

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
 Data File : VU032836.D
 Acq On : 18 Jun 2019 20:11
 Operator : JC/SP
 Sample : K3324-09DL 5X
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JR5DL

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\SOMULM061719WMA.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	1.180	24	28	33	rVB2	3734	3113	0.13%	0.031%
2	1.396	88	95	104	rBV	111338	116406	4.89%	1.145%
3	1.675	174	182	194	rVB	89781	110005	4.63%	1.082%
4	2.267	355	366	377	rVB	186229	283073	11.90%	2.785%
5	2.441	414	420	424	rBV5	1166	1541	0.06%	0.015%
6	2.553	451	455	457	rBV2	333	281	0.01%	0.003%
7	2.588	463	466	469	rBV	301	218	0.01%	0.002%
8	2.617	472	475	482	rVB4	861	1047	0.04%	0.010%
9	2.656	484	487	489	rBV3	369	225	0.01%	0.002%
10	2.695	496	499	505	rVB3	1249	1366	0.06%	0.013%
11	2.762	518	520	522	rBV	324	230	0.01%	0.002%
12	2.833	526	542	555	rVB	5752	12363	0.52%	0.122%
13	2.978	576	587	600	rVB	10874	20043	0.84%	0.197%
14	3.039	602	606	610	rBV2	371	292	0.01%	0.003%
15	3.174	641	648	650	rBV4	499	628	0.03%	0.006%
16	3.296	682	686	690	rBV2	243	246	0.01%	0.002%
17	3.334	695	698	700	rVB2	441	237	0.01%	0.002%
18	3.360	700	706	707	rBV2	425	372	0.02%	0.004%
19	3.421	721	725	727	rBV2	399	237	0.01%	0.002%
20	3.453	732	735	741	rVB2	468	312	0.01%	0.003%
21	3.592	775	778	781	rBV2	442	299	0.01%	0.003%
22	3.621	785	787	790	rBV2	288	203	0.01%	0.002%
23	3.752	823	828	830	rBV3	407	391	0.02%	0.004%
24	3.769	830	833	837	rVB3	202	206	0.01%	0.002%
25	3.862	860	862	869	rVB2	282	275	0.01%	0.003%
26	3.916	873	879	883	rVV3	520	554	0.02%	0.005%
27	4.055	918	922	928	rBV2	281	291	0.01%	0.003%
28	4.096	933	935	939	rVB	349	208	0.01%	0.002%
29	4.215	943	972	1005	rBV2	890431	2378160	100.00%	23.397%
30	4.511	1061	1064	1065	rBV2	413	218	0.01%	0.002%
31	4.640	1088	1104	1129	rBV	147081	342856	14.42%	3.373%
32	4.855	1168	1171	1173	rBV2	375	255	0.01%	0.003%
33	4.913	1187	1189	1194	rVB2	440	308	0.01%	0.003%
34	5.196	1272	1277	1280	rBV2	340	362	0.02%	0.004%

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 Title : VOC Analysis

35	5.331	1296	1319	1344	rBV2	292119	868603	36.52%	8.546%
36	5.498	1369	1371	1376	rVB3	348	228	0.01%	0.002%
37	5.547	1381	1386	1388	rBV2	772	656	0.03%	0.006%
38	5.672	1422	1425	1428	rVV3	321	219	0.01%	0.002%
39	5.881	1475	1490	1510	rBV	282974	550494	23.15%	5.416%
40	6.180	1569	1583	1607	rBV	230882	445113	18.72%	4.379%
41	6.325	1615	1628	1649	rBV	198246	391814	16.48%	3.855%
42	6.530	1687	1692	1693	rBV4	502	486	0.02%	0.005%
43	6.566	1699	1703	1705	rBV	425	364	0.02%	0.004%
44	6.608	1713	1716	1727	rVB5	821	1079	0.05%	0.011%
45	6.701	1732	1745	1774	rBV	129091	238398	10.02%	2.345%
46	6.826	1780	1784	1788	rBV4	484	524	0.02%	0.005%
47	6.849	1788	1791	1793	rBV2	660	515	0.02%	0.005%
48	6.923	1811	1814	1818	rBV3	436	401	0.02%	0.004%
49	6.990	1826	1835	1837	rBV3	528	741	0.03%	0.007%
50	7.083	1860	1864	1867	rBV2	451	348	0.01%	0.003%
51	7.112	1870	1873	1877	rBV3	205	212	0.01%	0.002%
52	7.154	1883	1886	1891	rVB4	596	435	0.02%	0.004%
53	7.222	1895	1907	1923	rBV	115800	206715	8.69%	2.034%
54	7.415	1952	1967	1978	rBV	26068	45656	1.92%	0.449%
55	7.559	1998	2012	2030	rBV	399894	696041	29.27%	6.848%
56	7.775	2077	2079	2084	rVB	390	298	0.01%	0.003%
57	7.846	2088	2101	2124	rBV	84391	147450	6.20%	1.451%
58	7.942	2129	2131	2136	rVV3	677	616	0.03%	0.006%
59	7.964	2136	2138	2140	rVV3	528	333	0.01%	0.003%
60	8.064	2167	2169	2173	rVB	443	288	0.01%	0.003%
61	8.093	2173	2178	2180	rBV3	528	413	0.02%	0.004%
62	8.151	2185	2196	2215	rBV	15311	27043	1.14%	0.266%
63	8.228	2215	2220	2222	rBV3	1415	1280	0.05%	0.013%
64	8.257	2222	2229	2234	rBV4	4917	6183	0.26%	0.061%
65	8.305	2234	2244	2267	rVV	250153	434799	18.28%	4.278%
66	8.411	2268	2277	2295	rVB	92470	147582	6.21%	1.452%
67	8.524	2305	2312	2321	rVB3	5183	8778	0.37%	0.086%
68	8.614	2334	2340	2348	rBV6	1195	2094	0.09%	0.021%
69	8.829	2402	2407	2411	rBV2	493	497	0.02%	0.005%
70	8.855	2411	2415	2417	rBV4	266	247	0.01%	0.002%
71	8.900	2417	2429	2451	rVV	67752	109466	4.60%	1.077%

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72	9.083	2473	2486	2515	rBV	419732	699614	29.42%	6.883%
73	9.273	2542	2545	2547	rBV	369	250	0.01%	0.002%
74	9.308	2553	2556	2558	rVB2	377	221	0.01%	0.002%
75	9.341	2564	2566	2569	rVB	431	235	0.01%	0.002%
76	9.765	2688	2698	2708	rBV4	3012	5073	0.21%	0.050%
77	9.810	2708	2712	2716	rVB2	407	298	0.01%	0.003%
78	9.952	2753	2756	2759	rBV	382	216	0.01%	0.002%
79	9.984	2763	2766	2770	rVB2	443	254	0.01%	0.002%
80	10.122	2807	2809	2817	rVB2	468	554	0.02%	0.005%
81	10.296	2857	2863	2867	rBV3	313	356	0.01%	0.004%
82	10.344	2875	2878	2881	rBV2	358	259	0.01%	0.003%
83	10.427	2891	2904	2922	rBV	284502	461312	19.40%	4.539%
84	10.530	2933	2936	2940	rBV2	372	305	0.01%	0.003%
85	10.562	2944	2946	2951	rBV2	347	215	0.01%	0.002%
86	10.611	2956	2961	2963	rVV3	381	333	0.01%	0.003%
87	10.710	2988	2992	2998	rVB2	389	386	0.02%	0.004%
88	11.045	3086	3096	3097	rBV	398	395	0.02%	0.004%
89	11.186	3135	3140	3143	rBV2	408	485	0.02%	0.005%
90	11.286	3169	3171	3175	rBV2	440	404	0.02%	0.004%
91	11.366	3194	3196	3201	rVB2	466	218	0.01%	0.002%
92	11.479	3219	3231	3258	rBV	435055	702058	29.52%	6.907%
93	11.855	3335	3348	3372	rBV	408382	675538	28.41%	6.646%
94	12.723	3615	3618	3621	rBV	312	262	0.01%	0.003%
95	13.032	3711	3714	3720	rBV3	331	353	0.01%	0.003%
96	13.504	3858	3861	3865	rBV3	379	334	0.01%	0.003%
97	13.675	3911	3914	3918	rBV3	398	237	0.01%	0.002%
98	13.897	3981	3983	3986	rBV2	441	313	0.01%	0.003%
99	13.922	3989	3991	3994	rVV2	399	224	0.01%	0.002%
100	14.514	4172	4175	4177	rBV2	520	270	0.01%	0.003%

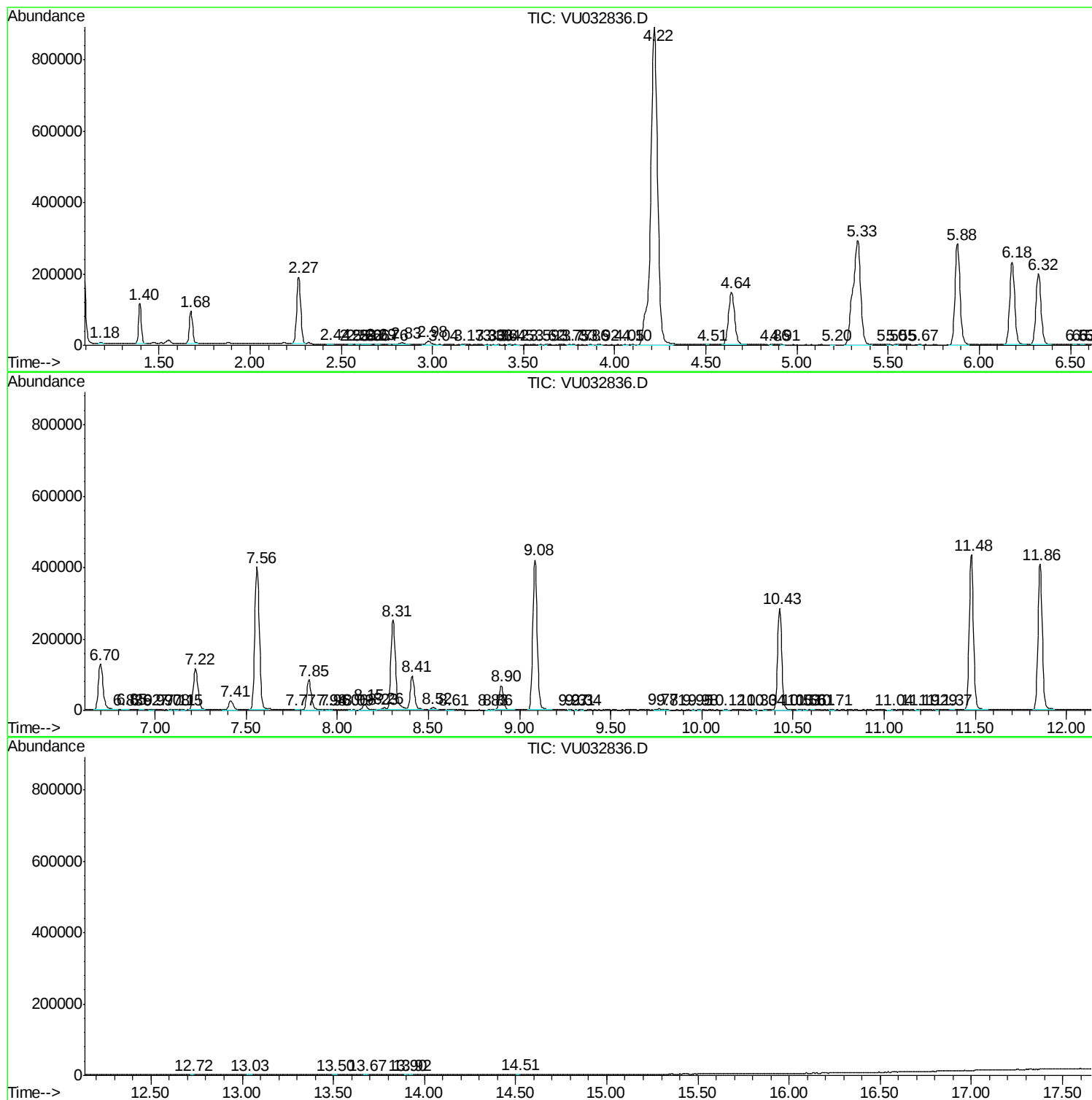
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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



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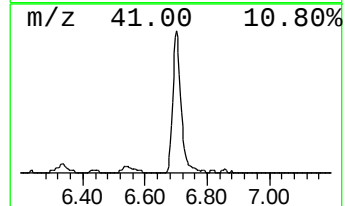
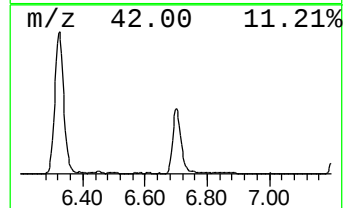
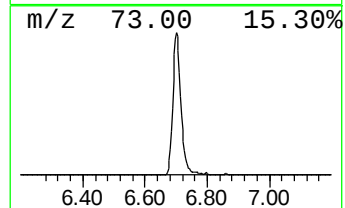
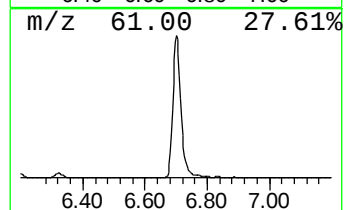
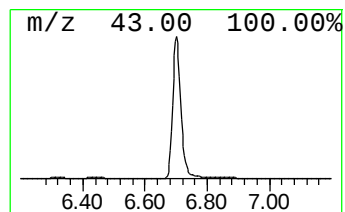
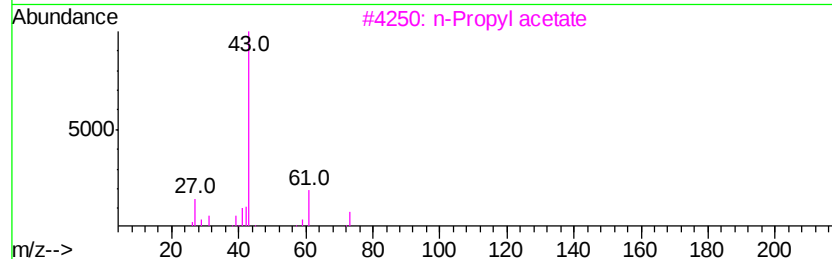
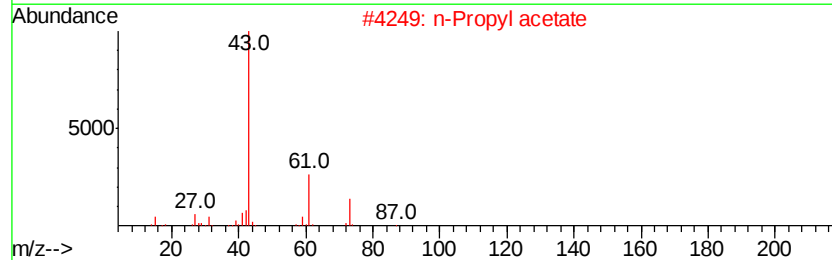
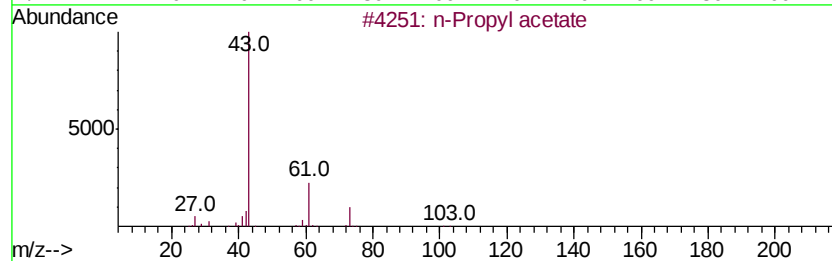
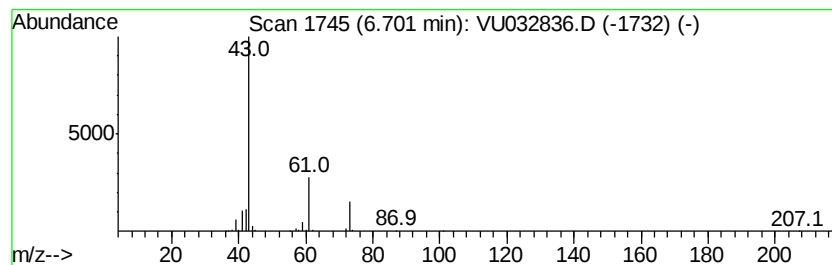
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	21.65 ug/L	238398	1,4-Difluorobenzene	5.88

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	64
4		Isopropyl acetate	102	C5H10O2	000108-21-4	36
5		Isobutylamine	73	C4H11N	000078-81-9	9



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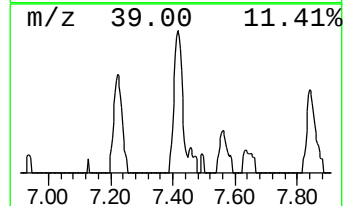
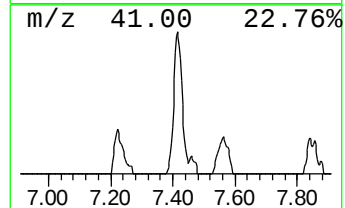
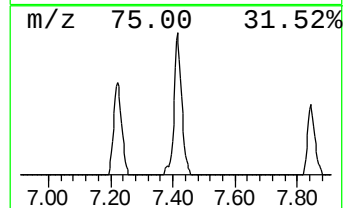
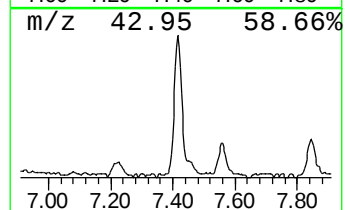
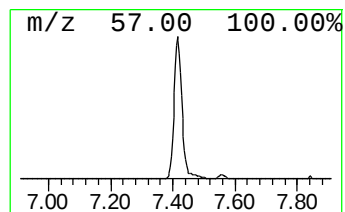
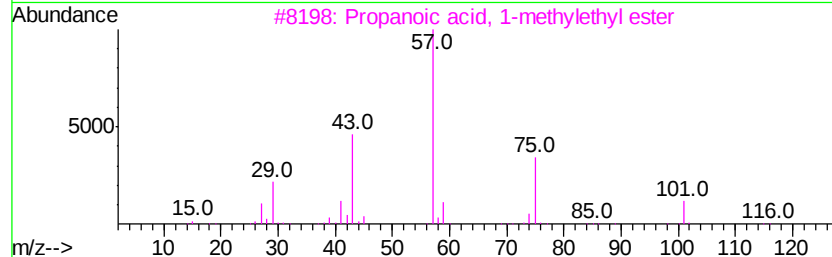
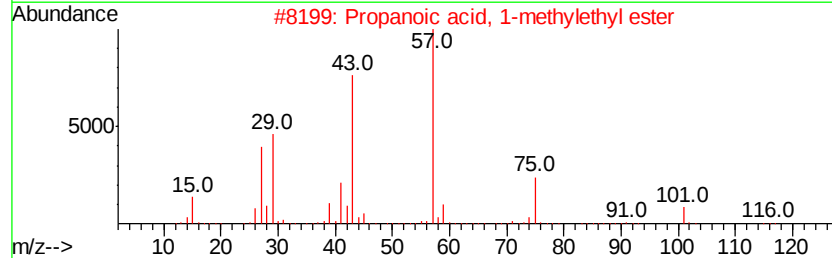
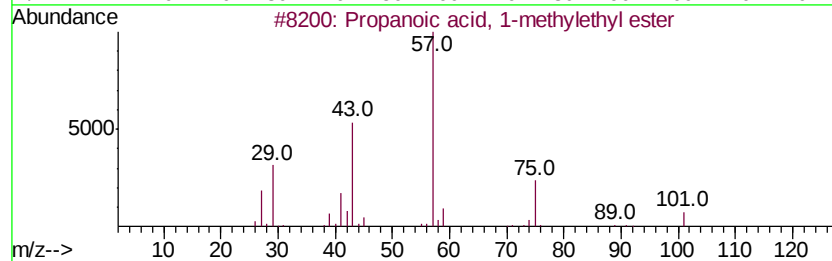
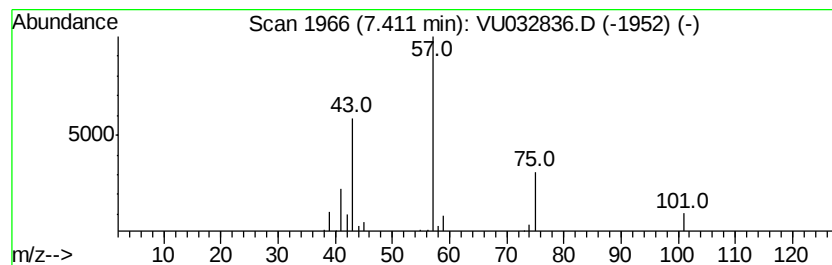
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Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	4.15 ug/L	45656	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42



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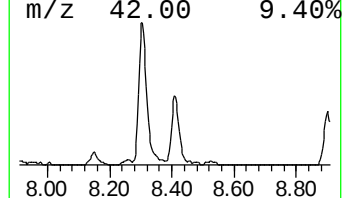
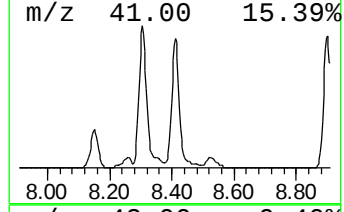
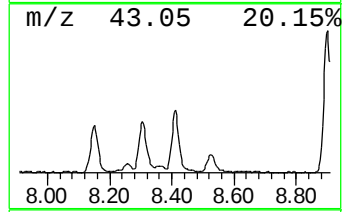
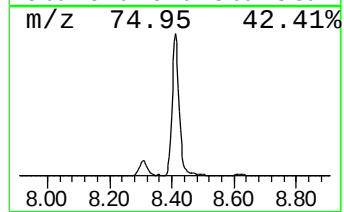
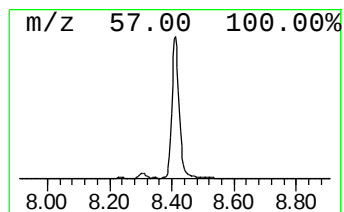
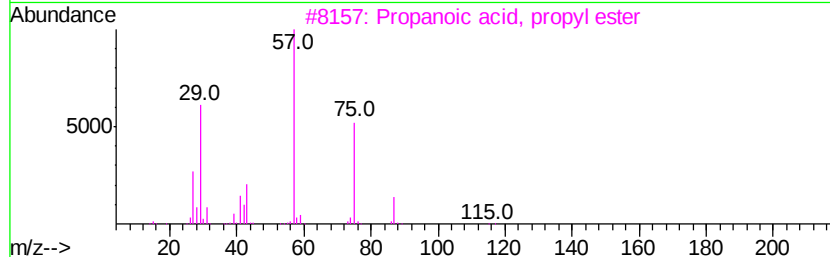
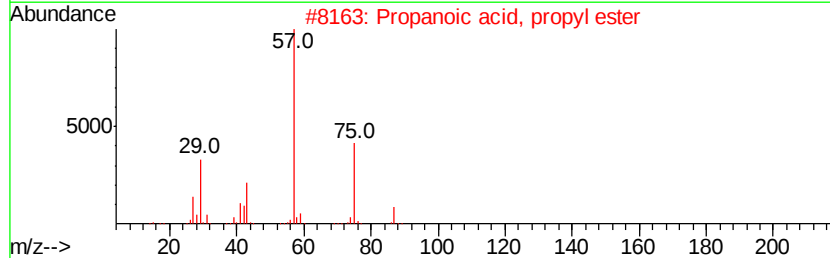
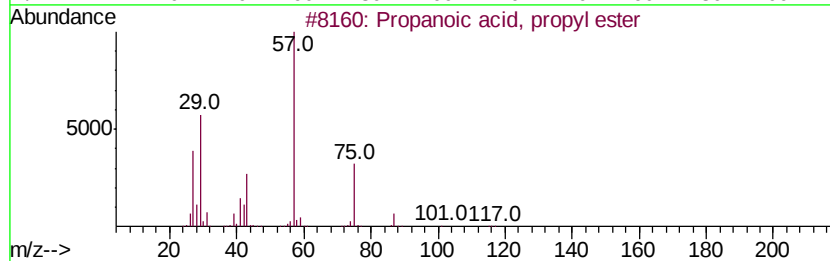
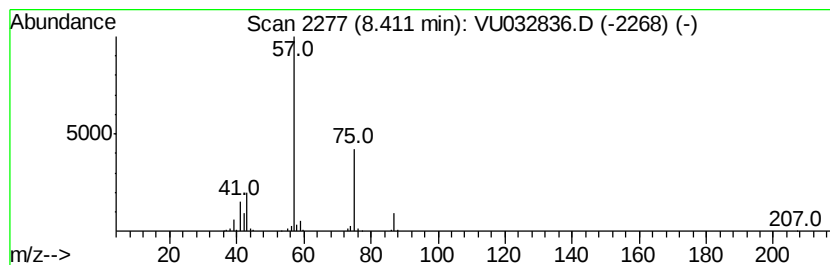
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Quant Title : VOC Analysis

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Peak Number 4 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	10.55 ug/L	147582	Chlorobenzene-d5	9.08

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	78
5		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032836.D
Acq On : 18 Jun 2019 20:11
Operator : JC/SP
Sample : K3324-09DL 5X
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR5DL

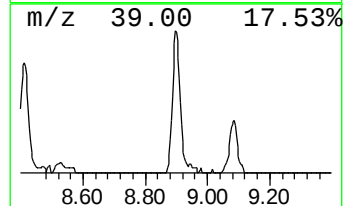
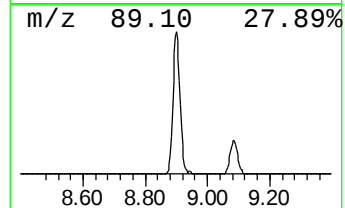
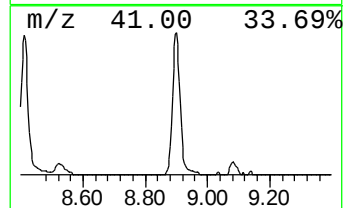
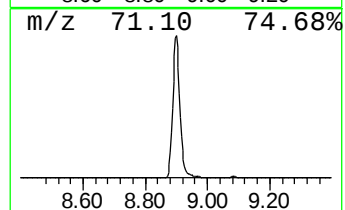
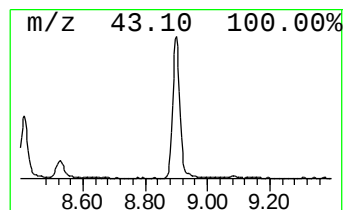
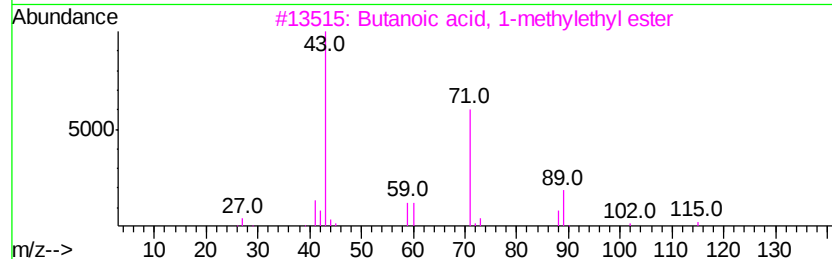
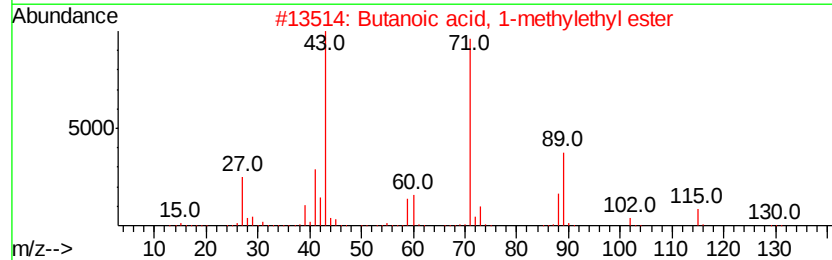
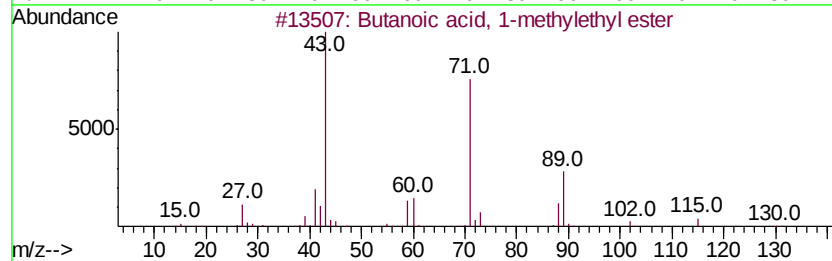
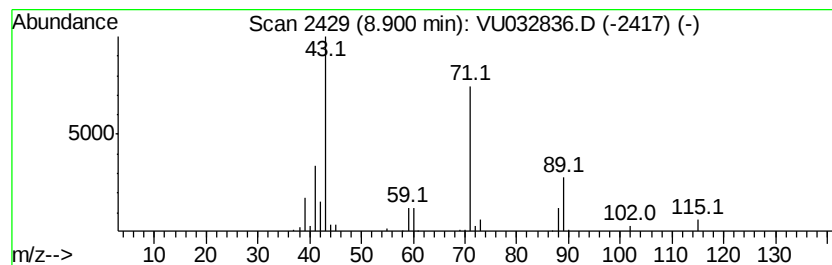
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Quant Title : VOC Analysis

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

Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	7.82 ug/L	109466	Chlorobenzene-d5	9.08

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	83
4		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	64
5		Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	64



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MSVOA_U
ClientSampleId :
C0JR5DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.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
n-Propyl acetate	6.70	21.6	ug/L	238398	1	5.88	550494	50.0
Propanoic acid, 1...	7.41	4.2	ug/L	45656	1	5.88	550494	50.0
Propanoic acid, p...	8.41	10.6	ug/L	147582	2	9.08	699614	50.0
Butanoic acid, 1-...	8.90	7.8	ug/L	109466	2	9.08	699614	50.0