

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092519\
 Data File : VU034824.D
 Acq On : 25 Sep 2019 23:52
 Operator : JC/SP
 Sample : K4983-14
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFDN4

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	1.392	87	94	105	rBV	295029	313289	8.70%	1.248%
2	1.540	135	140	150	rVB2	29507	40743	1.13%	0.162%
3	1.672	173	181	191	rBV	247591	312235	8.68%	1.244%
4	2.257	354	363	375	rVB	444768	668814	18.58%	2.665%
5	2.534	446	449	452	rBV4	1014	800	0.02%	0.003%
6	2.556	454	456	460	rVB5	1575	1118	0.03%	0.004%
7	2.611	464	473	479	rVV2	4284	6952	0.19%	0.028%
8	2.637	479	481	484	rVV2	1761	951	0.03%	0.004%
9	2.685	484	496	516	rVV	173728	317469	8.82%	1.265%
10	2.772	520	523	524	rBV3	1042	607	0.02%	0.002%
11	2.820	534	538	543	rBV8	1525	1480	0.04%	0.006%
12	2.862	547	551	553	rBV3	625	618	0.02%	0.002%
13	2.932	570	573	576	rVB4	1825	1042	0.03%	0.004%
14	3.022	598	601	603	rVV4	1024	627	0.02%	0.002%
15	3.106	623	627	629	rBV2	1430	1062	0.03%	0.004%
16	3.276	678	680	685	rVB4	1126	616	0.02%	0.002%
17	3.321	692	694	700	rBV6	1460	1254	0.03%	0.005%
18	3.363	704	707	709	rVB4	931	593	0.02%	0.002%
19	3.418	721	724	727	rVB4	1592	1070	0.03%	0.004%
20	3.440	727	731	734	rVB4	859	533	0.01%	0.002%
21	3.514	751	754	759	rVV4	1245	966	0.03%	0.004%
22	3.553	761	766	768	rBV4	983	1167	0.03%	0.005%
23	3.572	770	772	776	rVB4	920	553	0.02%	0.002%
24	3.598	776	780	782	rBV4	1070	590	0.02%	0.002%
25	3.672	800	803	805	rBV3	826	592	0.02%	0.002%
26	3.710	813	815	819	rVB4	817	558	0.02%	0.002%
27	3.849	854	858	861	rBV3	1625	1218	0.03%	0.005%
28	3.871	861	865	867	rBV3	771	529	0.01%	0.002%
29	3.907	874	876	882	rVB4	1018	751	0.02%	0.003%
30	3.936	882	885	888	rBV3	1007	686	0.02%	0.003%
31	4.006	899	907	911	rVB7	1257	1346	0.04%	0.005%
32	4.151	938	952	983	rBV2	225822	616884	17.14%	2.458%
33	4.399	1025	1029	1031	rBV4	911	735	0.02%	0.003%
34	4.444	1038	1043	1048	rBV7	1297	1453	0.04%	0.006%

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

35	4.624	1079	1099	1118	rBV	340825	814706	22.64%	3.247%
36	4.791	1149	1151	1155	rVB4	2245	1239	0.03%	0.005%
37	4.964	1201	1205	1206	rBV3	1647	1204	0.03%	0.005%
38	5.000	1214	1216	1219	rVB3	1282	669	0.02%	0.003%
39	5.025	1221	1224	1227	rBV4	1101	602	0.02%	0.002%
40	5.138	1255	1259	1261	rBV4	663	543	0.02%	0.002%
41	5.218	1281	1284	1288	rVB4	1092	791	0.02%	0.003%
42	5.318	1288	1315	1340	rBV2	724443	2151793	59.79%	8.575%
43	5.460	1356	1359	1364	rBV5	1993	1695	0.05%	0.007%
44	5.530	1368	1381	1399	rBV2	86506	187792	5.22%	0.748%
45	5.739	1441	1446	1448	rBV4	1728	1164	0.03%	0.005%
46	5.865	1467	1485	1503	rBV	595438	1326706	36.86%	5.287%
47	6.308	1609	1623	1643	rVB2	498893	998888	27.75%	3.980%
48	6.681	1727	1739	1774	rBV	1967158	3599111	100.00%	14.342%
49	7.205	1890	1902	1926	rBV	283964	527670	14.66%	2.103%
50	7.398	1952	1962	1974	rBV	227377	382214	10.62%	1.523%
51	7.543	1994	2007	2026	rBV	1015769	1802643	50.09%	7.183%
52	7.829	2084	2096	2117	rBV3	254541	473750	13.16%	1.888%
53	8.083	2173	2175	2178	rBV4	1392	920	0.03%	0.004%
54	8.135	2179	2191	2207	rBV	429057	717801	19.94%	2.860%
55	8.215	2208	2216	2218	rBV3	21907	29373	0.82%	0.117%
56	8.289	2230	2239	2262	rVB	875250	1488092	41.35%	5.930%
57	8.395	2262	2272	2291	rVB	712032	1125000	31.26%	4.483%
58	8.511	2301	2308	2323	rVB2	35663	58993	1.64%	0.235%
59	8.762	2384	2386	2389	rBV3	1313	958	0.03%	0.004%
60	8.791	2393	2395	2400	rVB5	1472	819	0.02%	0.003%
61	8.884	2409	2424	2446	rBV	894238	1447165	40.21%	5.767%
62	9.067	2465	2481	2517	rVB	839064	1462458	40.63%	5.828%
63	9.463	2602	2604	2606	rBV2	987	526	0.01%	0.002%
64	9.588	2633	2643	2657	rBV	21666	39666	1.10%	0.158%
65	9.746	2681	2692	2716	rBV	117432	205506	5.71%	0.819%
66	9.916	2741	2745	2746	rBV3	3316	2378	0.07%	0.009%
67	10.057	2784	2789	2792	rBV4	1611	1656	0.05%	0.007%
68	10.408	2885	2898	2916	rBV	667899	1095704	30.44%	4.366%
69	10.549	2936	2942	2944	rBV6	2307	2604	0.07%	0.010%
70	10.655	2972	2975	2979	rBV5	1939	1803	0.05%	0.007%
71	10.749	2998	3004	3006	rBV6	2823	2959	0.08%	0.012%

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72	10.848	3032	3035	3036	rBV2	1244	545	0.02%	0.002%
73	10.887	3042	3047	3049	rBV4	2009	1644	0.05%	0.007%
74	10.983	3075	3077	3084	rVB7	958	889	0.02%	0.004%
75	11.131	3116	3123	3135	rVB9	4802	7660	0.21%	0.031%
76	11.247	3156	3159	3162	rBV2	1276	923	0.03%	0.004%
77	11.299	3172	3175	3180	rBV6	1813	1512	0.04%	0.006%
78	11.385	3198	3202	3205	rBV6	1686	1255	0.03%	0.005%
79	11.459	3212	3225	3248	rBV	775570	1286075	35.73%	5.125%
80	11.836	3330	3342	3366	rBV	869430	1475865	41.01%	5.881%
81	12.115	3426	3429	3431	rBV4	1998	1348	0.04%	0.005%
82	12.163	3442	3444	3449	rVB2	2240	1392	0.04%	0.006%
83	12.237	3463	3467	3470	rBV5	2020	1721	0.05%	0.007%
84	12.276	3476	3479	3485	rVB6	2166	2196	0.06%	0.009%
85	12.311	3488	3490	3494	rBV3	1534	1257	0.03%	0.005%
86	12.575	3569	3572	3574	rBV4	1842	1181	0.03%	0.005%
87	12.842	3652	3655	3659	rBV3	1220	1039	0.03%	0.004%
88	12.922	3676	3680	3685	rBV7	1823	1808	0.05%	0.007%
89	12.945	3685	3687	3690	rBV3	1531	1051	0.03%	0.004%
90	13.061	3718	3723	3724	rBV5	2075	1663	0.05%	0.007%
91	13.118	3739	3741	3748	rVB7	3080	2591	0.07%	0.010%
92	13.292	3791	3795	3798	rBV4	2667	2045	0.06%	0.008%
93	13.311	3798	3801	3803	rVV3	1719	1002	0.03%	0.004%
94	13.733	3924	3932	3938	rBV4	11173	18107	0.50%	0.072%
95	14.356	4124	4126	4129	rBV3	1778	1366	0.04%	0.005%
96	14.482	4162	4165	4167	rBV4	2169	1136	0.03%	0.005%
97	14.665	4220	4222	4226	rBV5	1836	878	0.02%	0.003%
98	15.051	4335	4342	4352	rBV7	8542	15415	0.43%	0.061%
99	15.527	4488	4490	4495	rBV5	2276	1870	0.05%	0.007%
100	15.681	4536	4538	4542	rBV4	2848	1695	0.05%	0.007%

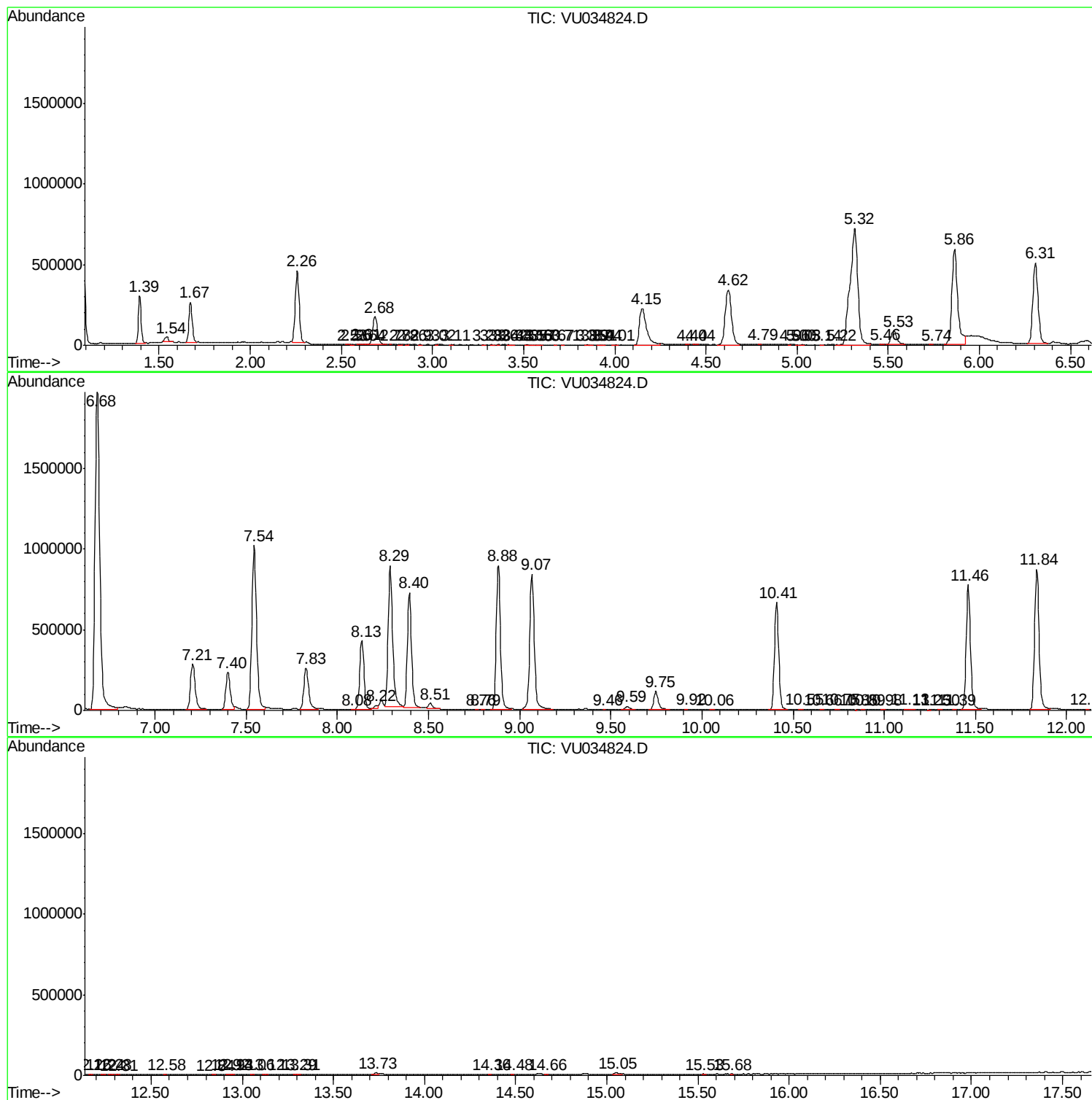
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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



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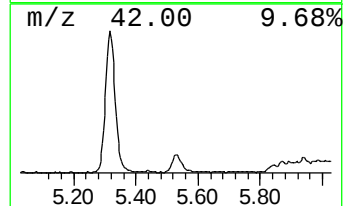
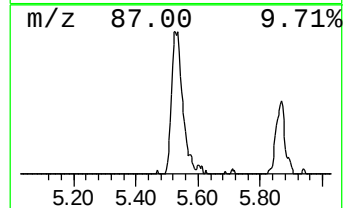
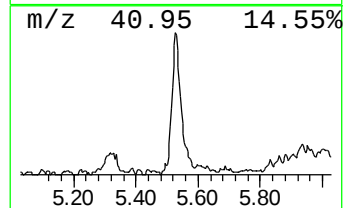
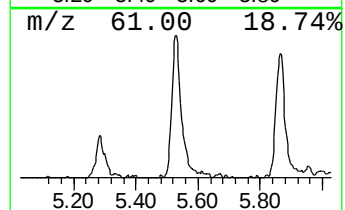
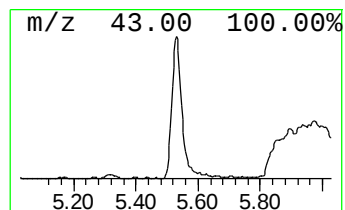
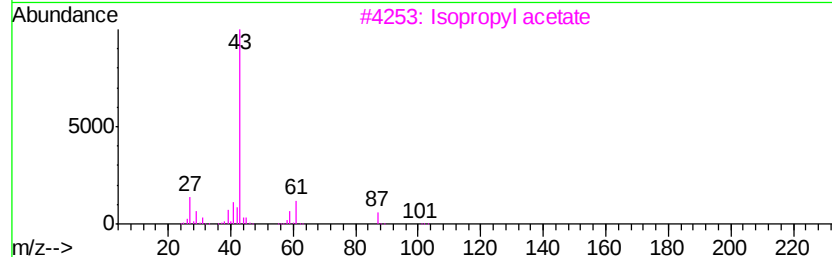
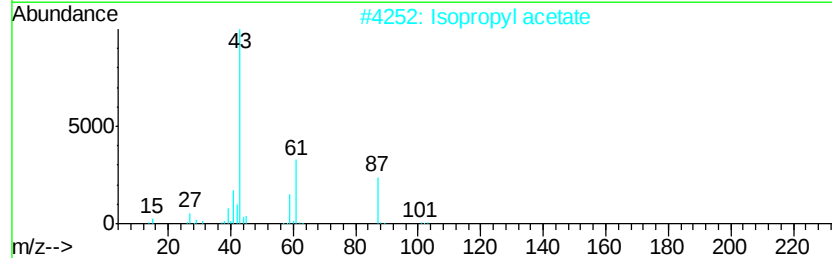
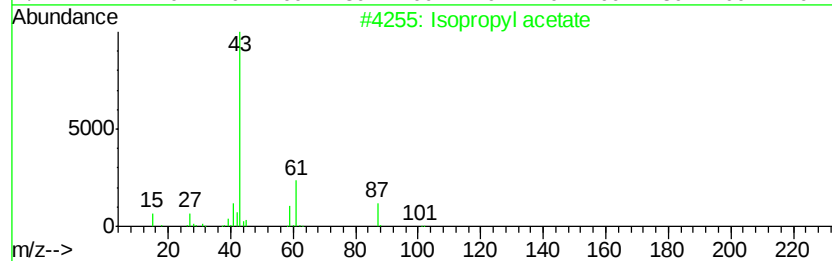
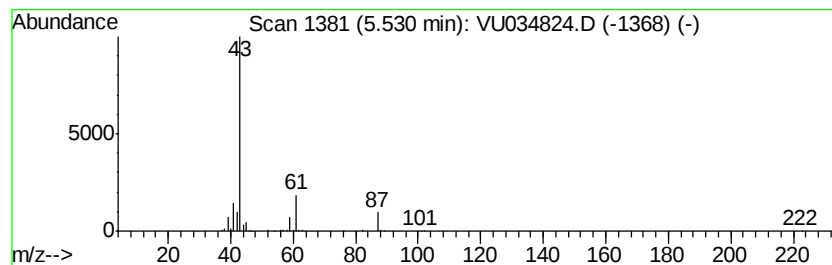
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.53	7.08 ug/L	187792	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	72
3		Isopropyl acetate	102	C5H10O2	000108-21-4	64
4		Isopropyl acetate	102	C5H10O2	000108-21-4	64
5		n-Propyl acetate	102	C5H10O2	000109-60-4	40



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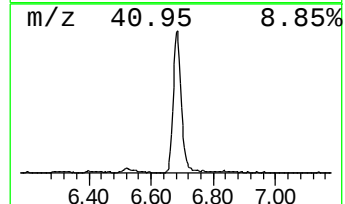
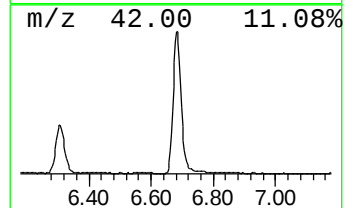
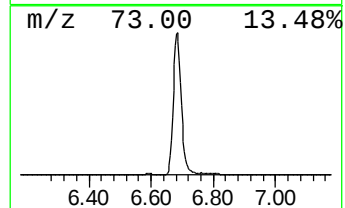
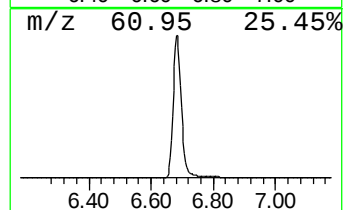
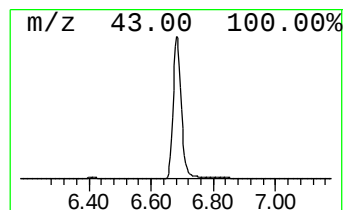
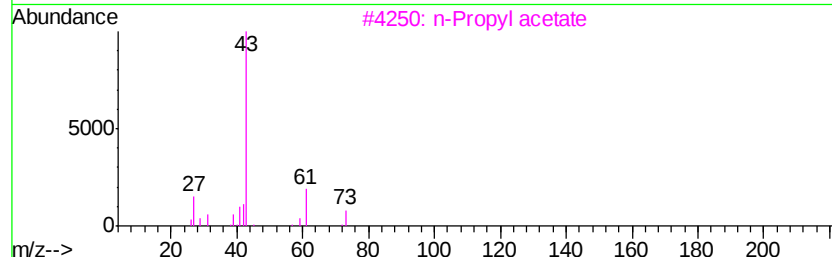
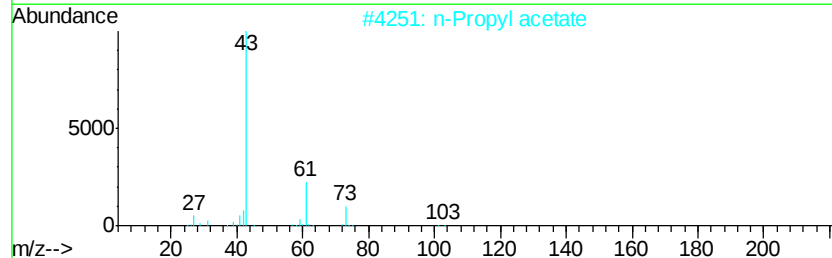
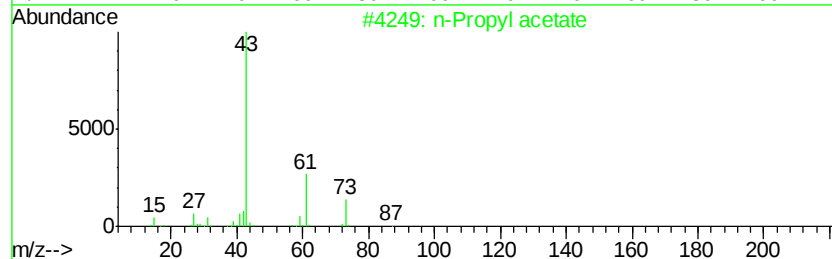
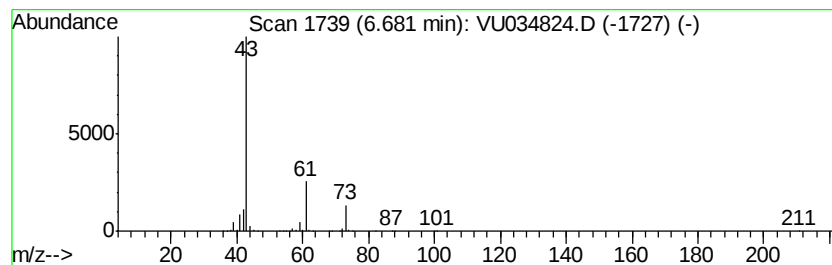
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Quant Title : VOC Analysis

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	135.64 ug/L	3599110	1,4-Difluorobenzene	5.86

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	78
4		Isopropyl acetate	102	C5H10O2	000108-21-4	36
5		Isopropyl acetate	102	C5H10O2	000108-21-4	9



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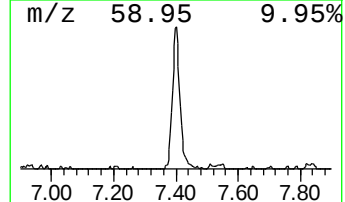
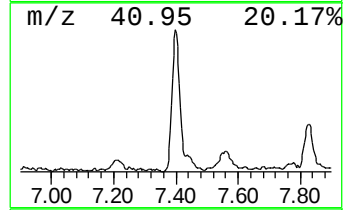
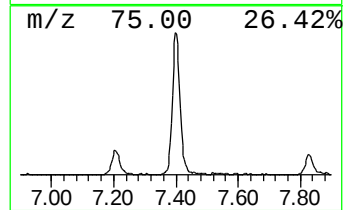
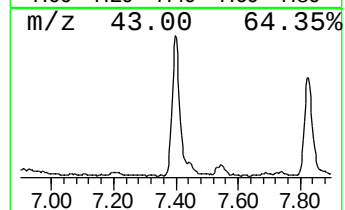
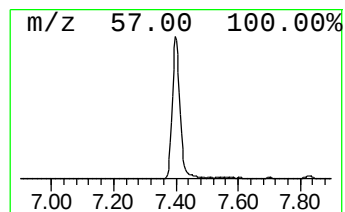
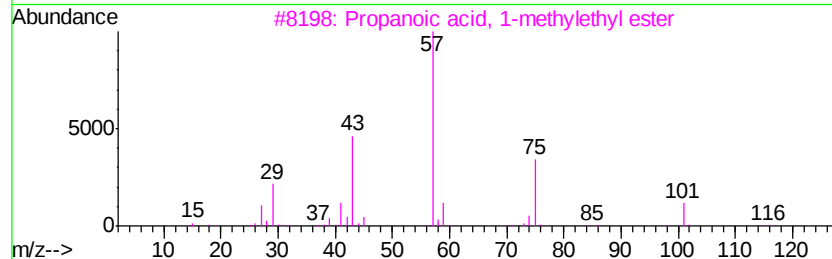
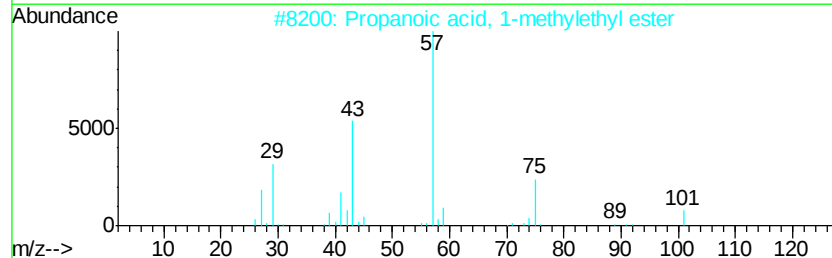
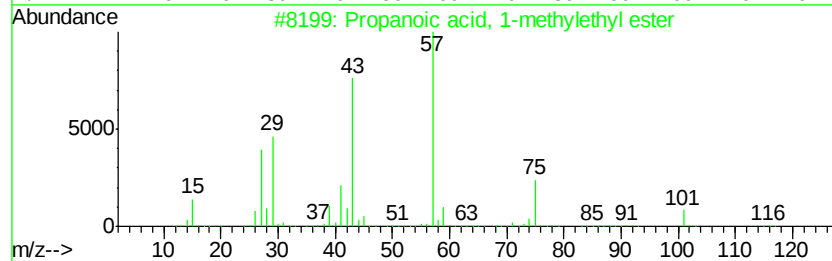
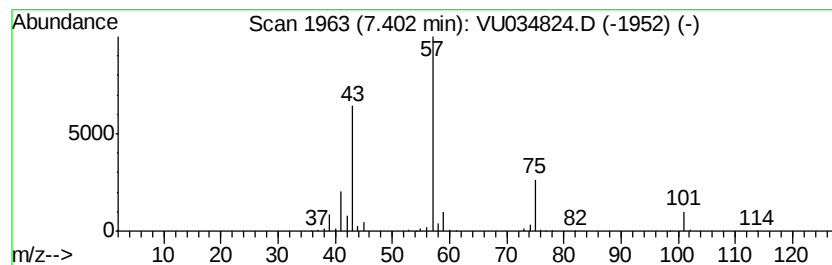
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Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	14.40 ug/L	382214	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	83	
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83	
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50	
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45	
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
Data File : VU034824.D
Acq On : 25 Sep 2019 23:52
Operator : JC/SP
Sample : K4983-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDN4

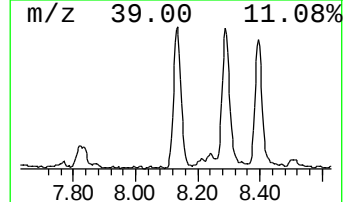
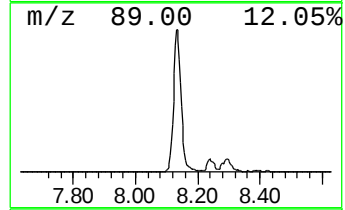
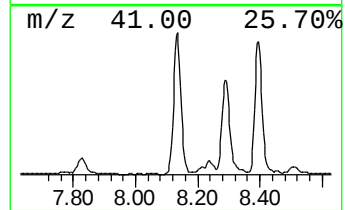
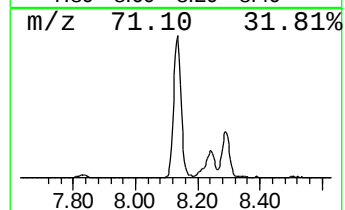
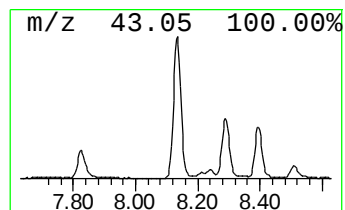
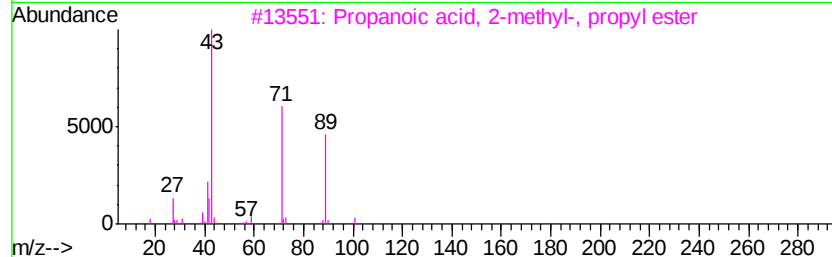
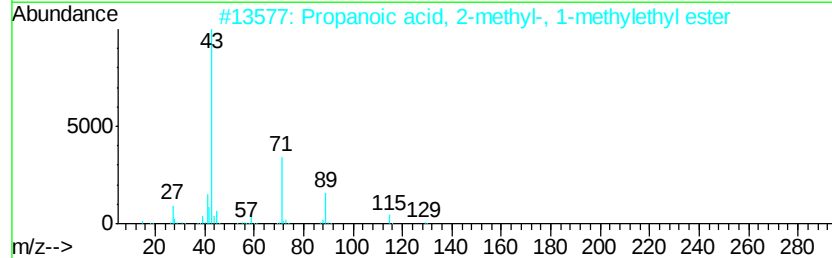
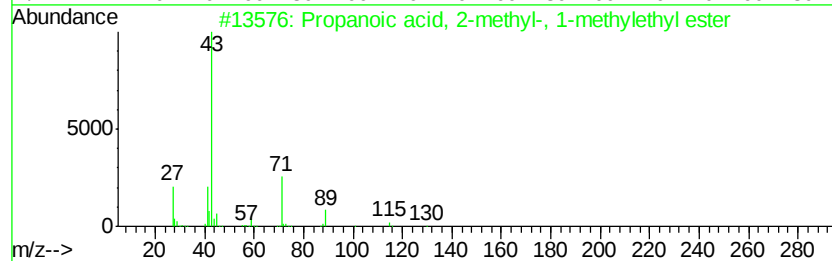
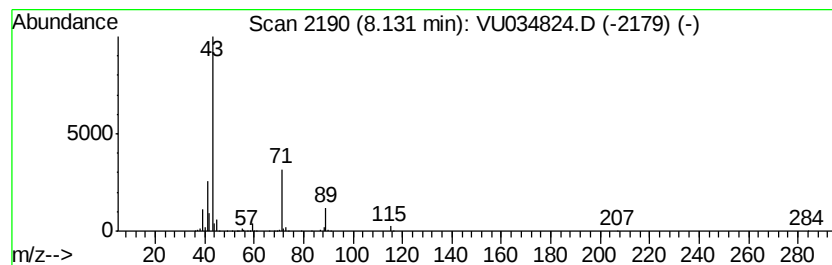
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Quant Title : VOC Analysis

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	24.54 ug/L	717801	Chlorobenzene-d5	9.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
5		3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
Data File : VU034824.D
Acq On : 25 Sep 2019 23:52
Operator : JC/SP
Sample : K4983-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDN4

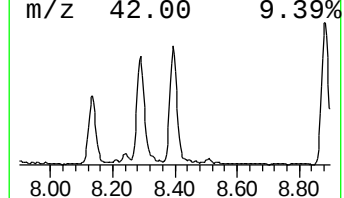
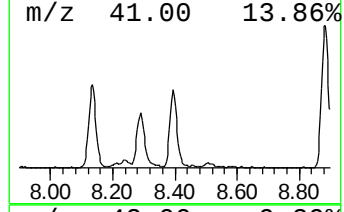
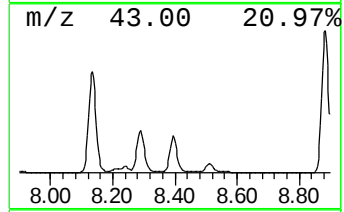
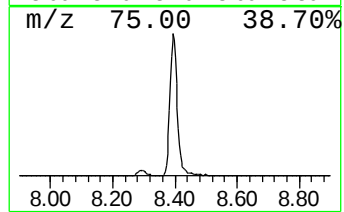
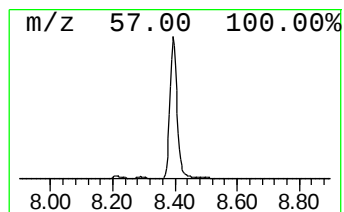
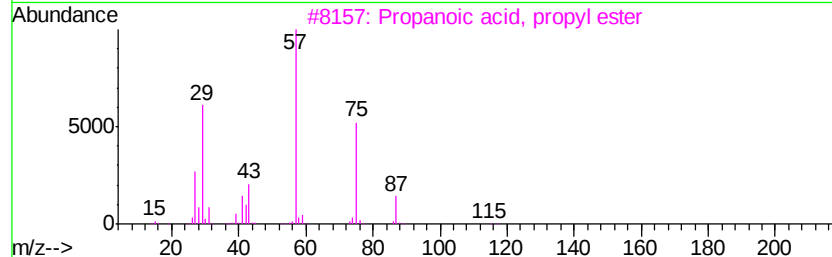
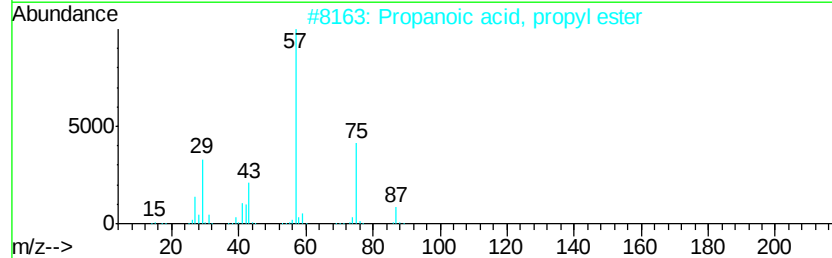
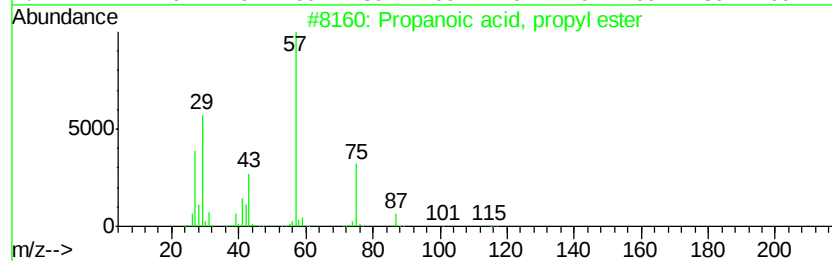
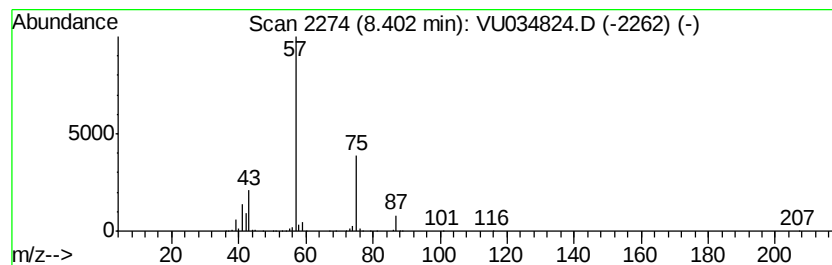
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Quant Title : VOC Analysis

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	38.46 ug/L	1125000	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	72
5		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	33



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092519\
Data File : VU034824.D
Acq On : 25 Sep 2019 23:52
Operator : JC/SP
Sample : K4983-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDN4

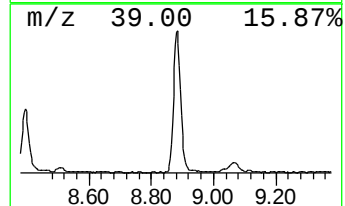
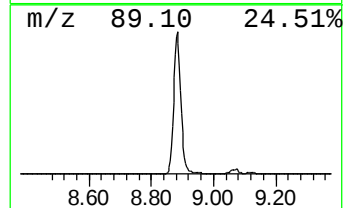
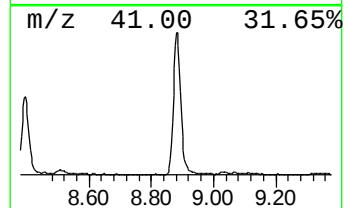
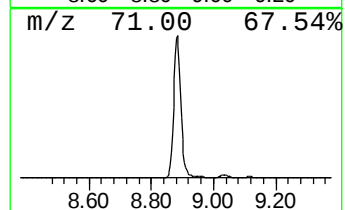
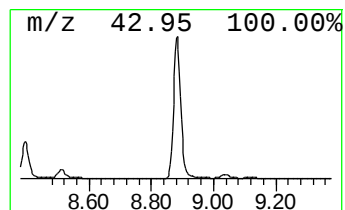
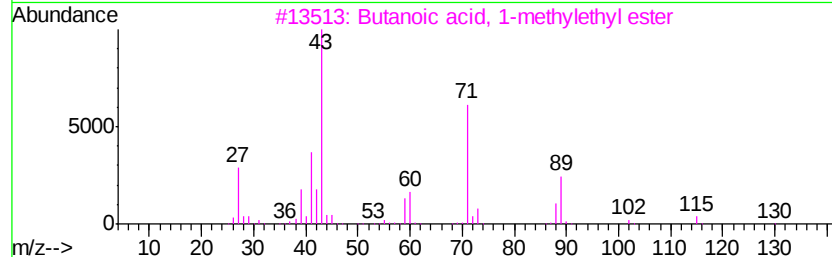
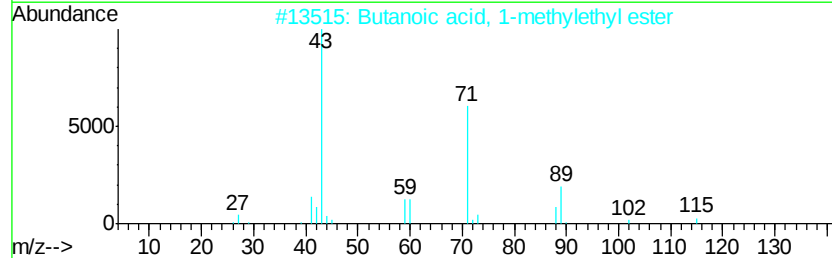
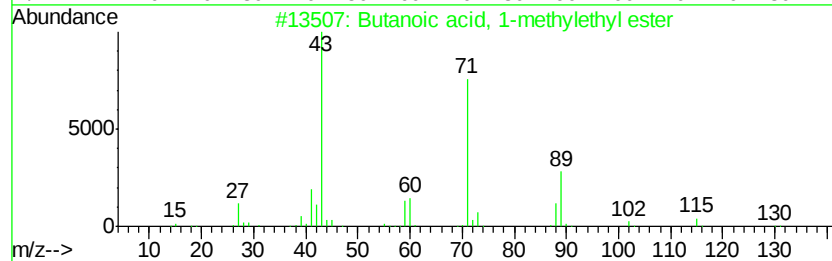
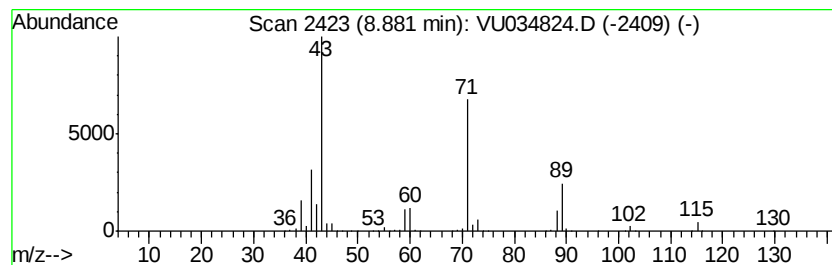
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Quant Title : VOC Analysis

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	49.48 ug/L	1447170	Chlorobenzene-d5	9.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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 : VU034824.D
Acq On : 25 Sep 2019 23:52
Operator : JC/SP
Sample : K4983-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDN4

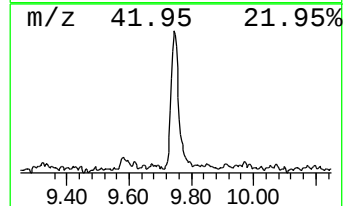
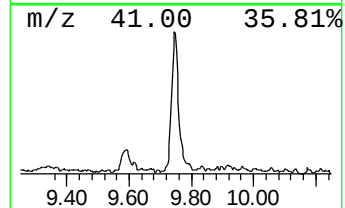
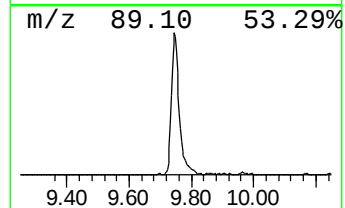
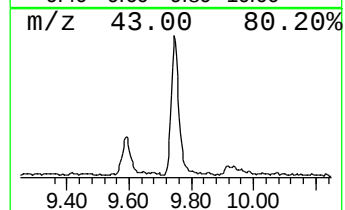
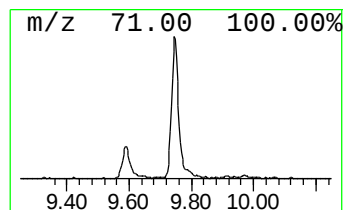
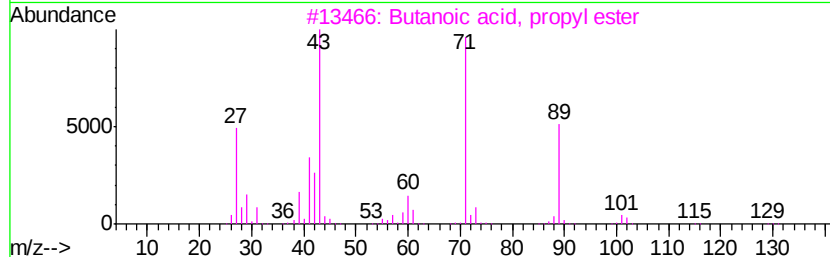
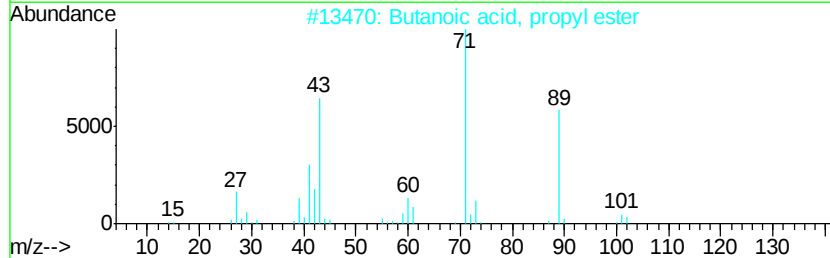
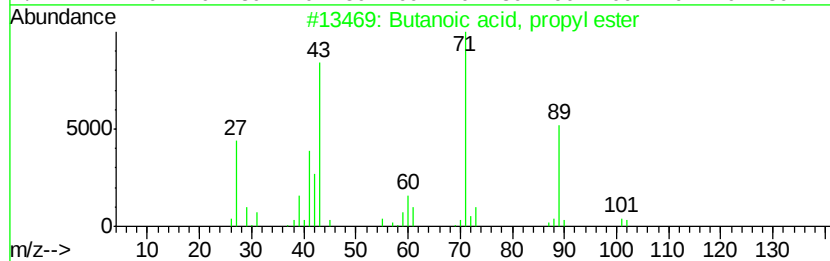
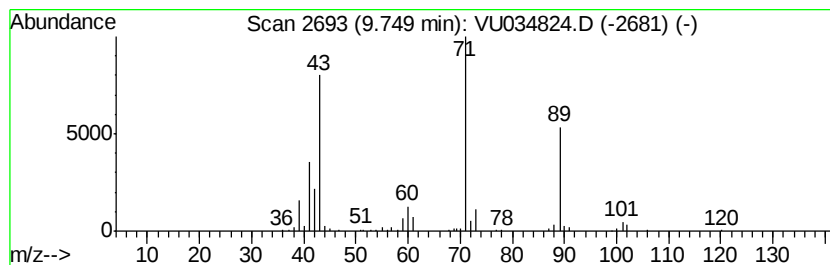
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Quant Title : VOC Analysis

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

Peak Number 8 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	7.03 ug/L	205506	Chlorobenzene-d5	9.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	91
2		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
3		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
4		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
5		Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092519\
Data File : VU034824.D
Acq On : 25 Sep 2019 23:52
Operator : JC/SP
Sample : K4983-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDN4

Quant Method : Z:\VOASRV\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	7.1	ug/L	187792	1	5.86	1326710	50.0
n-Propyl acetate	6.68	135.6	ug/L	3599110	1	5.86	1326710	50.0
Propanoic acid, 1...	7.40	14.4	ug/L	382214	1	5.86	1326710	50.0
Propanoic acid, 2...	8.13	24.5	ug/L	717801	2	9.07	1462460	50.0
Propanoic acid, p...	8.40	38.5	ug/L	1125000	2	9.07	1462460	50.0
Butanoic acid, 1-...	8.88	49.5	ug/L	1447170	2	9.07	1462460	50.0
Butanoic acid, pr...	9.75	7.0	ug/L	205506	2	9.07	1462460	50.0