

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
 Data File : VU032815.D
 Acq On : 18 Jun 2019 11:43
 Operator : JC/SP
 Sample : K3363-16
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JQ3

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	23	28	35	rVB	8197	7708	0.86%	0.081%
2	1.395	88	95	107	rVB	114022	116615	12.97%	1.218%
3	1.675	174	182	196	rBV	92808	115471	12.84%	1.206%
4	2.267	355	366	376	rBV	192300	290533	32.30%	3.035%
5	2.411	408	411	412	rBV	412	230	0.03%	0.002%
6	2.447	415	422	427	rVV4	1711	2564	0.29%	0.027%
7	2.691	490	498	512	rVB3	7440	12630	1.40%	0.132%
8	2.955	577	580	583	rVB2	455	299	0.03%	0.003%
9	2.974	583	586	588	rBV3	385	257	0.03%	0.003%
10	3.276	676	680	685	rVB4	528	457	0.05%	0.005%
11	3.305	685	689	692	rBV3	389	327	0.04%	0.003%
12	3.325	692	695	698	rBV2	407	305	0.03%	0.003%
13	3.630	784	790	793	rBV5	916	1186	0.13%	0.012%
14	3.710	812	815	818	rBV2	426	257	0.03%	0.003%
15	3.730	818	821	824	rVV3	354	263	0.03%	0.003%
16	3.749	824	827	830	rVB2	310	233	0.03%	0.002%
17	3.884	865	869	872	rBV3	434	374	0.04%	0.004%
18	3.907	872	876	878	rVV3	462	302	0.03%	0.003%
19	3.955	887	891	896	rBV3	389	505	0.06%	0.005%
20	4.026	909	913	919	rBV3	592	617	0.07%	0.006%
21	4.103	932	937	943	rVB4	482	497	0.06%	0.005%
22	4.167	943	957	981	rBV	88356	228927	25.45%	2.392%
23	4.495	1055	1059	1061	rBV2	354	335	0.04%	0.003%
24	4.559	1075	1079	1080	rBV	327	253	0.03%	0.003%
25	4.640	1087	1104	1130	rBV	152001	358326	39.84%	3.743%
26	4.749	1135	1138	1139	rVV2	388	267	0.03%	0.003%
27	4.781	1143	1148	1151	rVV3	447	362	0.04%	0.004%
28	4.836	1162	1165	1167	rBV3	411	287	0.03%	0.003%
29	4.868	1172	1175	1177	rBV	516	397	0.04%	0.004%
30	5.000	1210	1216	1220	rVB2	459	447	0.05%	0.005%
31	5.032	1223	1226	1229	rBV2	315	231	0.03%	0.002%
32	5.051	1229	1232	1238	rVB3	436	311	0.03%	0.003%
33	5.173	1265	1270	1274	rVB2	387	360	0.04%	0.004%
34	5.199	1274	1278	1280	rBV3	276	242	0.03%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
 Title : VOC Analysis

35	5.331	1296	1319	1346	rBV2	304621	899394	100.00%	9.396%
36	5.450	1354	1356	1364	rVB5	493	546	0.06%	0.006%
37	5.489	1364	1368	1373	rVV3	422	397	0.04%	0.004%
38	5.550	1377	1387	1405	rVV2	4896	11267	1.25%	0.118%
39	5.624	1408	1410	1415	rVV2	477	379	0.04%	0.004%
40	5.800	1461	1465	1471	rVB2	534	591	0.07%	0.006%
41	5.881	1476	1490	1515	rBV	294185	574537	63.88%	6.002%
42	6.064	1543	1547	1552	rVB2	305	295	0.03%	0.003%
43	6.180	1571	1583	1603	rBV	76503	147477	16.40%	1.541%
44	6.325	1614	1628	1650	rBV	205869	411800	45.79%	4.302%
45	6.421	1650	1658	1671	rBV2	6561	12725	1.41%	0.133%
46	6.537	1687	1694	1699	rBV4	1727	2823	0.31%	0.029%
47	6.575	1700	1706	1714	rVV2	4331	7238	0.80%	0.076%
48	6.697	1732	1744	1774	rBV	496373	885606	98.47%	9.252%
49	6.958	1819	1825	1827	rBV4	626	552	0.06%	0.006%
50	6.974	1827	1830	1833	rBV2	295	225	0.03%	0.002%
51	7.032	1844	1848	1854	rBV2	468	497	0.06%	0.005%
52	7.222	1895	1907	1925	rBV	125017	219485	24.40%	2.293%
53	7.344	1941	1945	1947	rVB5	335	241	0.03%	0.003%
54	7.415	1951	1967	1995	rBV	115267	200516	22.29%	2.095%
55	7.559	1999	2012	2027	rVV	413297	724061	80.51%	7.564%
56	7.630	2029	2034	2047	rVB2	13077	22092	2.46%	0.231%
57	7.768	2075	2077	2080	rBV3	455	302	0.03%	0.003%
58	7.842	2088	2100	2117	rBV	93467	161540	17.96%	1.688%
59	7.980	2142	2143	2147	rVB2	486	225	0.03%	0.002%
60	8.006	2149	2151	2158	rVB4	584	455	0.05%	0.005%
61	8.041	2158	2162	2165	rBV3	489	434	0.05%	0.005%
62	8.151	2184	2196	2208	rBV	58424	96757	10.76%	1.011%
63	8.222	2208	2218	2225	rBV3	34113	59981	6.67%	0.627%
64	8.305	2234	2244	2266	rVV	285077	474201	52.72%	4.954%
65	8.411	2267	2277	2294	rVB	304478	477654	53.11%	4.990%
66	8.521	2305	2311	2326	rVB	11486	19281	2.14%	0.201%
67	8.781	2389	2392	2395	rBV2	248	226	0.03%	0.002%
68	8.900	2416	2429	2451	rBV	223005	354567	39.42%	3.704%
69	9.083	2469	2486	2509	rBV	441337	731716	81.36%	7.644%
70	9.340	2560	2566	2568	rBV2	274	230	0.03%	0.002%
71	9.363	2569	2573	2574	rBV3	681	413	0.05%	0.004%

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72	9.456	2598	2602	2606	rBV3	273	252	0.03%	0.003%
73	9.601	2636	2647	2659	rBV6	3407	6323	0.70%	0.066%
74	9.765	2689	2698	2709	rBV4	6273	10420	1.16%	0.109%
75	9.922	2742	2747	2748	rBV2	435	352	0.04%	0.004%
76	10.112	2803	2806	2810	rVB2	354	278	0.03%	0.003%
77	10.205	2828	2835	2836	rBV2	263	273	0.03%	0.003%
78	10.244	2845	2847	2854	rVB3	330	309	0.03%	0.003%
79	10.283	2854	2859	2862	rBV3	265	262	0.03%	0.003%
80	10.427	2891	2904	2922	rBV	301394	477443	53.08%	4.988%
81	10.546	2938	2941	2945	rVB2	293	241	0.03%	0.003%
82	10.578	2945	2951	2956	rBV3	388	397	0.04%	0.004%
83	10.611	2957	2961	2967	rBV3	380	402	0.04%	0.004%
84	10.771	3005	3011	3012	rBV2	422	314	0.03%	0.003%
85	10.932	3053	3061	3064	rBV4	404	468	0.05%	0.005%
86	11.238	3154	3156	3160	rVB2	348	261	0.03%	0.003%
87	11.266	3161	3165	3172	rBV2	373	453	0.05%	0.005%
88	11.350	3187	3191	3196	rBV2	251	244	0.03%	0.003%
89	11.479	3219	3231	3256	rBV	460386	728785	81.03%	7.614%
90	11.855	3334	3348	3373	rBV	422033	697974	77.60%	7.292%
91	12.164	3441	3444	3447	rBV3	452	318	0.04%	0.003%
92	12.321	3491	3493	3498	rBV2	499	455	0.05%	0.005%
93	12.382	3509	3512	3515	rBV2	390	232	0.03%	0.002%
94	12.456	3532	3535	3540	rVB3	283	254	0.03%	0.003%
95	12.668	3596	3601	3603	rBV2	474	375	0.04%	0.004%
96	13.710	3922	3925	3930	rBV	418	345	0.04%	0.004%
97	13.954	3999	4001	4005	rBV2	392	361	0.04%	0.004%
98	14.556	4186	4188	4192	rBV2	488	316	0.04%	0.003%
99	14.970	4315	4317	4318	rBV	575	225	0.03%	0.002%
100	15.154	4371	4374	4376	rBV4	819	646	0.07%	0.007%

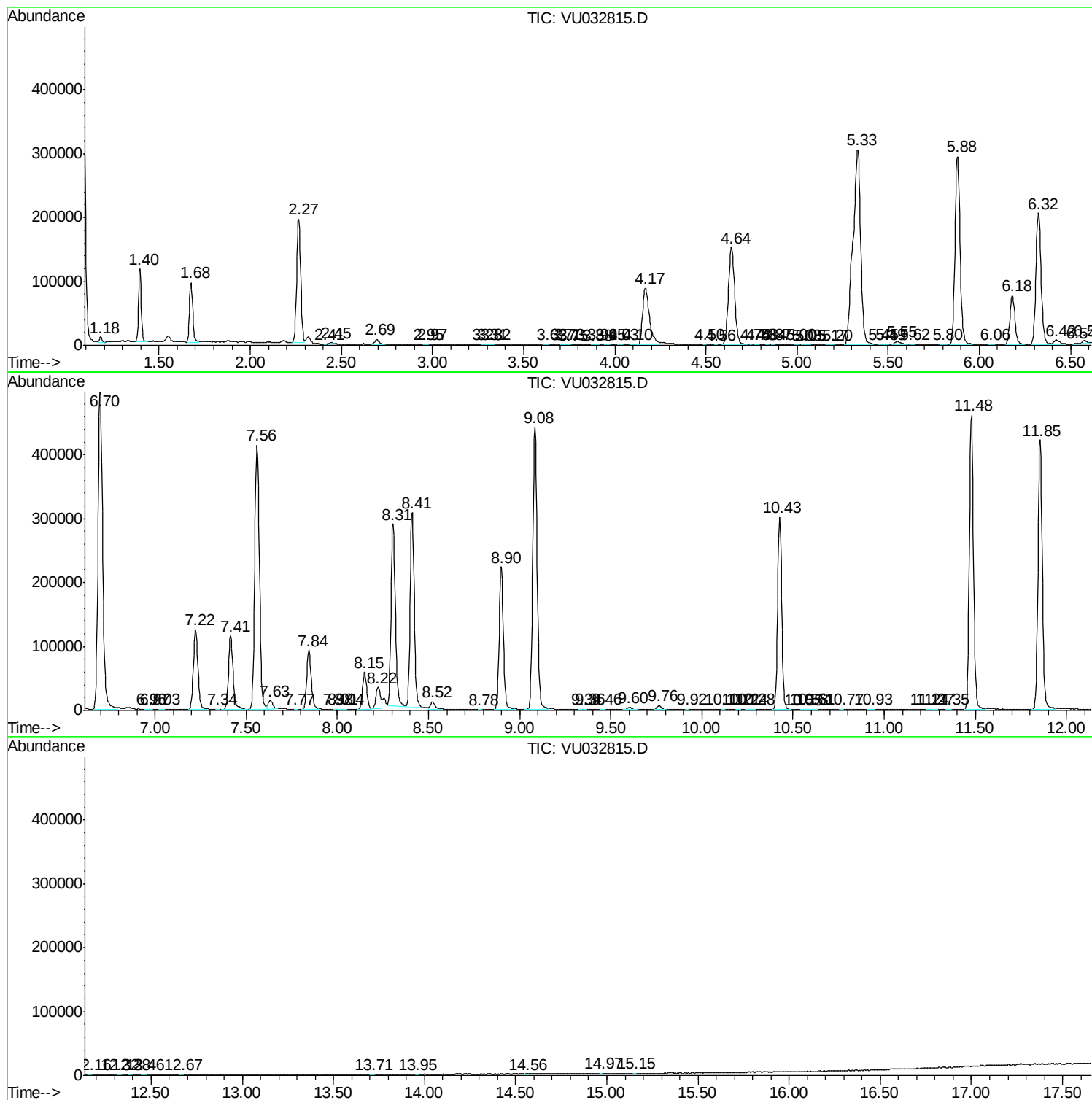
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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



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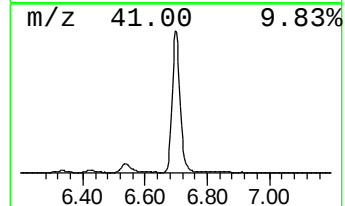
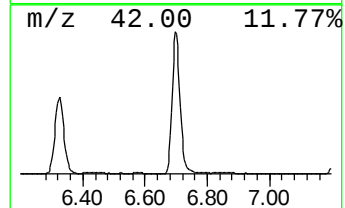
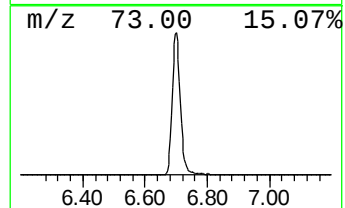
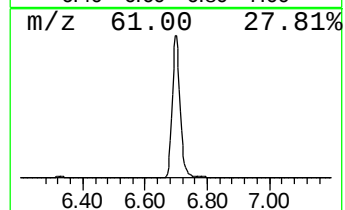
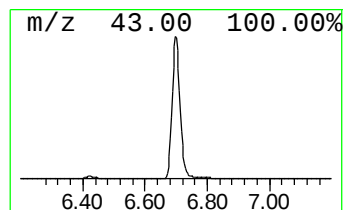
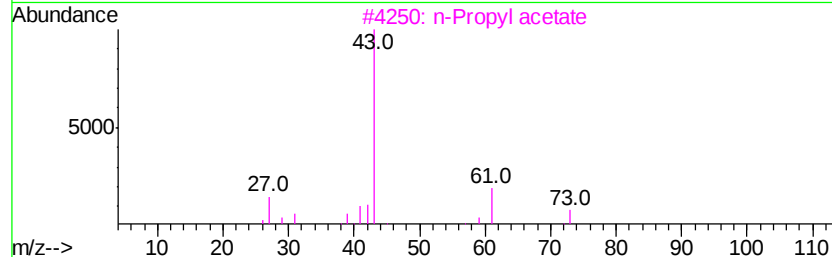
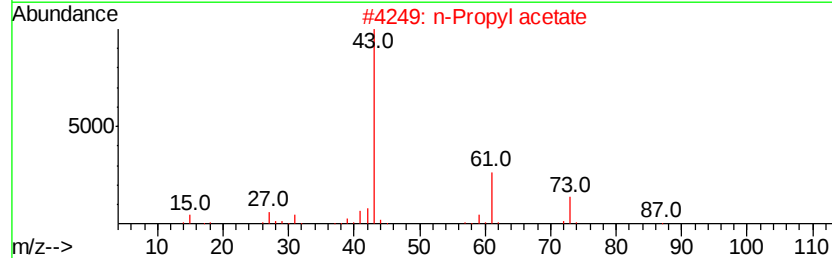
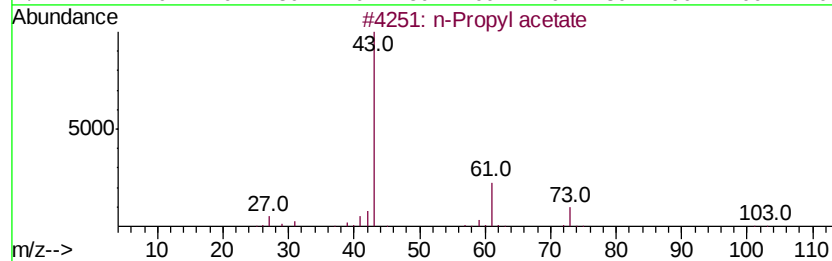
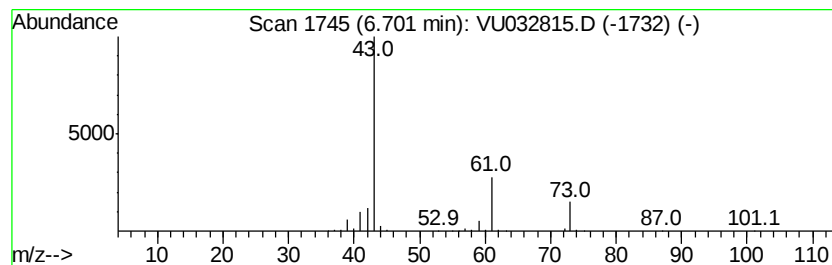
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	77.07 ug/L	885606	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	78
4		Isopropyl acetate	102	C5H10O2	000108-21-4	36
5		Isobutyl acetate	116	C6H12O2	000110-19-0	9



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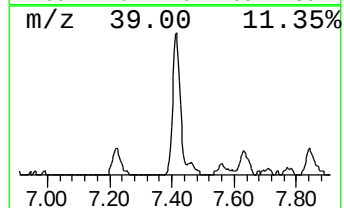
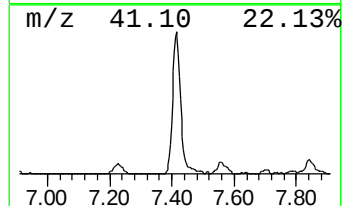
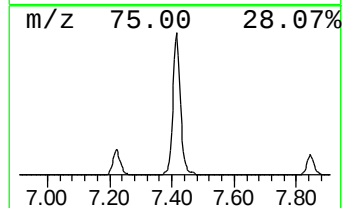
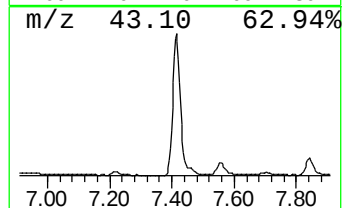
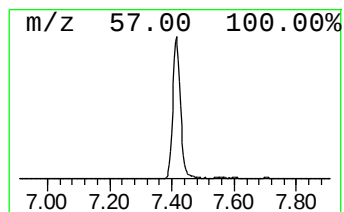
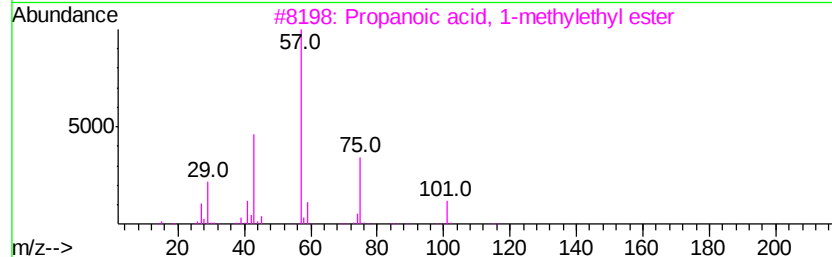
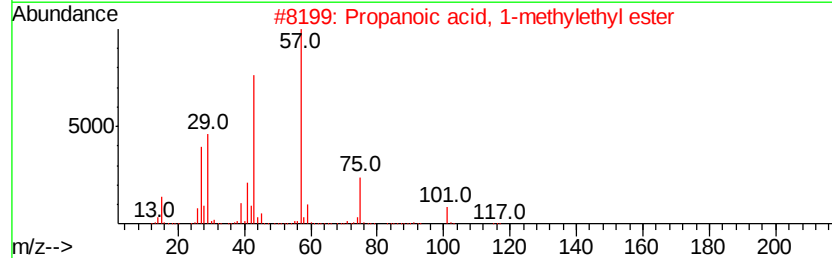
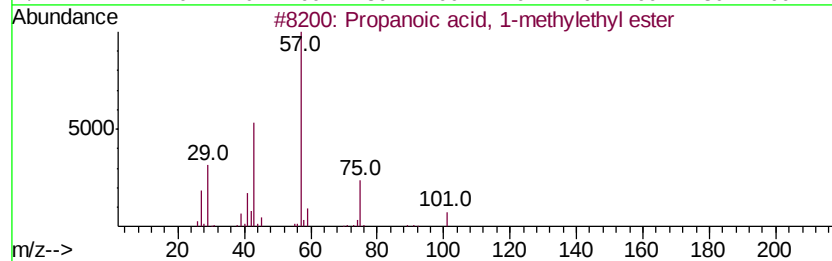
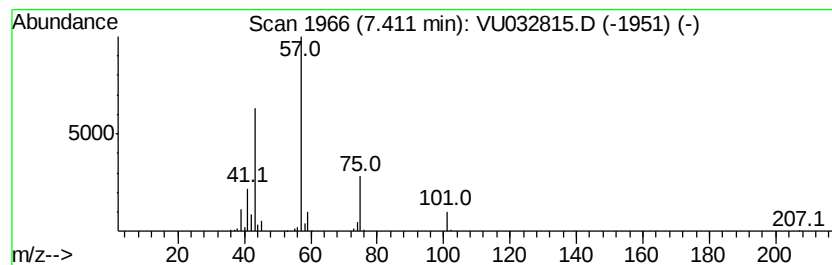
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Quant Title : VOC Analysis

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	17.45 ug/L	200516	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	86
2		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53



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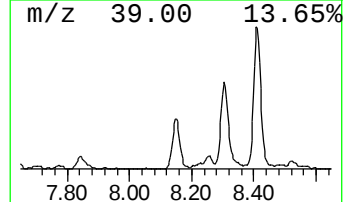
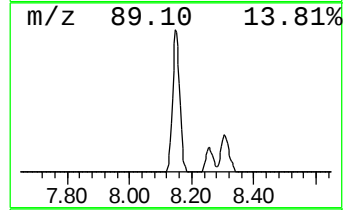
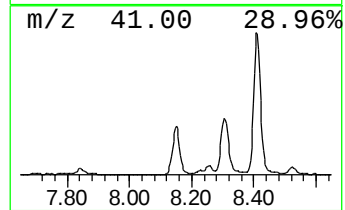
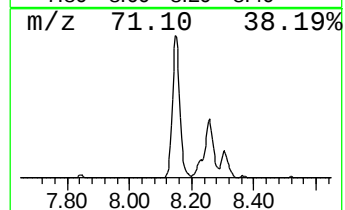
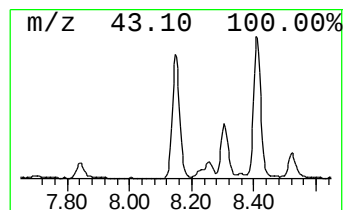
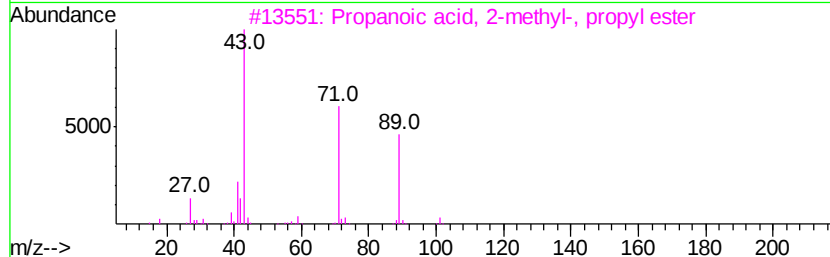
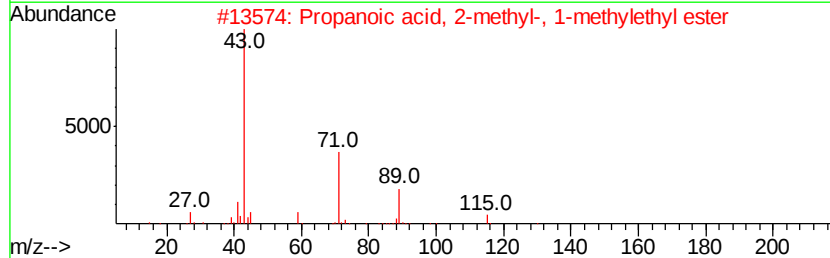
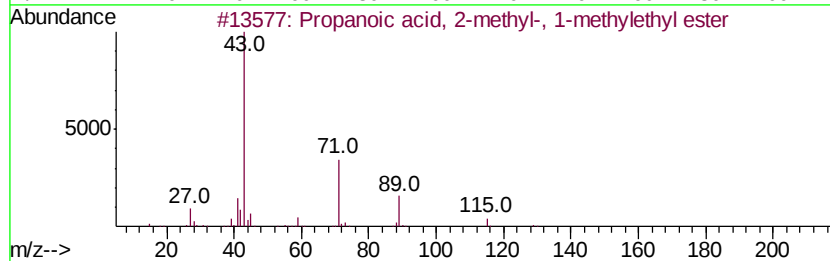
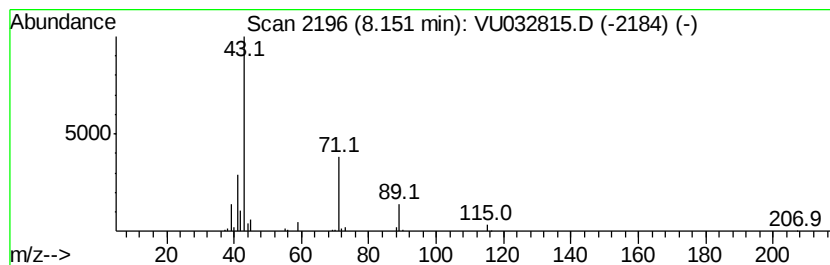
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Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	6.61 ug/L	96757	Chlorobenzene-d5	9.08

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	78	
3	Propanoic acid, 2-methyl-, propv...	130	C7H14O2	000644-49-5	78	
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	74	
5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032815.D
Acq On : 18 Jun 2019 11:43
Operator : JC/SP
Sample : K3363-16
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JQ3

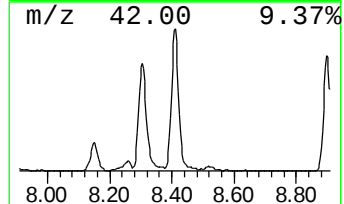
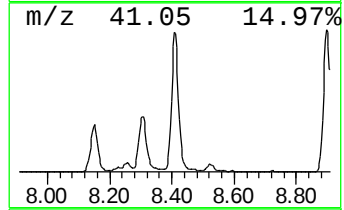
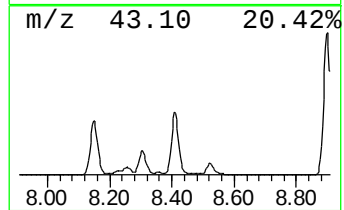
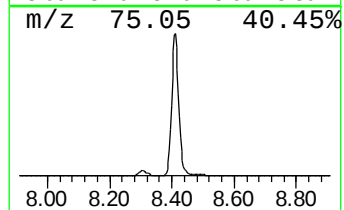
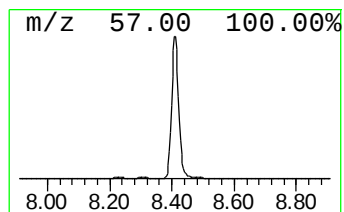
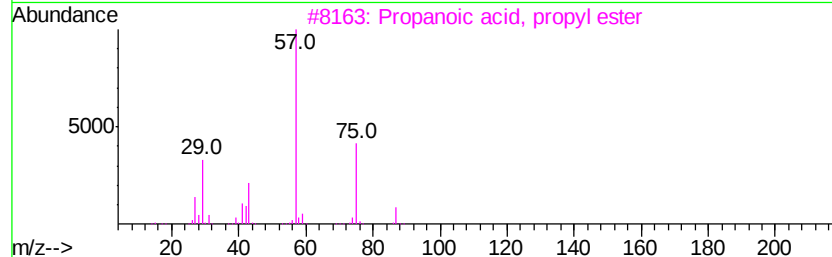
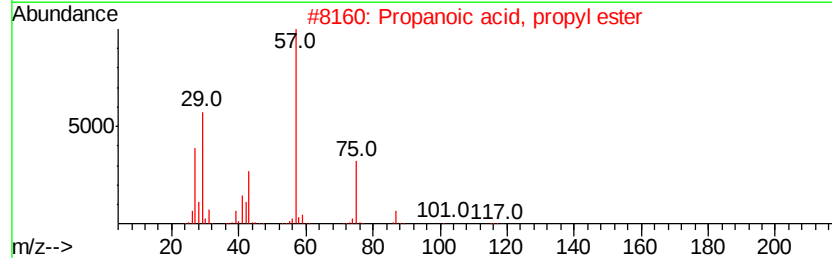
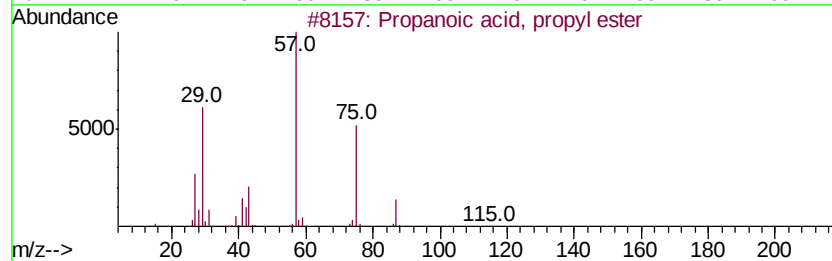
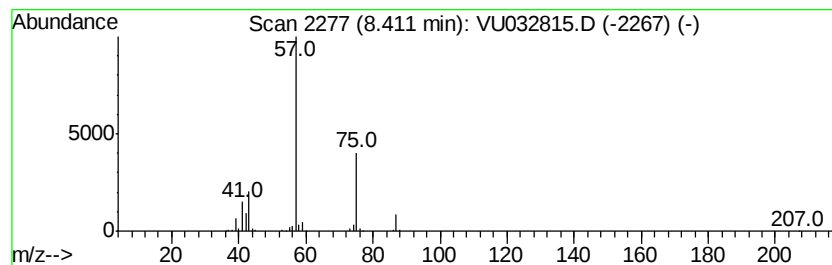
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	32.64 ug/L	477654	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		Trimethylaluminum	72	C3H9Al	000075-24-1	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032815.D
Acq On : 18 Jun 2019 11:43
Operator : JC/SP
Sample : K3363-16
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

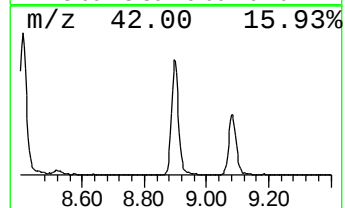
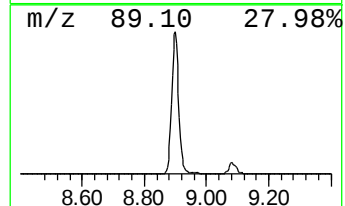
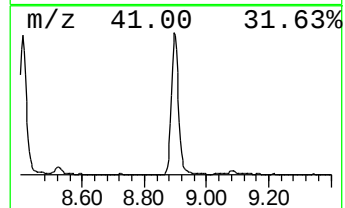
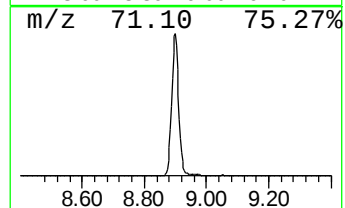
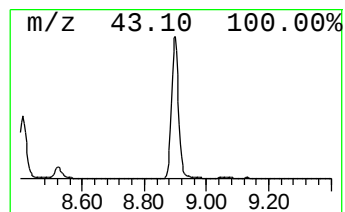
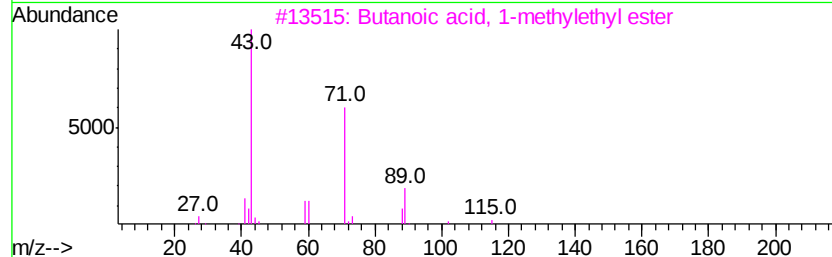
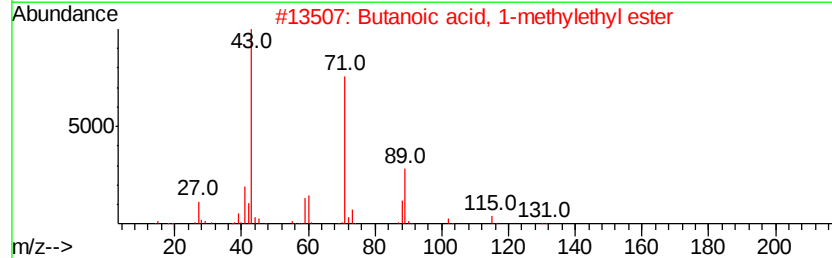
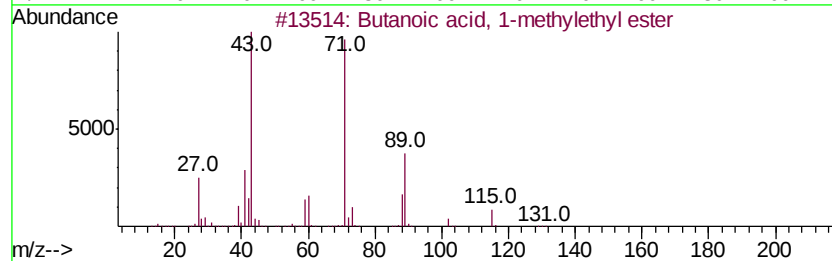
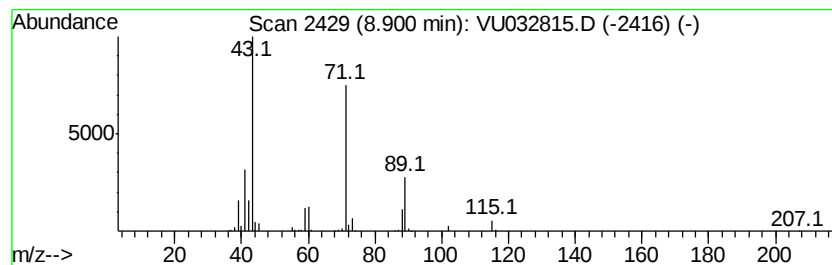
Instrument :
MSVOA_U
ClientSampleId :
C0JQ3

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 6 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.90	24.23 ug/L	354567	Chlorobenzene-d5	9.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	72	
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64	



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032815.D
Acq On : 18 Jun 2019 11:43
Operator : JC/SP
Sample : K3363-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JQ3

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	77.1	ug/L	885606	1	5.88	574537	50.0
Propanoic acid, 1...	7.41	17.4	ug/L	200516	1	5.88	574537	50.0
Propanoic acid, 2...	8.15	6.6	ug/L	96757	2	9.08	731716	50.0
Propanoic acid, p...	8.41	32.6	ug/L	477654	2	9.08	731716	50.0
Butanoic acid, 1-...	8.90	24.2	ug/L	354567	2	9.08	731716	50.0