

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092519\
 Data File : VU034818.D
 Acq On : 25 Sep 2019 21:31
 Operator : JC/SP
 Sample : K4983-08
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFDM3

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	23	27	32	rBV2	7917	7066	0.19%	0.027%
2	1.392	87	94	104	rBV	300956	319725	8.64%	1.219%
3	1.543	135	141	149	rVB3	31719	39972	1.08%	0.152%
4	1.672	173	181	194	rVB	256236	329268	8.90%	1.255%
5	2.257	354	363	374	rVB	438915	663304	17.93%	2.529%
6	2.531	446	448	452	rVB4	1333	809	0.02%	0.003%
7	2.685	483	496	518	rBV	260566	479301	12.95%	1.827%
8	2.833	540	542	544	rBV3	1791	725	0.02%	0.003%
9	2.900	560	563	565	rBV3	1140	743	0.02%	0.003%
10	2.923	565	570	574	rBV7	2382	2163	0.06%	0.008%
11	2.977	582	587	590	rBV7	1543	1285	0.03%	0.005%
12	3.074	614	617	618	rBV	894	476	0.01%	0.002%
13	3.116	626	630	631	rBV3	1678	1163	0.03%	0.004%
14	3.222	661	663	666	rBV2	1300	675	0.02%	0.003%
15	3.277	676	680	681	rBV2	854	520	0.01%	0.002%
16	3.286	681	683	686	rVV3	1275	1015	0.03%	0.004%
17	3.344	698	701	702	rBV3	772	513	0.01%	0.002%
18	3.370	706	709	712	rBV4	1327	1010	0.03%	0.004%
19	3.386	712	714	718	rVB3	997	699	0.02%	0.003%
20	3.408	718	721	722	rBV2	880	449	0.01%	0.002%
21	3.463	735	738	741	rBV2	1193	705	0.02%	0.003%
22	3.482	741	744	746	rVB3	863	409	0.01%	0.002%
23	3.502	746	750	752	rBV4	1090	855	0.02%	0.003%
24	3.518	752	755	758	rBV2	814	512	0.01%	0.002%
25	3.637	790	792	794	rBV2	1101	620	0.02%	0.002%
26	3.649	794	796	798	rBV2	1026	595	0.02%	0.002%
27	3.675	802	804	806	rVB3	875	433	0.01%	0.002%
28	3.691	806	809	813	rBV3	1313	1145	0.03%	0.004%
29	3.743	819	825	831	rBV8	1344	1580	0.04%	0.006%
30	3.772	831	834	837	rBV3	1063	721	0.02%	0.003%
31	3.810	843	846	851	rVB6	1064	832	0.02%	0.003%
32	3.858	858	861	865	rBV4	946	753	0.02%	0.003%
33	3.920	875	880	882	rBV4	790	760	0.02%	0.003%
34	3.942	885	887	890	rVB3	1241	693	0.02%	0.003%

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 Title : VOC Analysis

35	3.971	892	896	899	rBV4	798	768	0.02%	0.003%
36	4.003	904	906	909	rBV2	785	465	0.01%	0.002%
37	4.058	917	923	926	rBV6	1861	1971	0.05%	0.008%
38	4.084	929	931	934	rVB3	1271	512	0.01%	0.002%
39	4.151	938	952	980	rBV	225201	611032	16.51%	2.330%
40	4.511	1061	1064	1066	rBV2	1084	676	0.02%	0.003%
41	4.624	1081	1099	1119	rBV	347002	829896	22.43%	3.164%
42	4.955	1200	1202	1205	rBV4	1095	499	0.01%	0.002%
43	5.103	1245	1248	1251	rVB3	1504	1114	0.03%	0.004%
44	5.119	1251	1253	1256	rVB4	1225	747	0.02%	0.003%
45	5.148	1256	1262	1263	rBV4	1913	1628	0.04%	0.006%
46	5.180	1271	1272	1275	rVB3	855	482	0.01%	0.002%
47	5.231	1285	1288	1290	rVB3	1390	709	0.02%	0.003%
48	5.315	1290	1314	1336	rBV2	736888	2190202	59.19%	8.350%
49	5.527	1369	1380	1404	rBV2	89421	194142	5.25%	0.740%
50	5.672	1423	1425	1427	rBV2	1528	835	0.02%	0.003%
51	5.865	1470	1485	1503	rBV	593225	1276675	34.50%	4.867%
52	6.305	1610	1622	1646	rVB	507420	1023840	27.67%	3.903%
53	6.563	1695	1702	1704	rBV2	14901	18725	0.51%	0.071%
54	6.681	1727	1739	1772	rBV	2024001	3700361	100.00%	14.108%
55	7.083	1861	1864	1869	rBV7	1908	1143	0.03%	0.004%
56	7.206	1890	1902	1920	rBV	292407	531881	14.37%	2.028%
57	7.399	1951	1962	1974	rBV	244200	413499	11.17%	1.576%
58	7.543	1995	2007	2023	rBV	1001098	1759505	47.55%	6.708%
59	7.826	2085	2095	2115	rBV2	259462	469891	12.70%	1.791%
60	8.016	2152	2154	2157	rVB	1844	757	0.02%	0.003%
61	8.035	2157	2160	2164	rBV4	1478	1008	0.03%	0.004%
62	8.135	2179	2191	2207	rBV	457767	757552	20.47%	2.888%
63	8.212	2208	2215	2218	rBV4	24716	32640	0.88%	0.124%
64	8.289	2230	2239	2262	rVV	881204	1516245	40.98%	5.781%
65	8.395	2262	2272	2294	rVB	727251	1165551	31.50%	4.444%
66	8.508	2301	2307	2322	rVB	36089	63365	1.71%	0.242%
67	8.759	2381	2385	2391	rBV7	2068	2812	0.08%	0.011%
68	8.884	2412	2424	2446	rBV	933896	1507578	40.74%	5.748%
69	9.067	2462	2481	2508	rBV	831592	1450460	39.20%	5.530%
70	9.228	2524	2531	2543	rVB	18784	30581	0.83%	0.117%
71	9.353	2556	2570	2584	rBV	56479	105504	2.85%	0.402%

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72	9.553	2628	2632	2633	rBV3	1212	785	0.02%	0.003%
73	9.588	2635	2643	2660	rVV2	22151	42027	1.14%	0.160%
74	9.749	2683	2693	2720	rBV3	139623	271714	7.34%	1.036%
75	9.887	2733	2736	2737	rBV3	1540	1005	0.03%	0.004%
76	10.263	2850	2853	2856	rBV4	1062	858	0.02%	0.003%
77	10.408	2884	2898	2923	rBV	687831	1125949	30.43%	4.293%
78	10.569	2941	2948	2951	rBV5	4951	6371	0.17%	0.024%
79	10.662	2967	2977	2994	rBV3	22385	52146	1.41%	0.199%
80	10.749	2996	3004	3013	rVB3	16999	28458	0.77%	0.108%
81	10.948	3058	3066	3080	rVB2	14164	22757	0.61%	0.087%
82	11.128	3112	3122	3139	rBV	60031	96647	2.61%	0.368%
83	11.373	3194	3198	3199	rBV4	1988	1383	0.04%	0.005%
84	11.459	3213	3225	3244	rBV	755217	1245694	33.66%	4.749%
85	11.546	3246	3252	3268	rVB	28947	50634	1.37%	0.193%
86	11.746	3306	3314	3321	rBV3	14395	24049	0.65%	0.092%
87	11.836	3331	3342	3371	rVB	884185	1486013	40.16%	5.665%
88	12.340	3491	3499	3507	rBV8	4018	6919	0.19%	0.026%
89	12.594	3573	3578	3584	rBV9	4412	6461	0.17%	0.025%
90	12.684	3602	3606	3613	rVB5	8024	9093	0.25%	0.035%
91	13.054	3718	3721	3725	rBV6	2251	2096	0.06%	0.008%
92	13.106	3725	3737	3746	rVV6	15429	29272	0.79%	0.112%
93	13.266	3783	3787	3788	rBV2	4729	3062	0.08%	0.012%
94	13.379	3816	3822	3832	rVB2	8304	13241	0.36%	0.050%
95	13.488	3854	3856	3863	rVB7	3776	3261	0.09%	0.012%
96	13.594	3883	3889	3893	rBV7	2943	3865	0.10%	0.015%
97	13.729	3921	3931	3949	rBV	47990	104996	2.84%	0.400%
98	14.546	4183	4185	4187	rVB	2100	867	0.02%	0.003%
99	14.874	4278	4287	4299	rBV3	14949	30172	0.82%	0.115%
100	15.051	4332	4342	4352	rBV6	16074	33114	0.89%	0.126%

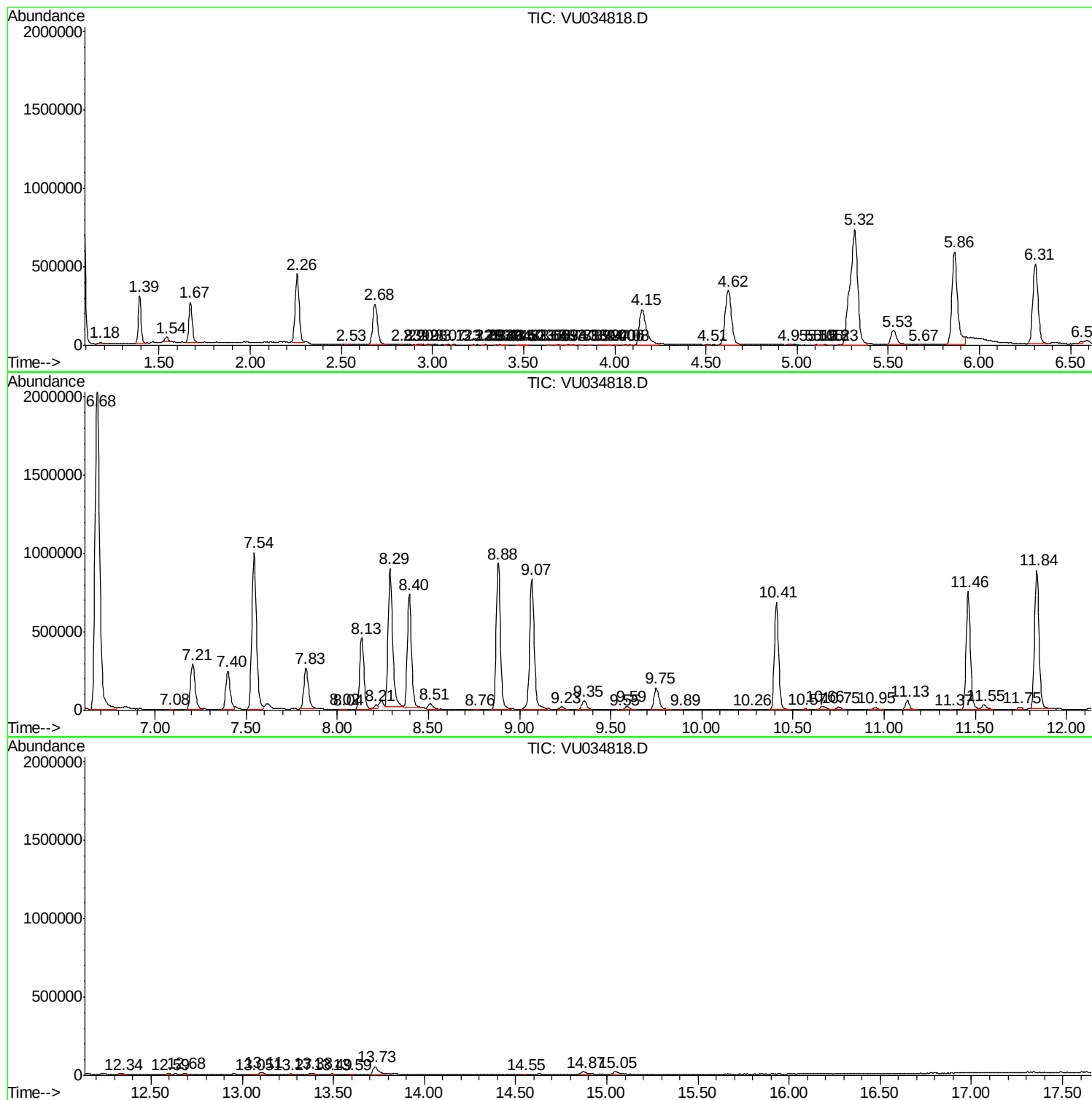
Sum of corrected areas: 26229654

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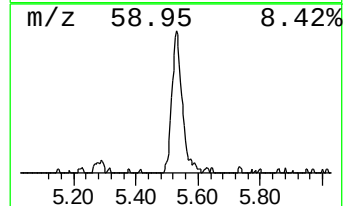
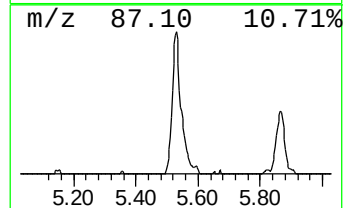
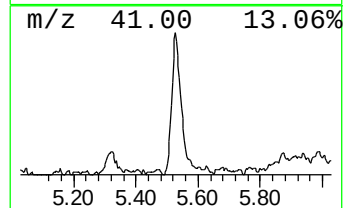
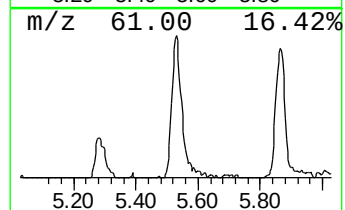
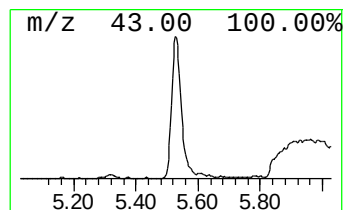
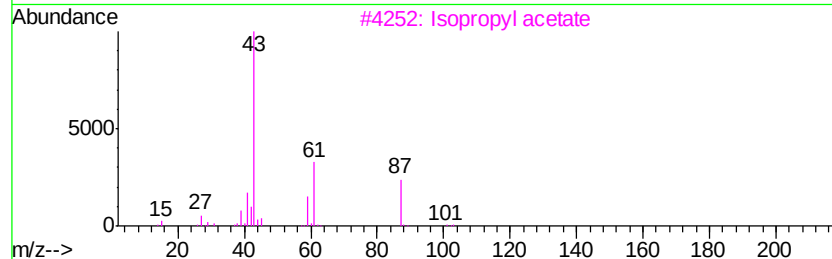
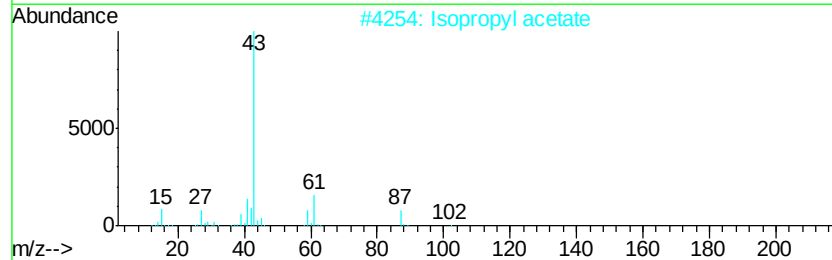
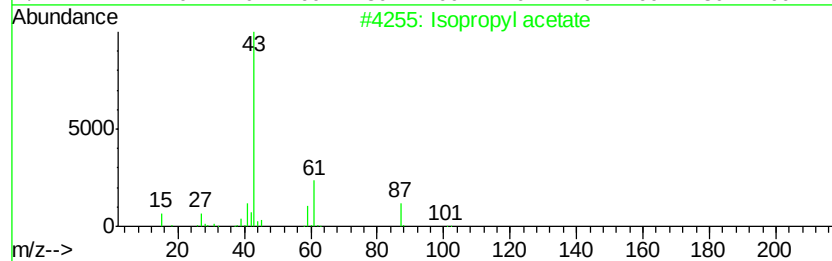
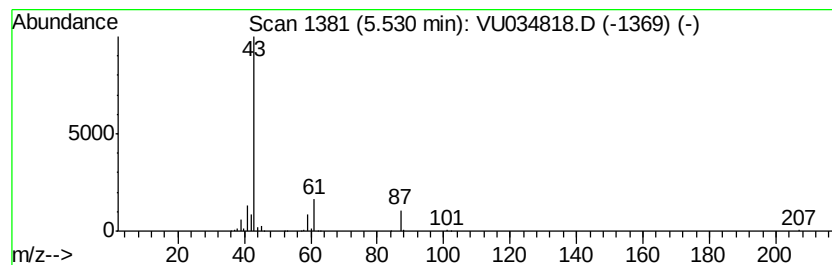
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.53	7.60 ug/L	194142	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	40
4		Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9
5		Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9



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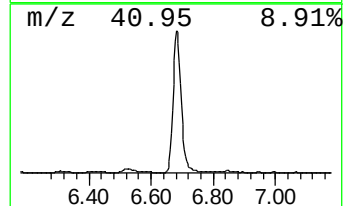
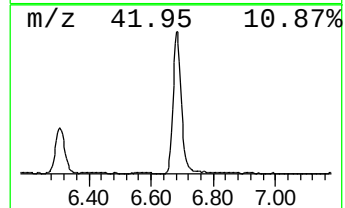
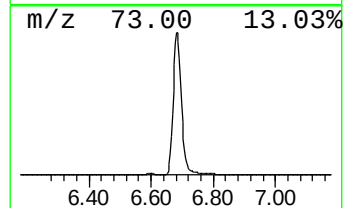
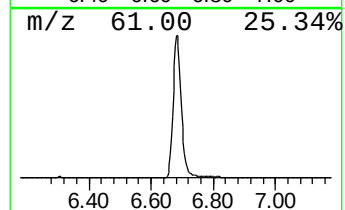
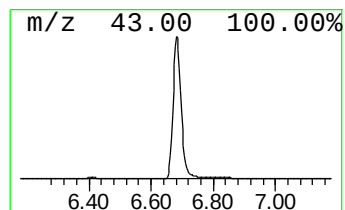
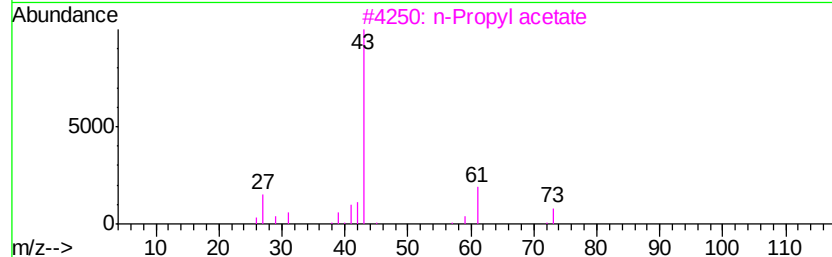
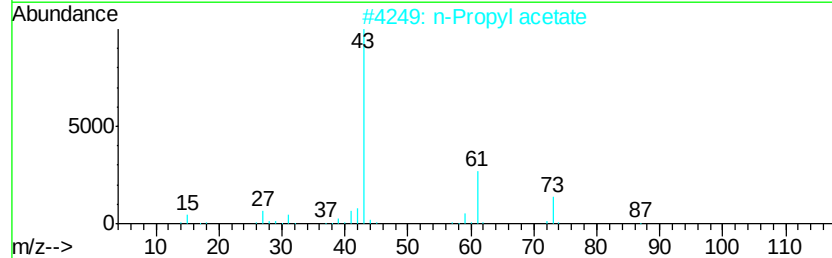
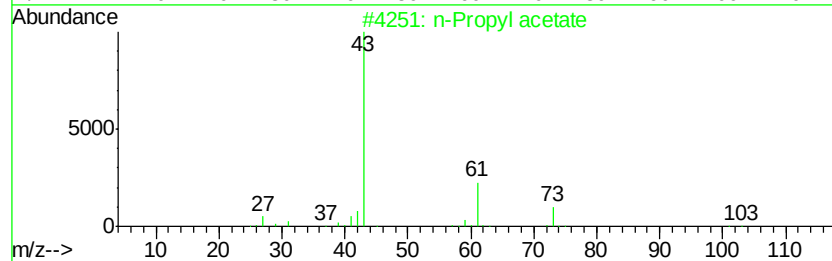
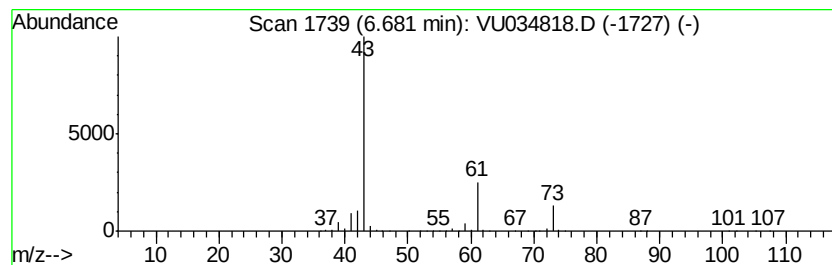
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Quant Title : VOC Analysis

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	144.92 ug/L	3700360	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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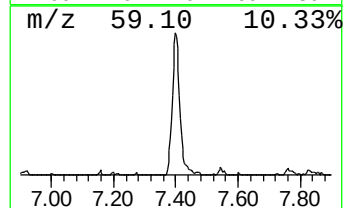
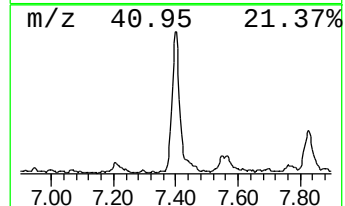
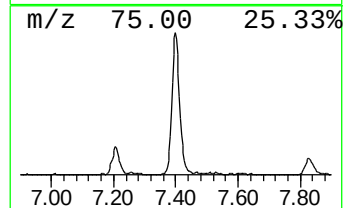
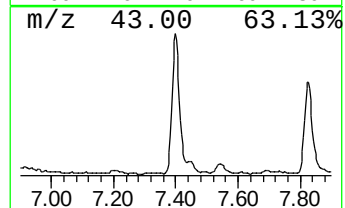
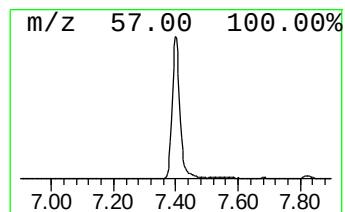
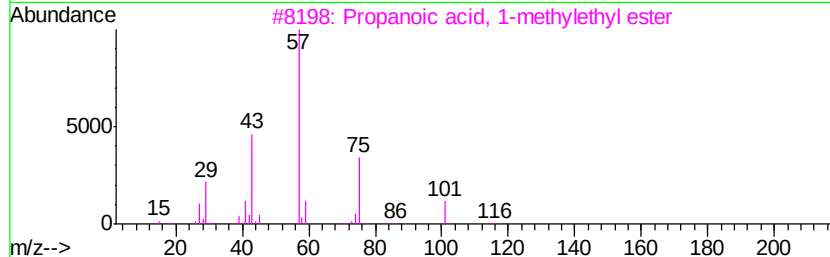
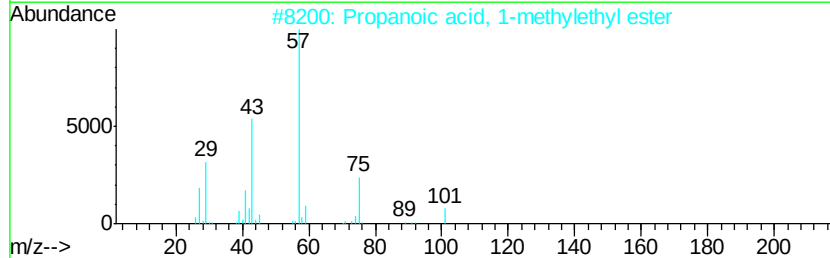
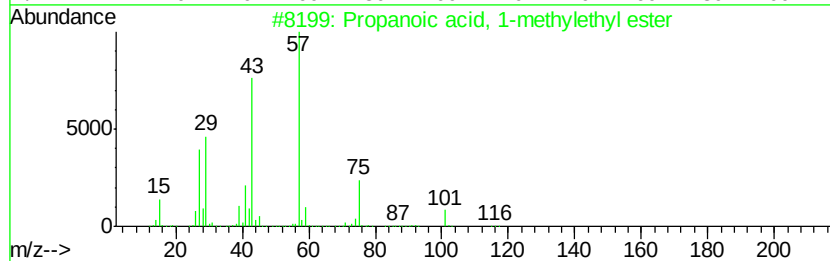
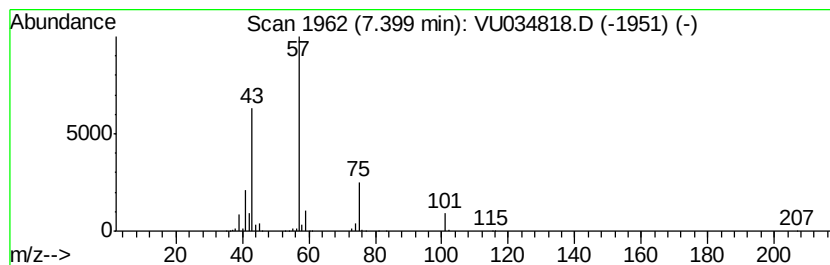
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Quant Title : VOC Analysis

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	16.19 ug/L	413499	1,4-Difluorobenzene	5.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2		000637-78-5	78
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2		000637-78-5	72
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2		000637-78-5	72
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2		000637-78-5	64
5	Propanoic acid, propyl ester	116	C6H12O2		000106-36-5	36



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
Data File : VU034818.D
Acq On : 25 Sep 2019 21:31
Operator : JC/SP
Sample : K4983-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDM3

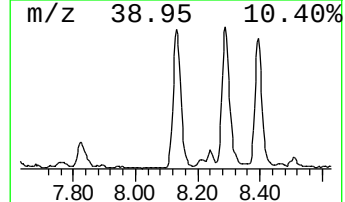
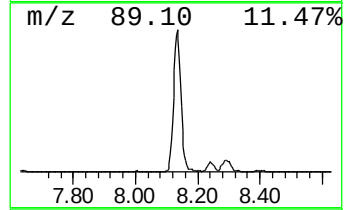
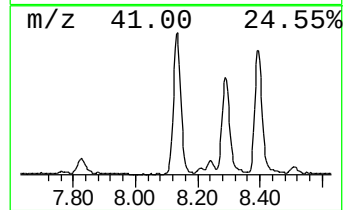
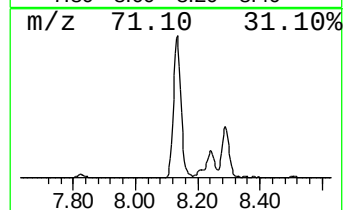
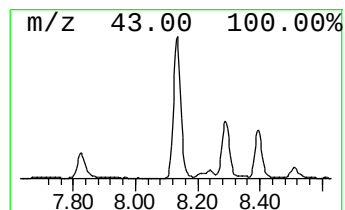
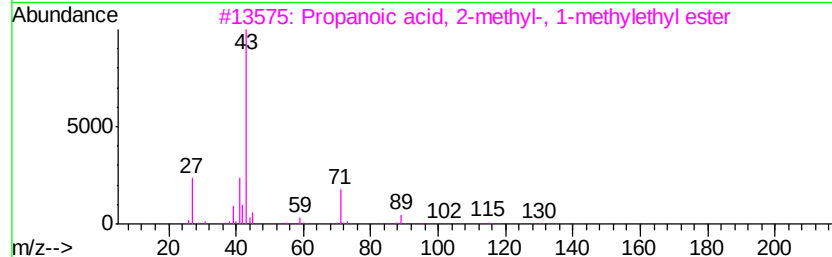
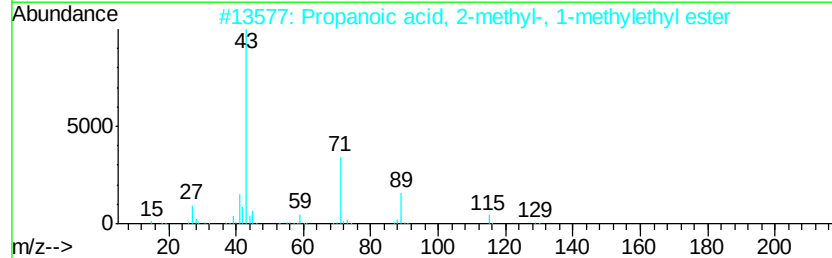
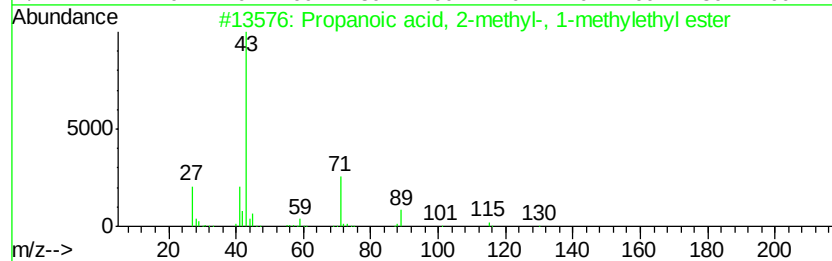
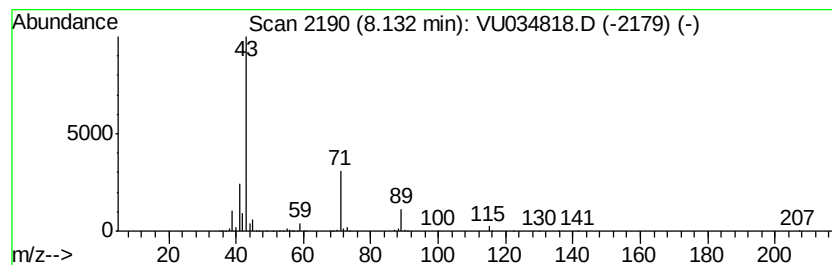
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Quant Title : VOC Analysis

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	26.11 ug/L	757552	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-, 1-met...	130	C7H14O2	000617-50-5	78		
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64		
5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	56		



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
Data File : VU034818.D
Acq On : 25 Sep 2019 21:31
Operator : JC/SP
Sample : K4983-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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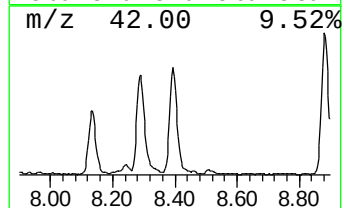
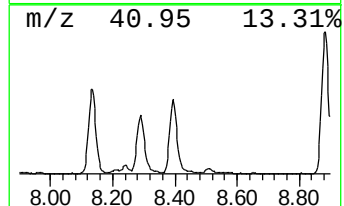
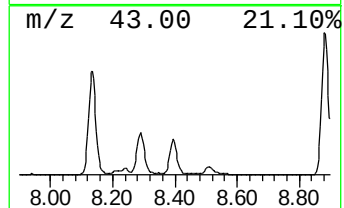
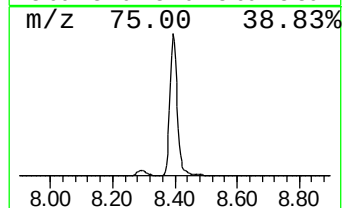
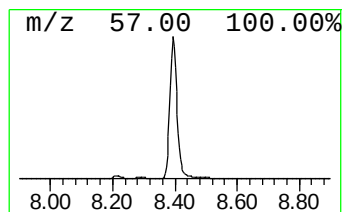
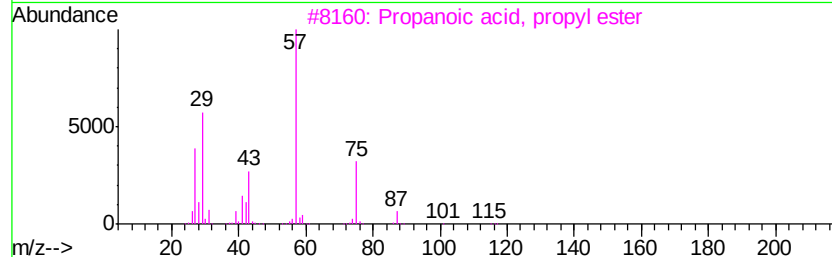
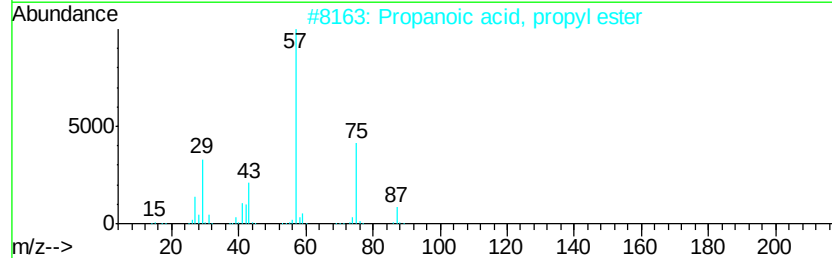
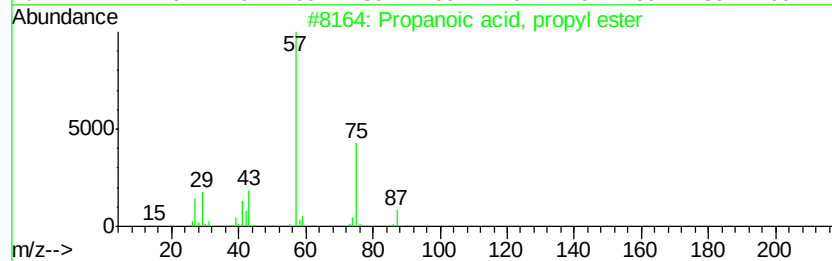
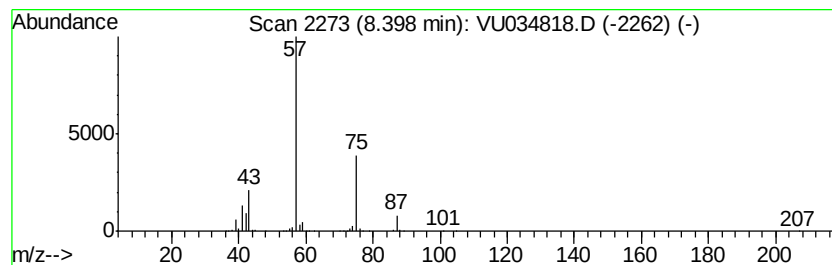
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Quant Title : VOC Analysis

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	40.18 ug/L	1165550	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	83
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
5		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
Data File : VU034818.D
Acq On : 25 Sep 2019 21:31
Operator : JC/SP
Sample : K4983-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDM3

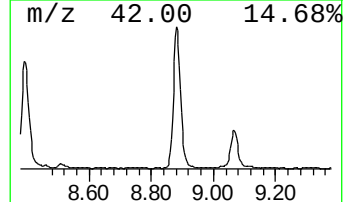
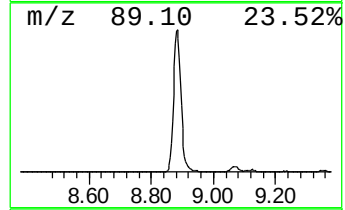
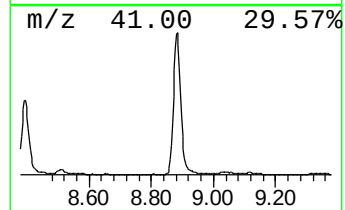
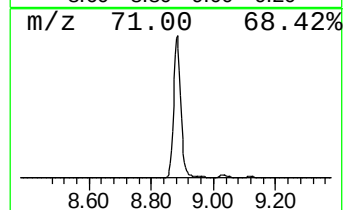
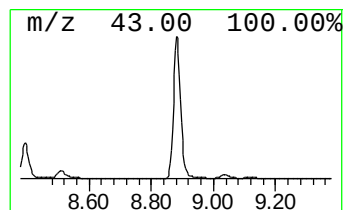
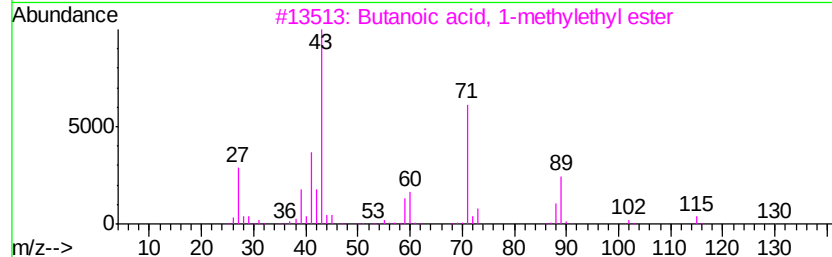
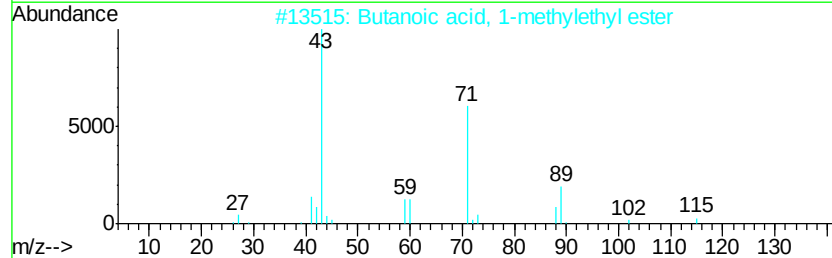
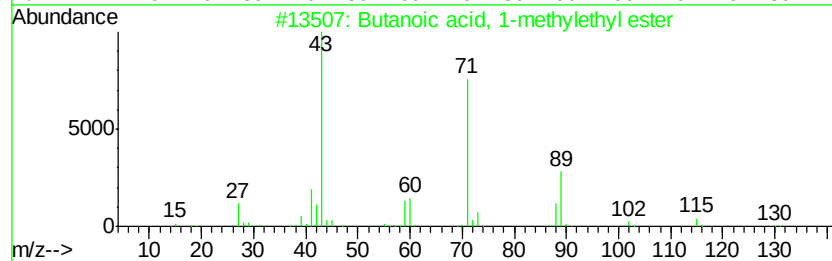
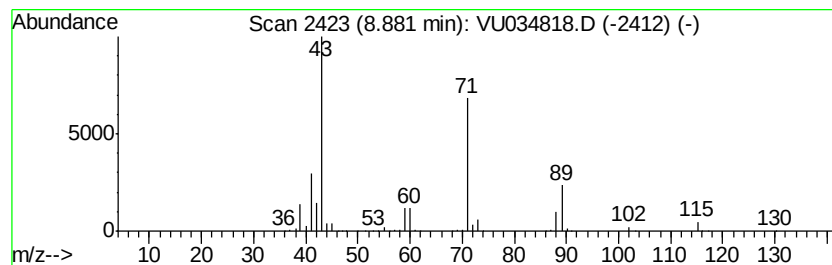
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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	51.97 ug/L	1507580	Chlorobenzene-d5	9.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
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-, propy...	130	C7H14O2	000644-49-5	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
Data File : VU034818.D
Acq On : 25 Sep 2019 21:31
Operator : JC/SP
Sample : K4983-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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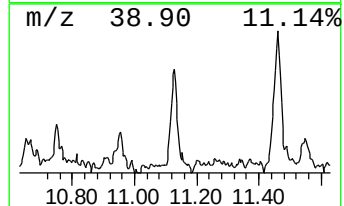
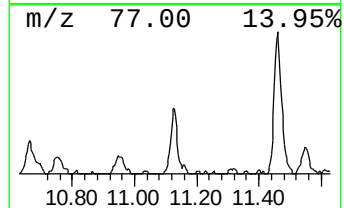
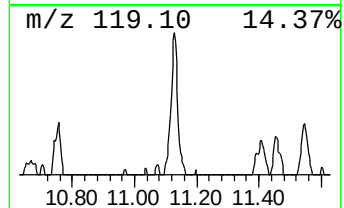
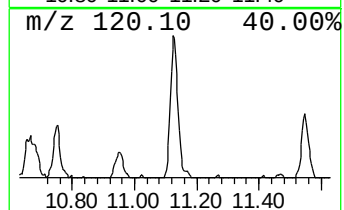
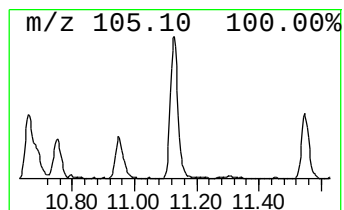
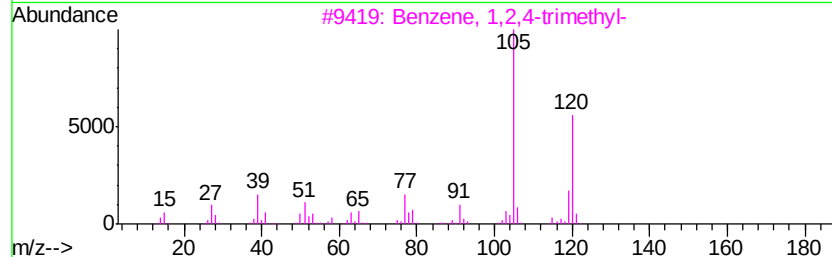
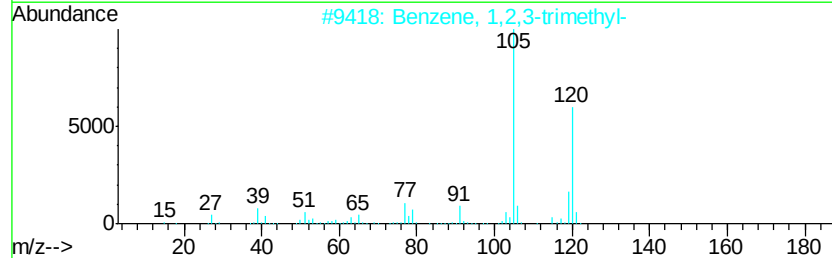
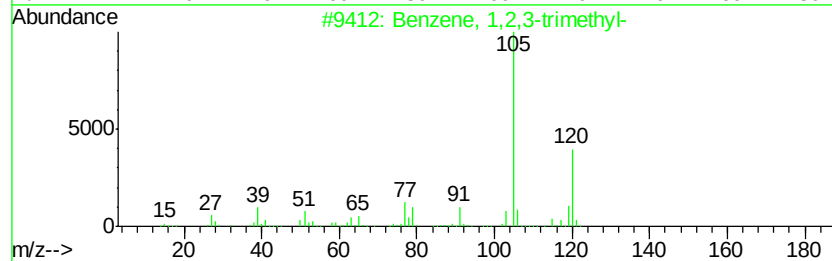
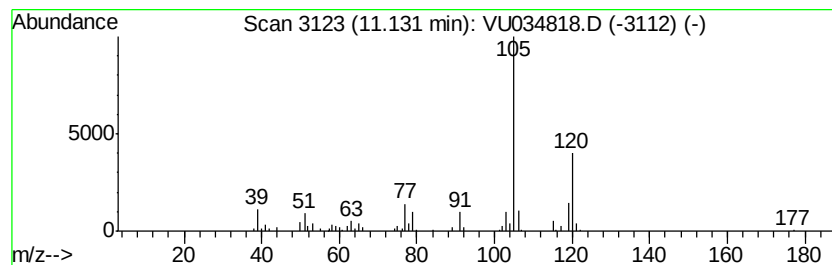
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Quant Title : VOC Analysis

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

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.13	3.88 ug/L	96647	1,4-Dichlorobenzene-d4	11.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
5		Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
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Acq On : 25 Sep 2019 21:31
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Sample : K4983-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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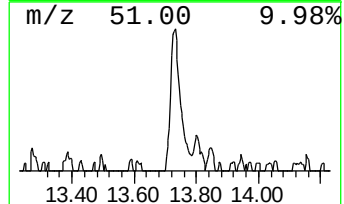
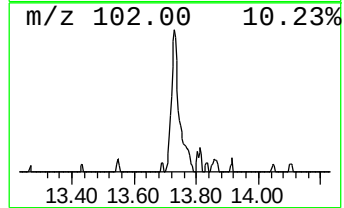
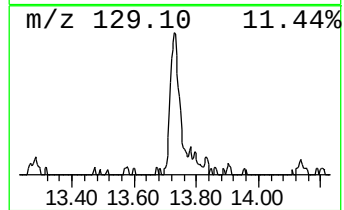
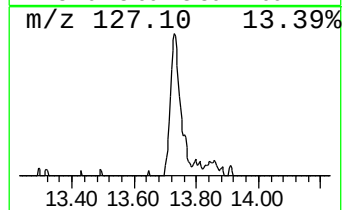
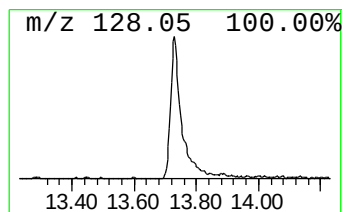
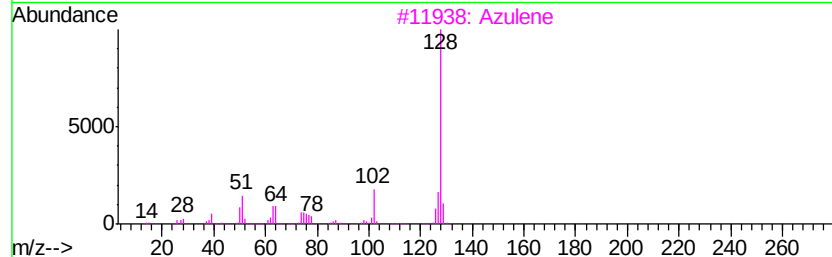
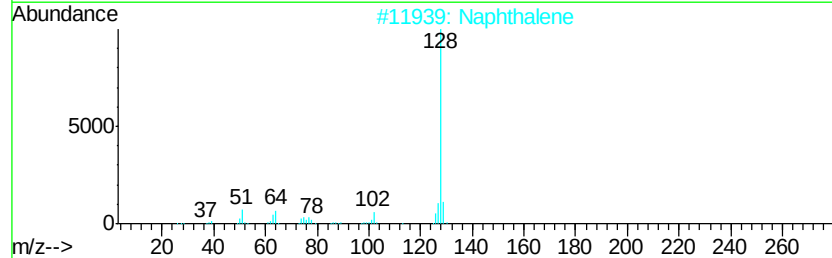
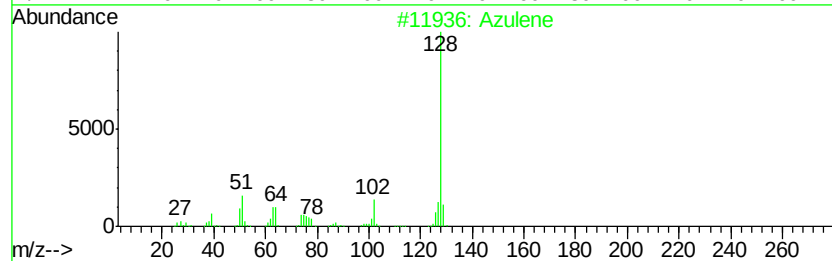
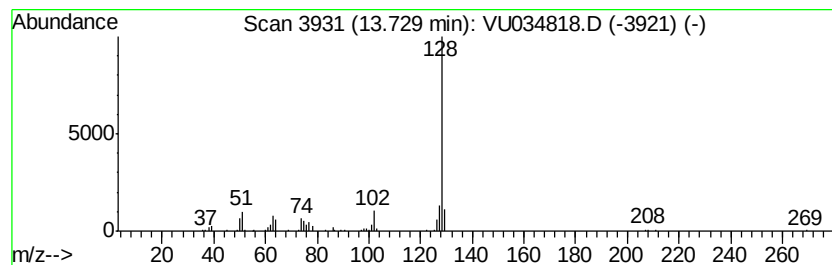
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Quant Title : VOC Analysis

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

Peak Number 9 Azulene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.21 ug/L	104996	1,4-Dichlorobenzene-d4	11.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Azulene	128	C10H8	000275-51-4	94
2		Naphthalene	128	C10H8	000091-20-3	91
3		Azulene	128	C10H8	000275-51-4	91
4		Azulene	128	C10H8	000275-51-4	91
5		Naphthalene	128	C10H8	000091-20-3	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU092519\
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 29 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl acetate	5.53	7.6	ug/L	194142	1	5.86	1276680	50.0
n-Propyl acetate	6.68	144.9	ug/L	3700360	1	5.86	1276680	50.0
Propanoic acid, 1...	7.40	16.2	ug/L	413499	1	5.86	1276680	50.0
Propanoic acid, 2...	8.13	26.1	ug/L	757552	2	9.07	1450460	50.0
Propanoic acid, p...	8.40	40.2	ug/L	1165550	2	9.07	1450460	50.0
Butanoic acid, 1-...	8.88	52.0	ug/L	1507580	2	9.07	1450460	50.0
Benzene, 1,2,3-tr...	11.13	3.9	ug/L	96647	3	11.46	1245690	50.0
Azulene	13.73	4.2	ug/L	104996	3	11.46	1245690	50.0