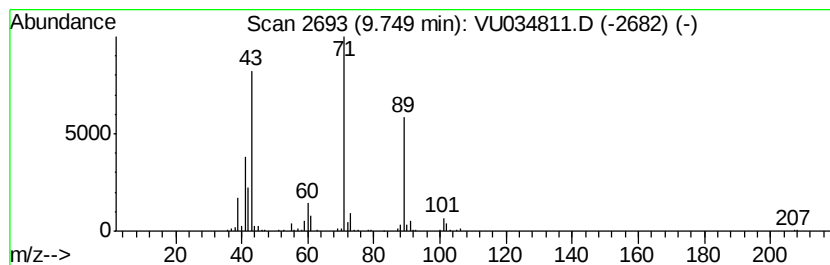
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 Butanoic acid, propyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	8.76 ug/L	263119	Chlorobenzene-d5	9.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
3		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	83
4		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	80
5		Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	74



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU092519\
Data File : VU034811.D
Acq On : 25 Sep 2019 18:47
Operator : JC/SP
Sample : PB123366TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB03

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.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	5.53	7.7	ug/L	198032	1	5.86	1289980	50.0
n-Propyl acetate	6.68	151.1	ug/L	3896890	1	5.86	1289980	50.0
Propanoic acid, 1...	7.40	18.2	ug/L	468646	1	5.86	1289980	50.0
Propanoic acid, 2...	8.13	28.6	ug/L	858925	2	9.07	1501000	50.0
Propanoic acid, p...	8.40	43.5	ug/L	1307130	2	9.07	1501000	50.0
Butanoic acid, 1-...	8.88	56.9	ug/L	1708270	2	9.07	1501000	50.0
Butanoic acid, pr...	9.75	8.8	ug/L	263119	2	9.07	1501000	50.0