

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
 Data File : VU032830.D
 Acq On : 18 Jun 2019 17:30
 Operator : JC/SP
 Sample : K3379-01
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JT1

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	34	rVB2	4403	3735	0.42%	0.041%
2	1.396	87	95	109	rBV	118854	119635	13.54%	1.299%
3	1.469	113	118	125	rVV	9807	10156	1.15%	0.110%
4	1.675	174	182	199	rVB	92447	114378	12.95%	1.242%
5	2.267	355	366	376	rBV	190986	288306	32.64%	3.131%
6	2.444	411	421	439	rVB	4345	9205	1.04%	0.100%
7	2.553	447	455	459	rBV5	689	1082	0.12%	0.012%
8	2.614	466	474	488	rBV2	3703	6762	0.77%	0.073%
9	2.695	490	499	510	rVV3	7461	12255	1.39%	0.133%
10	2.749	514	516	520	rVB2	588	350	0.04%	0.004%
11	2.775	520	524	526	rBV2	460	353	0.04%	0.004%
12	3.074	613	617	619	rBV2	356	258	0.03%	0.003%
13	3.219	660	662	666	rVB2	388	273	0.03%	0.003%
14	3.386	711	714	717	rBV2	335	239	0.03%	0.003%
15	3.421	722	725	728	rBV2	401	317	0.04%	0.003%
16	3.437	728	730	734	rVB2	349	256	0.03%	0.003%
17	3.489	743	746	749	rBV2	387	260	0.03%	0.003%
18	3.621	784	787	788	rBV	620	318	0.04%	0.003%
19	3.717	809	817	821	rBV3	288	417	0.05%	0.005%
20	3.813	841	847	854	rBV3	376	564	0.06%	0.006%
21	4.100	931	936	942	rVB3	313	377	0.04%	0.004%
22	4.167	942	957	990	rBV	97760	254987	28.87%	2.769%
23	4.579	1082	1085	1087	rVV3	420	300	0.03%	0.003%
24	4.640	1087	1104	1133	rVV	148229	350730	39.70%	3.809%
25	4.878	1173	1178	1182	rBV3	389	564	0.06%	0.006%
26	4.929	1189	1194	1196	rBV2	360	293	0.03%	0.003%
27	5.016	1218	1221	1224	rBV	341	257	0.03%	0.003%
28	5.035	1224	1227	1231	rVB3	386	277	0.03%	0.003%
29	5.096	1239	1246	1248	rBV3	273	303	0.03%	0.003%
30	5.334	1293	1320	1347	rBV2	298027	883373	100.00%	9.593%
31	5.546	1375	1386	1399	rBV3	5032	10957	1.24%	0.119%
32	5.778	1454	1458	1461	rBV2	308	258	0.03%	0.003%
33	5.881	1475	1490	1514	rBV	271021	536379	60.72%	5.825%
34	6.173	1577	1581	1589	rVB7	1202	1615	0.18%	0.018%

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 Title : VOC Analysis

35	6.325	1614	1628	1648	rBV	199260	398262	45.08%	4.325%
36	6.421	1650	1658	1669	rVV2	7026	12490	1.41%	0.136%
37	6.530	1685	1692	1695	rBV5	2459	3125	0.35%	0.034%
38	6.575	1699	1706	1713	rVV2	5600	8659	0.98%	0.094%
39	6.701	1731	1745	1775	rBV	437411	787267	89.12%	8.550%
40	6.977	1827	1831	1832	rBV2	443	262	0.03%	0.003%
41	7.077	1859	1862	1864	rBV2	361	239	0.03%	0.003%
42	7.106	1868	1871	1874	rBV2	379	252	0.03%	0.003%
43	7.148	1879	1884	1885	rVB2	481	395	0.04%	0.004%
44	7.157	1885	1887	1889	rBV2	424	243	0.03%	0.003%
45	7.222	1895	1907	1928	rBV	104523	187829	21.26%	2.040%
46	7.415	1954	1967	1991	rVV	120541	211172	23.91%	2.293%
47	7.559	1999	2012	2029	rBV	416032	716829	81.15%	7.785%
48	7.701	2048	2056	2065	rVB6	1745	3117	0.35%	0.034%
49	7.765	2072	2076	2077	rBV2	718	559	0.06%	0.006%
50	7.842	2089	2100	2123	rBV	76617	135071	15.29%	1.467%
51	8.090	2175	2177	2180	rVB	665	344	0.04%	0.004%
52	8.148	2180	2195	2209	rBV	67093	111282	12.60%	1.209%
53	8.225	2211	2219	2223	rBV2	9312	13447	1.52%	0.146%
54	8.305	2234	2244	2266	rVB	328729	547209	61.95%	5.943%
55	8.411	2266	2277	2294	rVB	310341	481709	54.53%	5.231%
56	8.521	2307	2311	2326	rVB2	7423	11998	1.36%	0.130%
57	8.717	2367	2372	2376	rVB4	501	485	0.05%	0.005%
58	8.739	2376	2379	2382	rBV2	478	321	0.04%	0.003%
59	8.759	2382	2385	2390	rVB3	518	447	0.05%	0.005%
60	8.897	2414	2428	2455	rBV	256586	403421	45.67%	4.381%
61	9.083	2466	2486	2507	rBV	415242	689575	78.06%	7.489%
62	9.244	2533	2536	2541	rVB2	642	535	0.06%	0.006%
63	9.337	2561	2565	2568	rBV3	339	254	0.03%	0.003%
64	9.498	2610	2615	2619	rBV2	461	528	0.06%	0.006%
65	9.598	2639	2646	2657	rBV3	5588	9567	1.08%	0.104%
66	9.675	2666	2670	2676	rBV2	524	512	0.06%	0.006%
67	9.762	2689	2697	2706	rBV2	4696	7707	0.87%	0.084%
68	9.897	2735	2739	2744	rBV2	269	287	0.03%	0.003%
69	9.926	2744	2748	2751	rVV2	278	259	0.03%	0.003%
70	9.945	2751	2754	2761	rVB3	349	398	0.05%	0.004%
71	10.048	2782	2786	2788	rBV2	301	277	0.03%	0.003%

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72	10.103	2798	2803	2809	rVB6	425	637	0.07%	0.007%
73	10.173	2823	2825	2827	rBV	334	235	0.03%	0.003%
74	10.209	2830	2836	2838	rBV3	400	374	0.04%	0.004%
75	10.289	2859	2861	2865	rVB2	508	286	0.03%	0.003%
76	10.360	2879	2883	2887	rVB3	381	319	0.04%	0.003%
77	10.427	2891	2904	2923	rBV	298060	482868	54.66%	5.244%
78	10.543	2935	2940	2943	rBV4	329	259	0.03%	0.003%
79	10.694	2984	2987	2992	rBV3	453	402	0.05%	0.004%
80	10.894	3043	3049	3052	rVV3	446	421	0.05%	0.005%
81	11.154	3126	3130	3137	rVB5	1076	1221	0.14%	0.013%
82	11.231	3150	3154	3155	rBV2	403	257	0.03%	0.003%
83	11.347	3186	3190	3198	rBV5	322	313	0.04%	0.003%
84	11.479	3218	3231	3251	rBV	423560	676361	76.57%	7.345%
85	11.710	3301	3303	3307	rBV3	470	361	0.04%	0.004%
86	11.781	3322	3325	3330	rVB3	587	414	0.05%	0.004%
87	11.855	3335	3348	3369	rBV	412575	680700	77.06%	7.392%
88	12.057	3409	3411	3414	rVB3	493	251	0.03%	0.003%
89	12.324	3490	3494	3500	rBV4	584	769	0.09%	0.008%
90	12.408	3517	3520	3524	rBV4	421	412	0.05%	0.004%
91	12.475	3538	3541	3542	rBV	378	240	0.03%	0.003%
92	12.553	3563	3565	3571	rVB2	339	321	0.04%	0.003%
93	12.582	3571	3574	3579	rBV4	459	481	0.05%	0.005%
94	12.604	3579	3581	3586	rBV2	443	321	0.04%	0.003%
95	12.710	3612	3614	3617	rBV	398	248	0.03%	0.003%
96	13.260	3782	3785	3788	rBV3	418	280	0.03%	0.003%
97	13.308	3796	3800	3809	rVB5	540	772	0.09%	0.008%
98	13.652	3905	3907	3912	rBV4	356	266	0.03%	0.003%
99	13.832	3961	3963	3966	rBV2	518	296	0.03%	0.003%
100	15.321	4419	4426	4432	rBV5	1169	1835	0.21%	0.020%

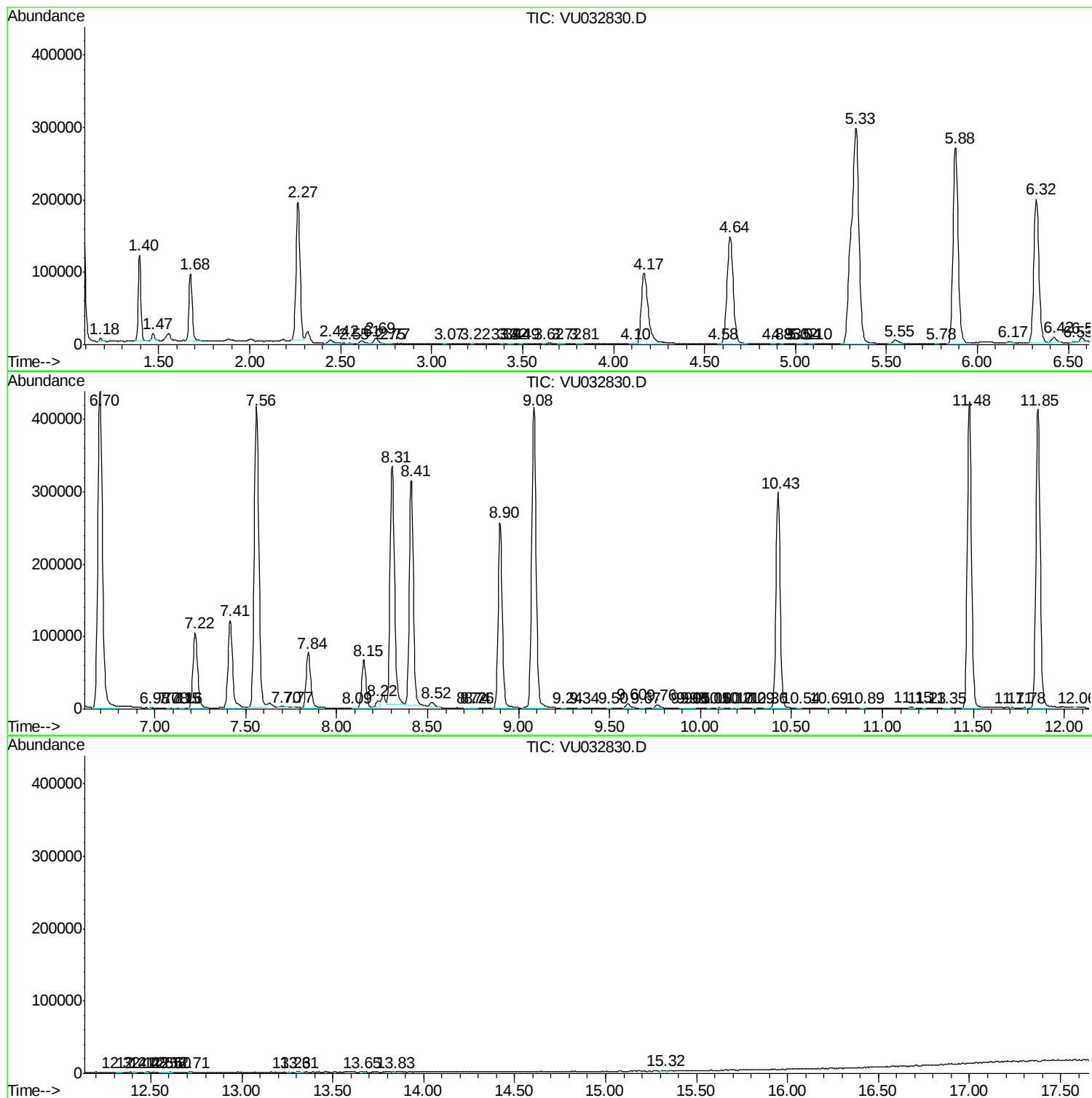
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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



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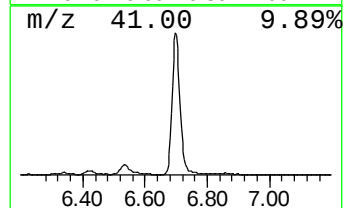
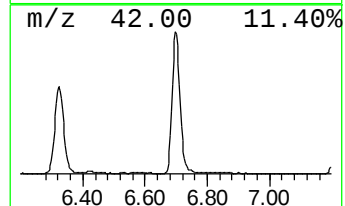
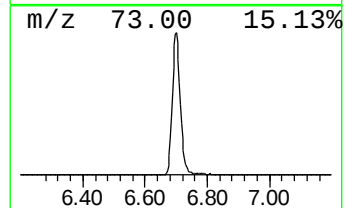
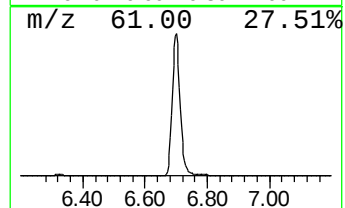
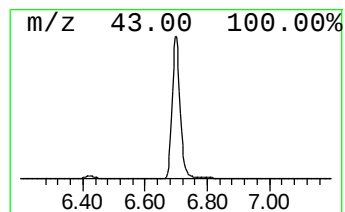
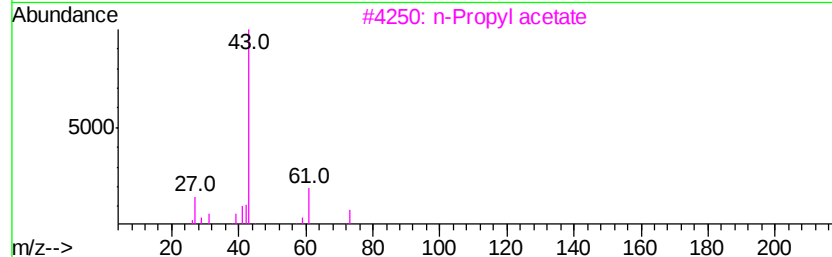
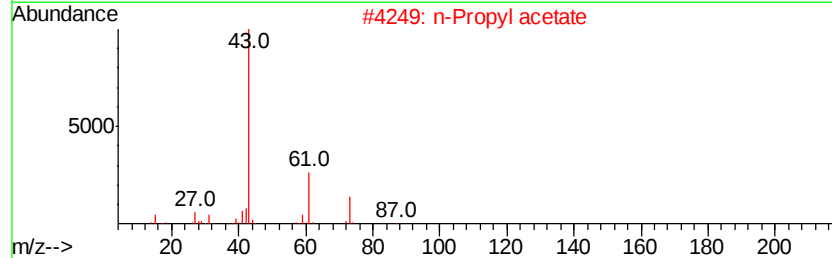
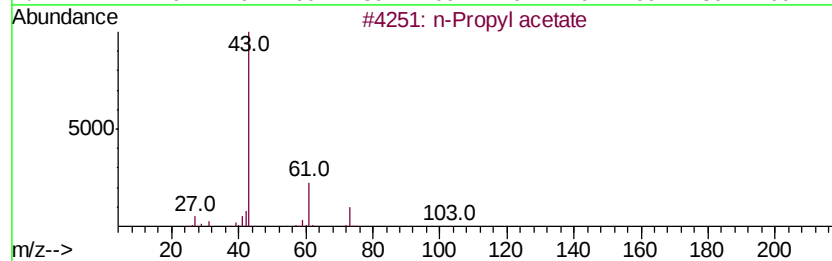
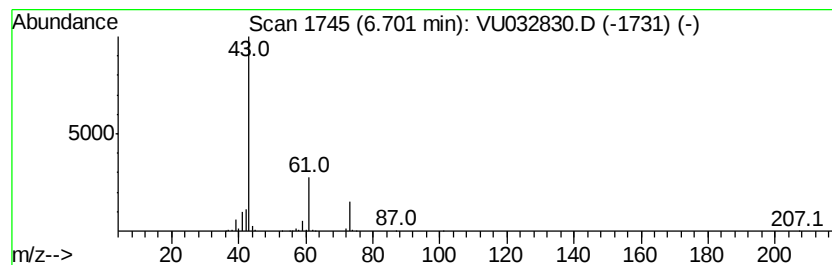
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	73.39 ug/L	787267	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		Isobutylamine	73	C4H11N	000078-81-9	9



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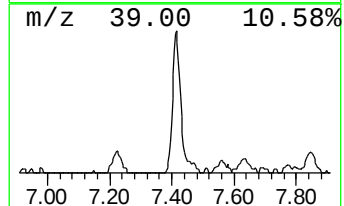
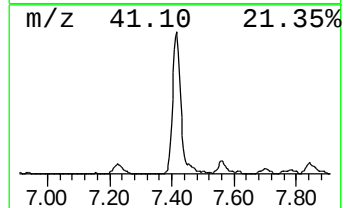
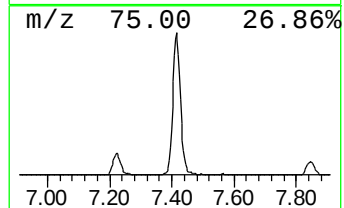
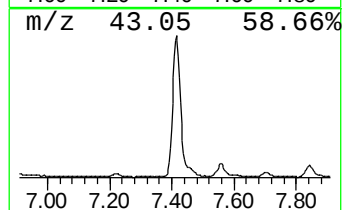
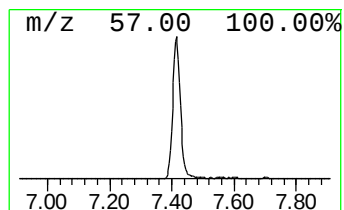
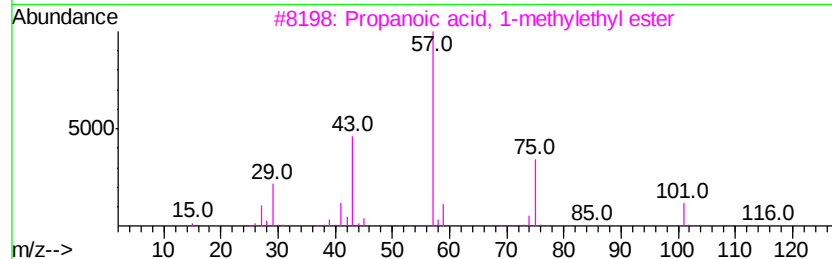
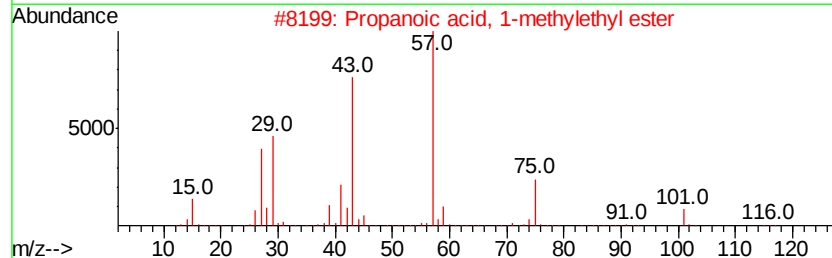
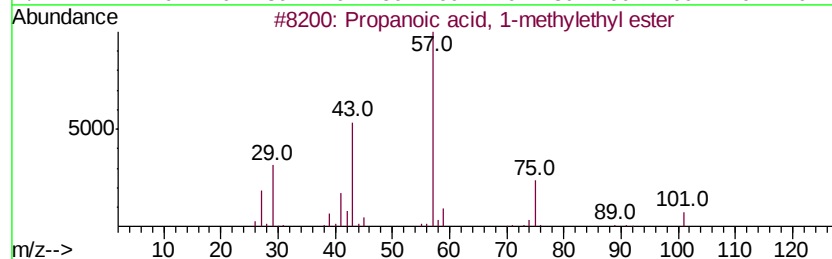
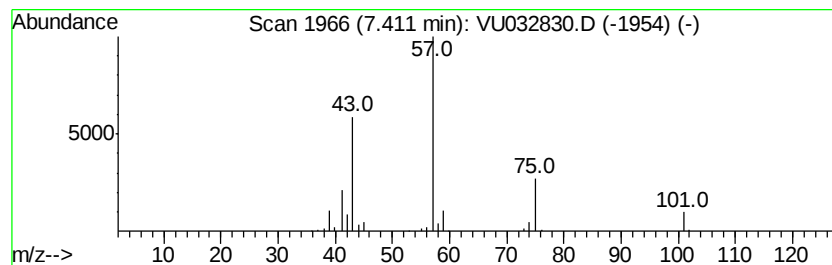
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Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	19.69 ug/L	211172	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	78
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	45



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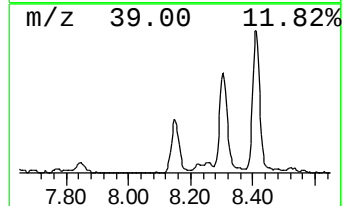
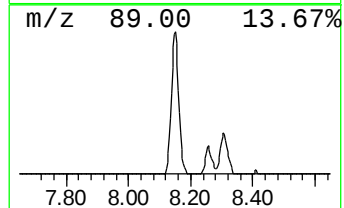
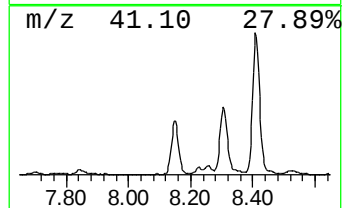
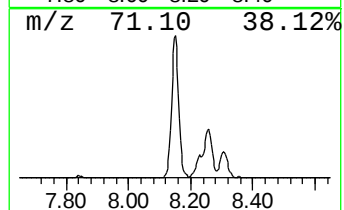
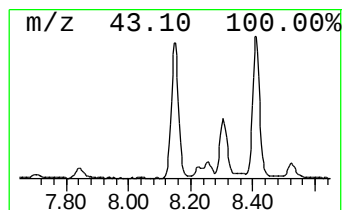
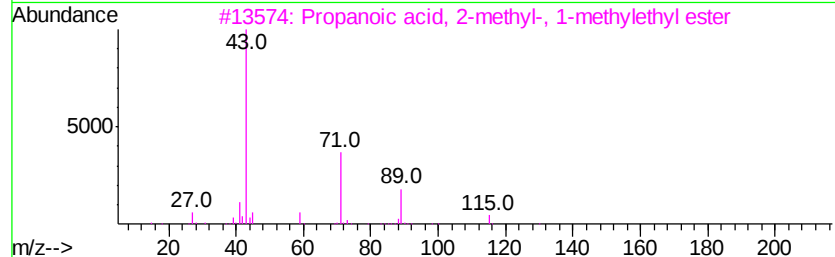
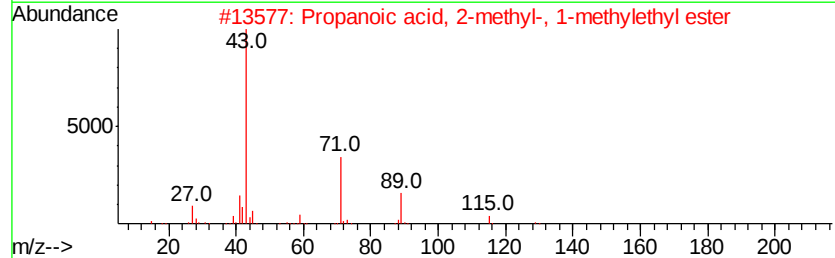
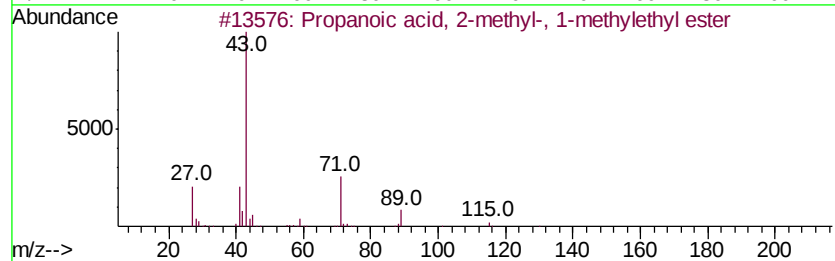
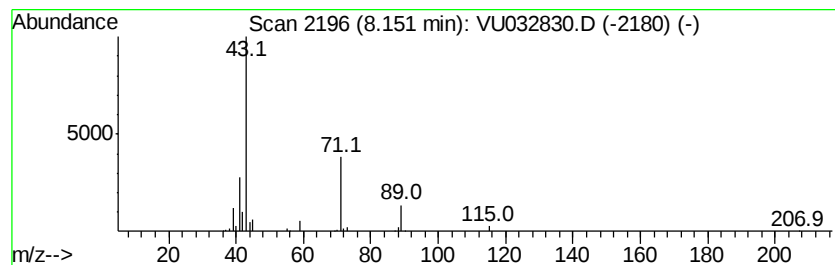
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	8.07 ug/L	111282	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	83
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032830.D
Acq On : 18 Jun 2019 17:30
Operator : JC/SP
Sample : K3379-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JT1

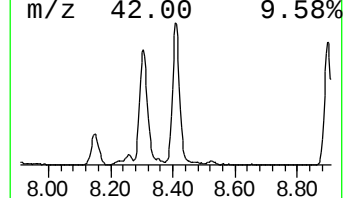
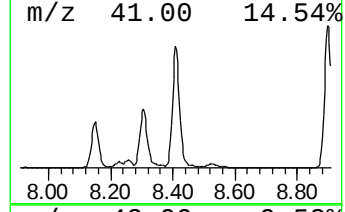
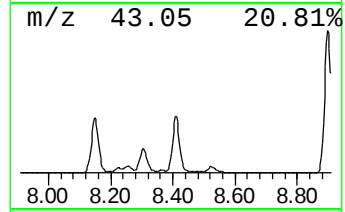
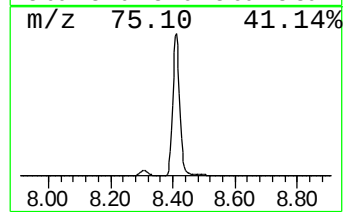
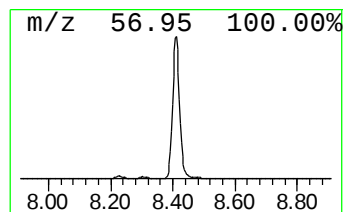
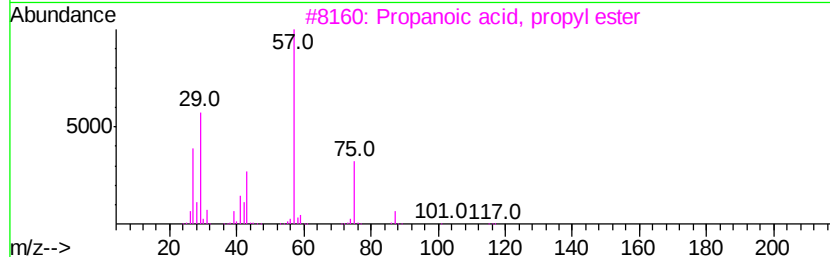
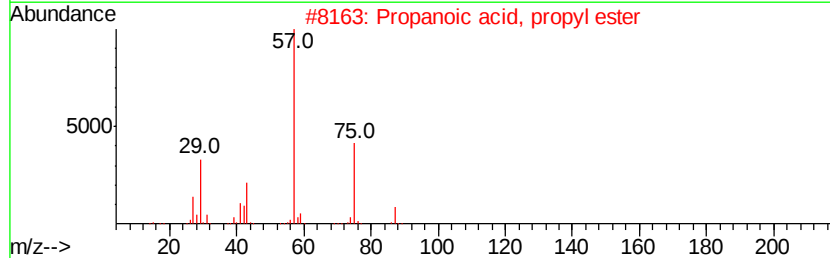
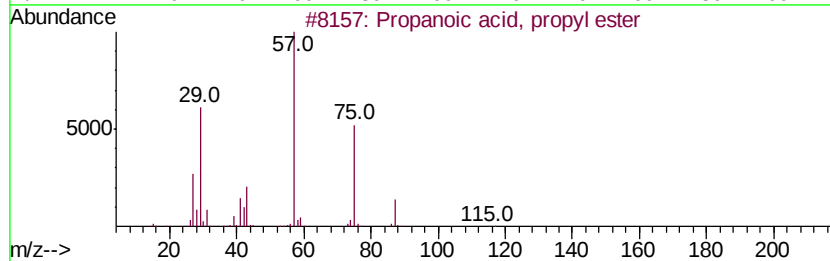
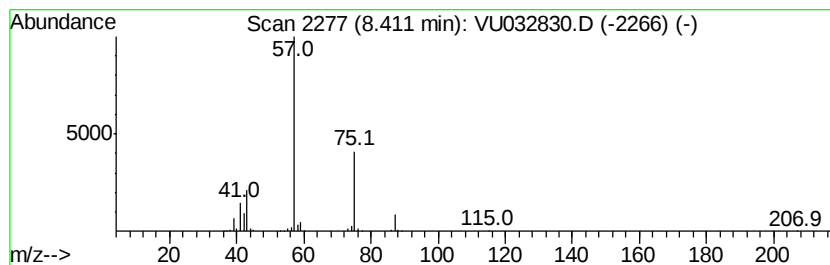
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Quant Title : VOC Analysis

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	34.93 ug/L	481709	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 : VU032830.D
Acq On : 18 Jun 2019 17:30
Operator : JC/SP
Sample : K3379-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 24 Sample Multiplier: 1

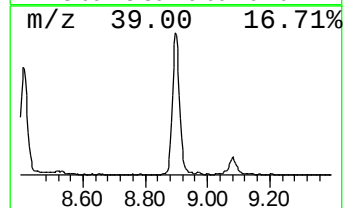
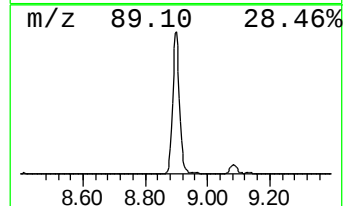
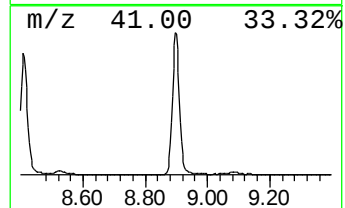
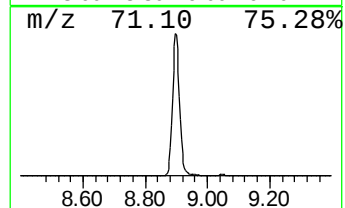
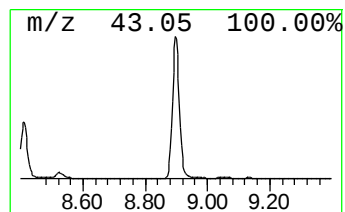
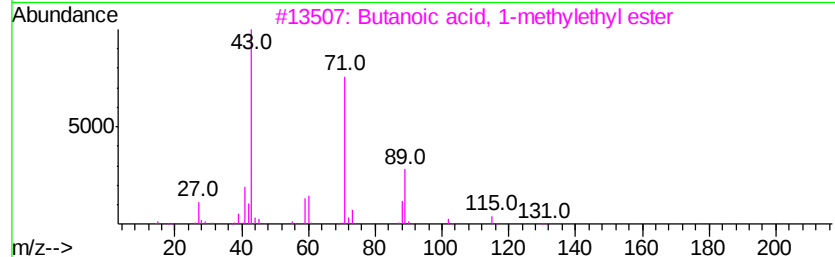
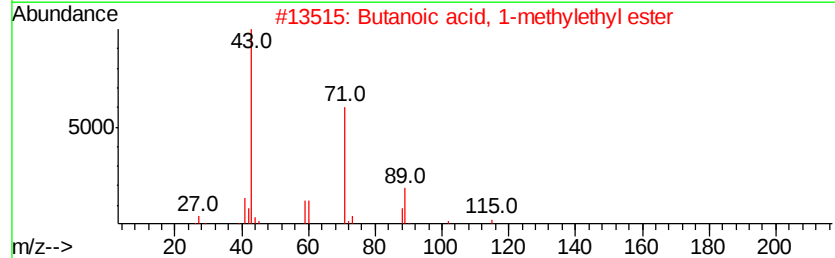
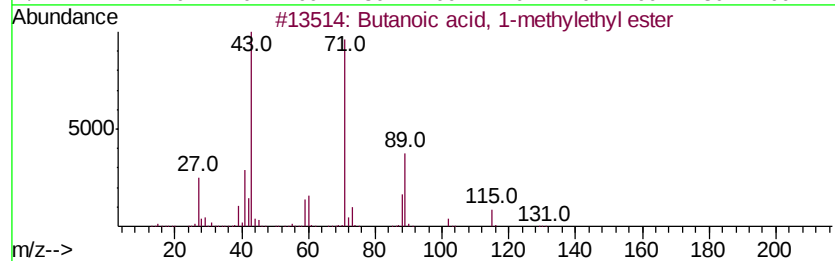
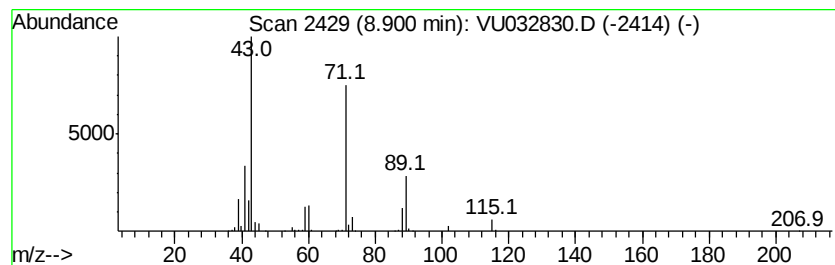
Instrument :
MSVOA_U
ClientSampleId :
C0JT1

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	29.25 ug/L	403421	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	90
4		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	72
5		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032830.D
Acq On : 18 Jun 2019 17:30
Operator : JC/SP
Sample : K3379-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JT1

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	73.4	ug/L	787267	1	5.88	536379	50.0
Propanoic acid, 1...	7.41	19.7	ug/L	211172	1	5.88	536379	50.0
Propanoic acid, 2...	8.15	8.1	ug/L	111282	2	9.08	689575	50.0
Propanoic acid, p...	8.41	34.9	ug/L	481709	2	9.08	689575	50.0
Butanoic acid, 1-...	8.90	29.3	ug/L	403421	2	9.08	689575	50.0