

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
 Data File : VU032820.D
 Acq On : 18 Jun 2019 13:37
 Operator : JC/SP
 Sample : K3363-21
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JR2

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	36	rBV	7778	7078	0.19%	0.056%
2	1.396	87	95	112	rBV2	257432	282035	7.43%	2.231%
3	1.470	112	118	127	rBV	10258	11919	0.31%	0.094%
4	1.672	174	181	197	rVB	97242	123620	3.26%	0.978%
5	2.267	355	366	377	rBV2	208038	325729	8.58%	2.576%
6	2.614	466	474	490	rBV	2402	5149	0.14%	0.041%
7	2.695	490	499	508	rVV	7189	10864	0.29%	0.086%
8	2.978	577	587	603	rVB	14434	26153	0.69%	0.207%
9	3.042	603	607	611	rBV3	346	400	0.01%	0.003%
10	3.177	642	649	650	rBV5	633	716	0.02%	0.006%
11	3.331	693	697	700	rBV3	468	447	0.01%	0.004%
12	3.405	716	720	723	rBV2	463	314	0.01%	0.002%
13	3.428	723	727	731	rBV4	532	621	0.02%	0.005%
14	3.489	741	746	751	rBV2	332	438	0.01%	0.003%
15	3.592	775	778	781	rBV3	389	270	0.01%	0.002%
16	3.614	782	785	789	rVB3	455	355	0.01%	0.003%
17	3.643	789	794	797	rBV	554	400	0.01%	0.003%
18	3.659	797	799	803	rVB2	403	293	0.01%	0.002%
19	3.730	819	821	825	rVB3	341	236	0.01%	0.002%
20	3.756	825	829	831	rBV	279	231	0.01%	0.002%
21	3.929	879	883	886	rBV2	280	281	0.01%	0.002%
22	4.006	903	907	909	rBV2	381	234	0.01%	0.002%
23	4.100	930	936	939	rBV3	566	405	0.01%	0.003%
24	4.215	945	972	1013	rBV2	1473191	3795375	100.00%	30.017%
25	4.486	1054	1056	1057	rBV2	502	231	0.01%	0.002%
26	4.640	1088	1104	1128	rVB	156175	361171	9.52%	2.856%
27	4.743	1134	1136	1138	rVB2	538	240	0.01%	0.002%
28	4.762	1138	1142	1147	rBV4	436	421	0.01%	0.003%
29	4.875	1174	1177	1179	rBV2	393	257	0.01%	0.002%
30	4.939	1194	1197	1200	rVB4	574	286	0.01%	0.002%
31	4.997	1213	1215	1219	rBV3	426	350	0.01%	0.003%
32	5.080	1237	1241	1245	rVB3	426	407	0.01%	0.003%
33	5.106	1245	1249	1251	rBV	641	445	0.01%	0.004%
34	5.331	1293	1319	1350	rBV2	312126	921221	24.27%	7.286%

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 Title : VOC Analysis

35	5.550	1378	1387	1401	rBV3	5029	10232	0.27%	0.081%
36	5.666	1420	1423	1426	rVB3	383	261	0.01%	0.002%
37	5.772	1451	1456	1457	rBV3	300	251	0.01%	0.002%
38	5.788	1457	1461	1463	rVV2	426	376	0.01%	0.003%
39	5.878	1476	1489	1513	rBV	291268	570714	15.04%	4.514%
40	6.048	1536	1542	1544	rBV3	684	728	0.02%	0.006%
41	6.183	1574	1584	1598	rVB6	9032	18876	0.50%	0.149%
42	6.325	1613	1628	1650	rBV	209727	420065	11.07%	3.322%
43	6.421	1651	1658	1673	rVB	3950	8291	0.22%	0.066%
44	6.534	1685	1693	1697	rBV2	2346	3237	0.09%	0.026%
45	6.575	1702	1706	1714	rVB2	2612	3974	0.10%	0.031%
46	6.698	1732	1744	1779	rBV	378046	686085	18.08%	5.426%
47	6.974	1825	1830	1833	rBV5	393	271	0.01%	0.002%
48	7.080	1860	1863	1866	rVB3	472	302	0.01%	0.002%
49	7.222	1895	1907	1931	rBV	110544	197818	5.21%	1.564%
50	7.415	1951	1967	1977	rBV	101041	172706	4.55%	1.366%
51	7.559	1999	2012	2040	rBV	429617	745009	19.63%	5.892%
52	7.842	2089	2100	2124	rBV	88866	153061	4.03%	1.211%
53	8.006	2146	2151	2153	rVB2	685	482	0.01%	0.004%
54	8.029	2153	2158	2159	rBV3	291	246	0.01%	0.002%
55	8.087	2173	2176	2179	rBV2	348	226	0.01%	0.002%
56	8.151	2185	2196	2212	rVV	57874	95222	2.51%	0.753%
57	8.257	2214	2229	2234	rVV5	7575	13626	0.36%	0.108%
58	8.305	2234	2244	2266	rVV	304302	526646	13.88%	4.165%
59	8.411	2267	2277	2297	rVB	125341	200459	5.28%	1.585%
60	8.524	2305	2312	2326	rVB3	6272	11732	0.31%	0.093%
61	8.617	2337	2341	2343	rBV2	477	389	0.01%	0.003%
62	8.772	2385	2389	2390	rBV	336	233	0.01%	0.002%
63	8.900	2416	2429	2449	rBV	170711	271405	7.15%	2.146%
64	9.026	2464	2468	2469	rBV2	363	224	0.01%	0.002%
65	9.083	2473	2486	2512	rVV	438822	724060	19.08%	5.726%
66	9.238	2532	2534	2540	rVB4	527	447	0.01%	0.004%
67	9.267	2540	2543	2547	rBV4	366	327	0.01%	0.003%
68	9.392	2576	2582	2592	rVB3	583	814	0.02%	0.006%
69	9.440	2592	2597	2598	rBV2	662	533	0.01%	0.004%
70	9.472	2602	2607	2610	rBV3	513	497	0.01%	0.004%
71	9.498	2611	2615	2620	rVB4	522	513	0.01%	0.004%

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72	9.604	2643	2648	2652	rVV5	556	564	0.01%	0.004%
73	9.762	2690	2697	2709	rBV5	1976	3180	0.08%	0.025%
74	9.881	2729	2734	2742	rVV3	328	506	0.01%	0.004%
75	9.961	2756	2759	2762	rBV2	366	310	0.01%	0.002%
76	10.077	2789	2795	2797	rBV3	449	383	0.01%	0.003%
77	10.286	2856	2860	2863	rVB4	403	328	0.01%	0.003%
78	10.347	2876	2879	2885	rVB2	259	247	0.01%	0.002%
79	10.424	2891	2903	2924	rBV	304247	488478	12.87%	3.863%
80	10.598	2953	2957	2960	rBV3	324	301	0.01%	0.002%
81	10.743	2997	3002	3004	rBV2	282	227	0.01%	0.002%
82	10.784	3011	3015	3023	rBV3	429	455	0.01%	0.004%
83	10.820	3023	3026	3029	rBV3	431	279	0.01%	0.002%
84	10.845	3031	3034	3037	rBV2	310	238	0.01%	0.002%
85	11.193	3139	3142	3145	rBV	356	237	0.01%	0.002%
86	11.479	3219	3231	3252	rBV	445927	717778	18.91%	5.677%
87	11.720	3300	3306	3309	rBV4	432	531	0.01%	0.004%
88	11.746	3312	3314	3318	rVV3	386	254	0.01%	0.002%
89	11.855	3334	3348	3370	rBV	428533	707143	18.63%	5.593%
90	12.180	3447	3449	3453	rBV2	453	320	0.01%	0.003%
91	12.279	3478	3480	3485	rBV2	333	276	0.01%	0.002%
92	12.418	3520	3523	3526	rBV2	283	225	0.01%	0.002%
93	12.546	3560	3563	3566	rBV4	303	257	0.01%	0.002%
94	12.620	3583	3586	3590	rBV2	513	394	0.01%	0.003%
95	13.746	3934	3936	3942	rBV3	347	322	0.01%	0.003%
96	13.980	4007	4009	4014	rBV3	454	312	0.01%	0.002%
97	14.096	4041	4045	4049	rBV3	582	563	0.01%	0.004%
98	14.337	4118	4120	4123	rVB2	959	426	0.01%	0.003%
99	14.450	4152	4155	4157	rBV2	562	437	0.01%	0.003%
100	14.537	4179	4182	4184	rBV2	569	366	0.01%	0.003%

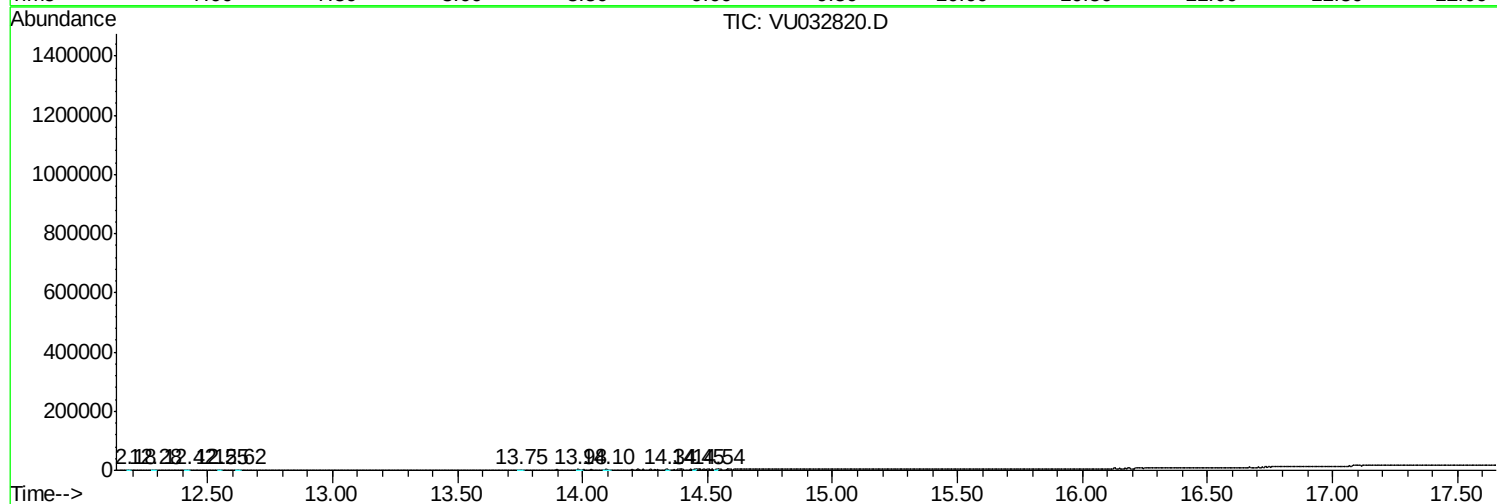
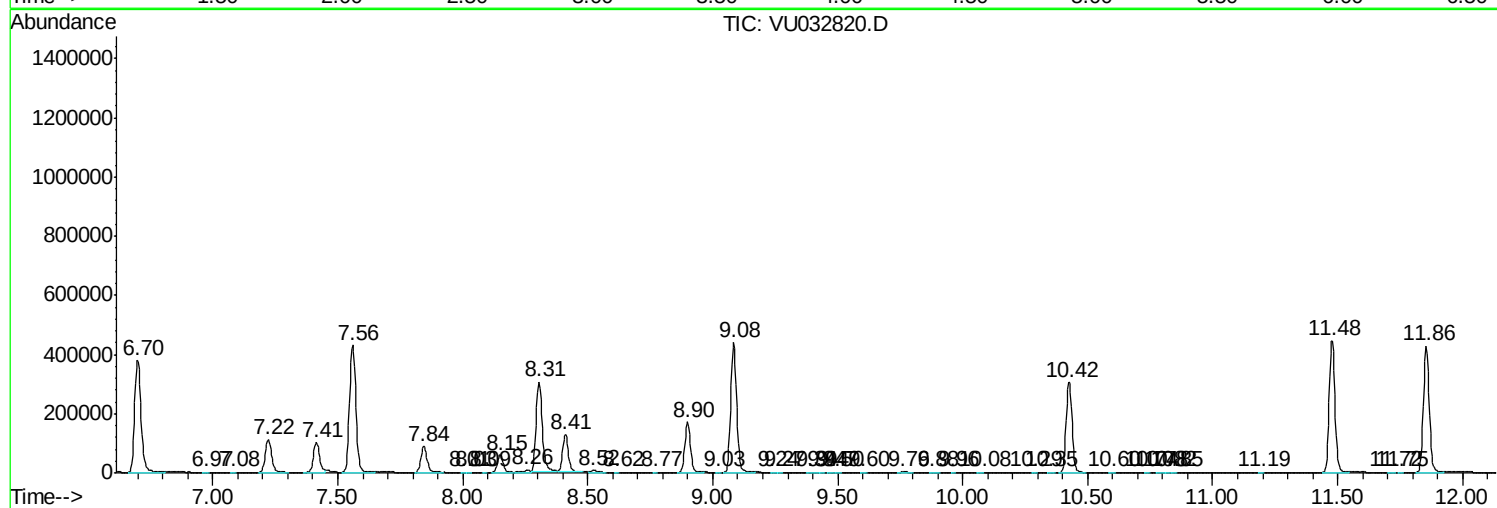
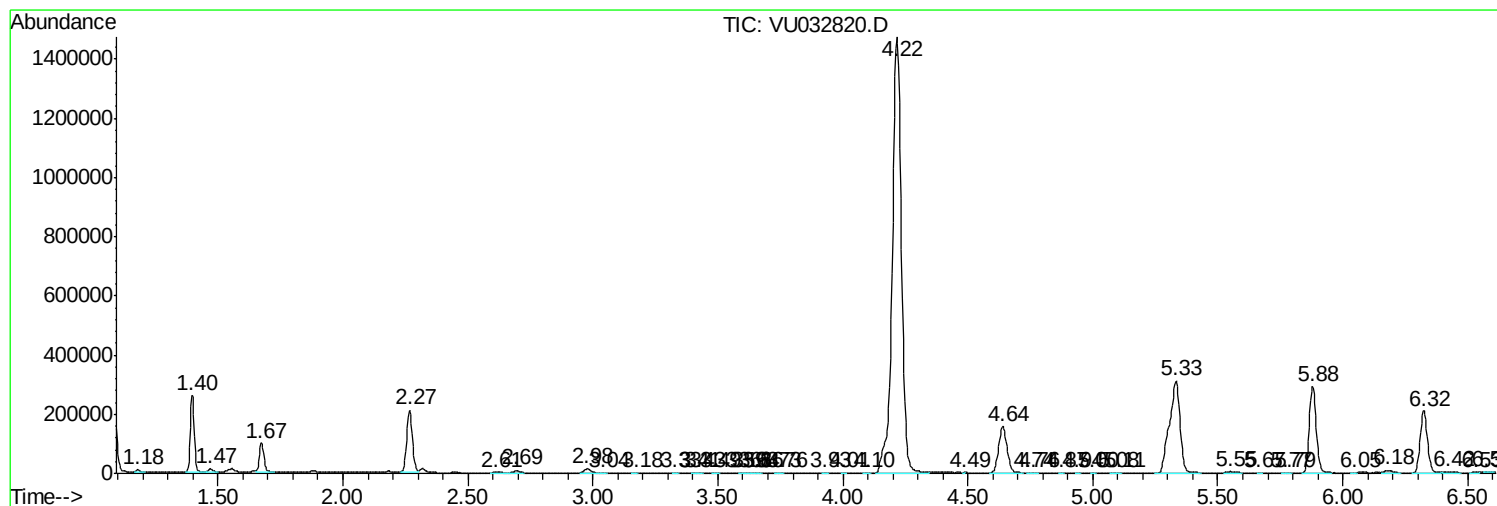
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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



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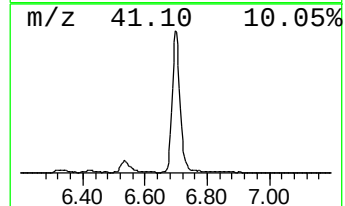
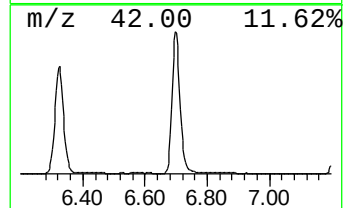
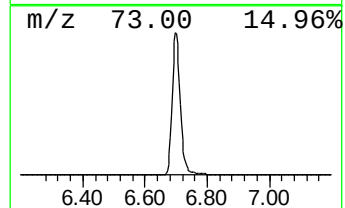
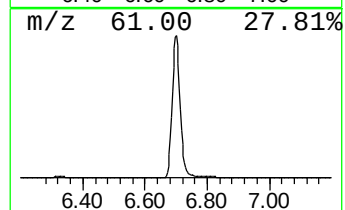
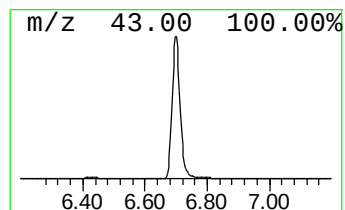
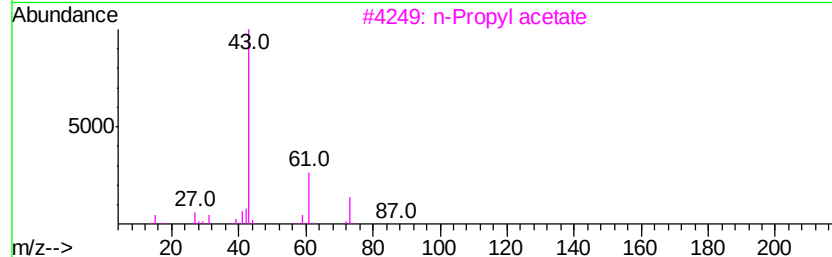
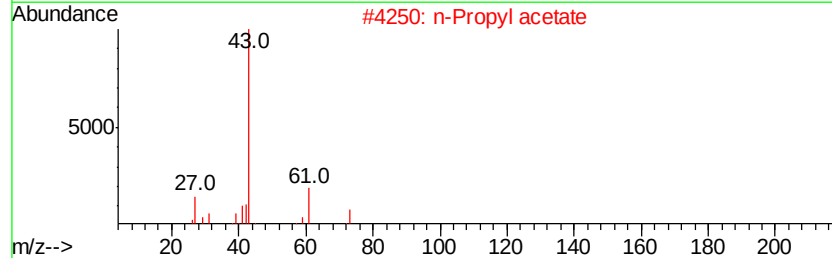
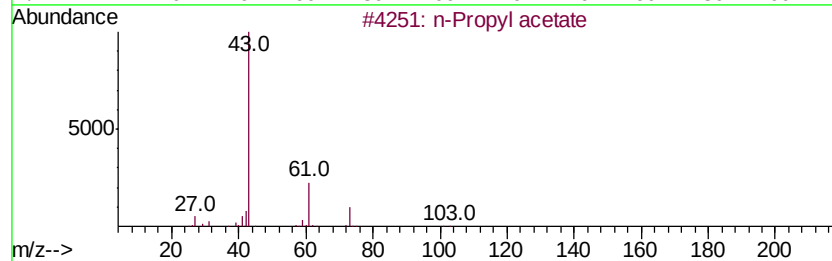
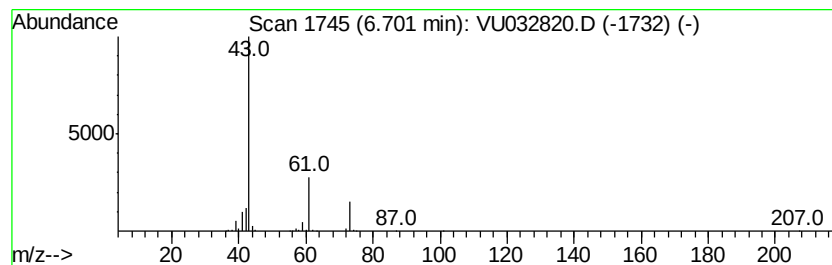
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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	60.11 ug/L	686085	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		Isopropyl acetate	102	C5H10O2	000108-21-4	33



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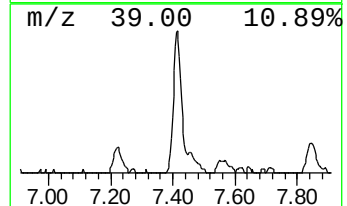
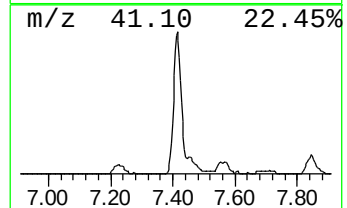
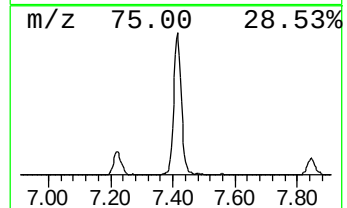
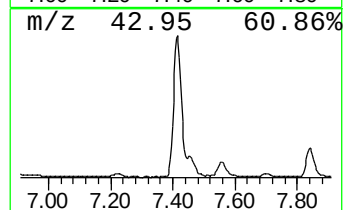
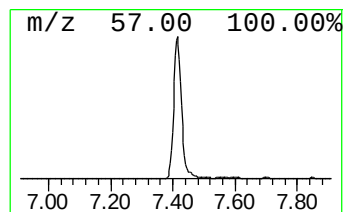
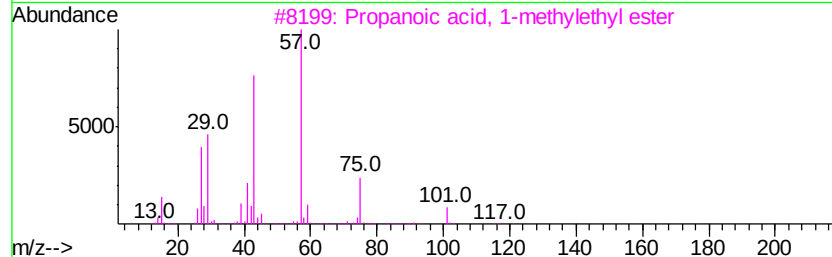
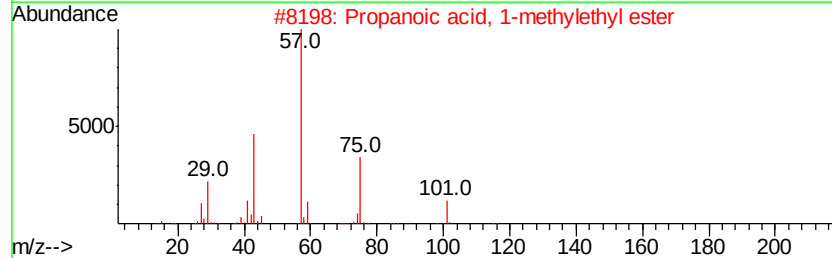
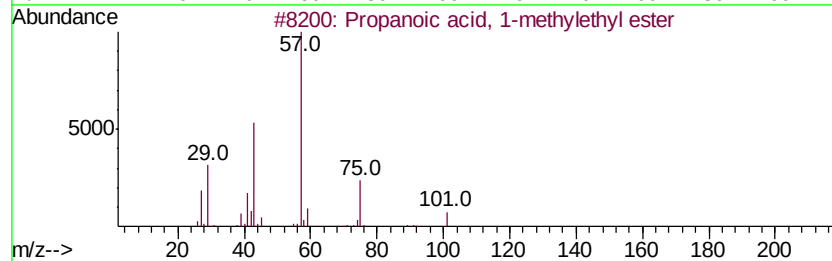
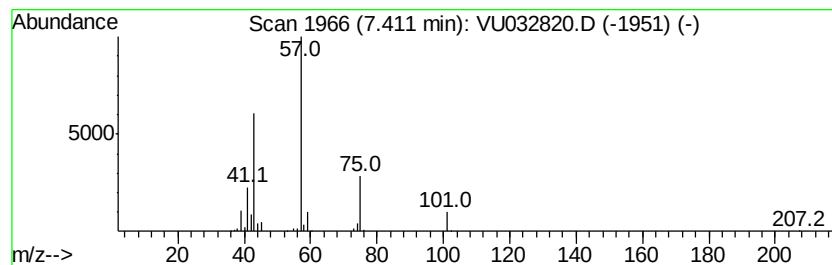
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Quant Title : VOC Analysis

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	15.13 ug/L	172706	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	74
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



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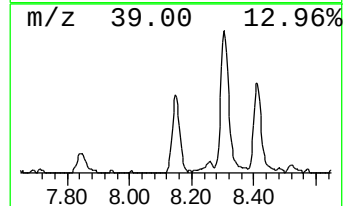
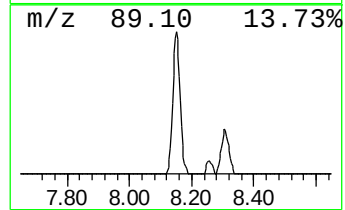
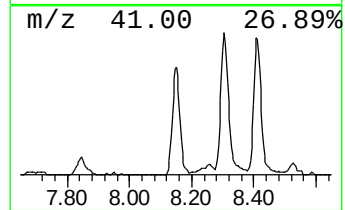
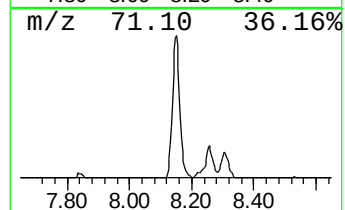
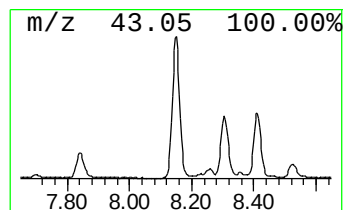
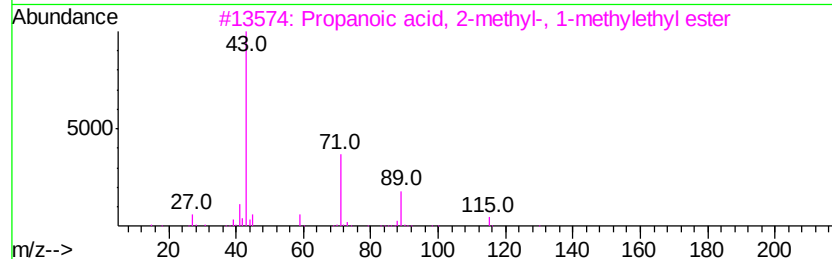
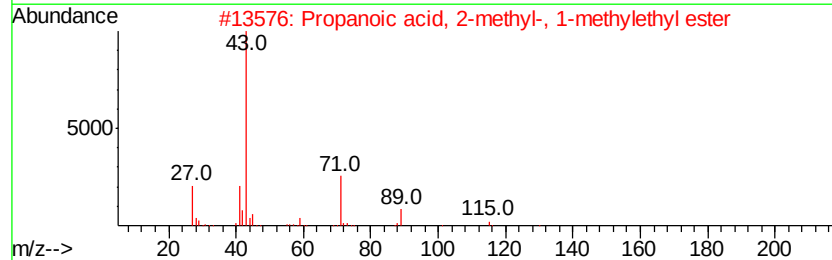
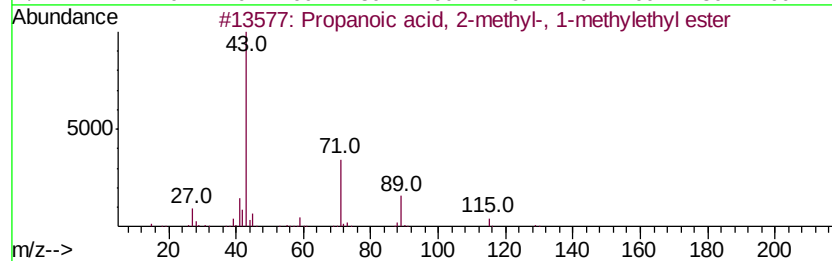
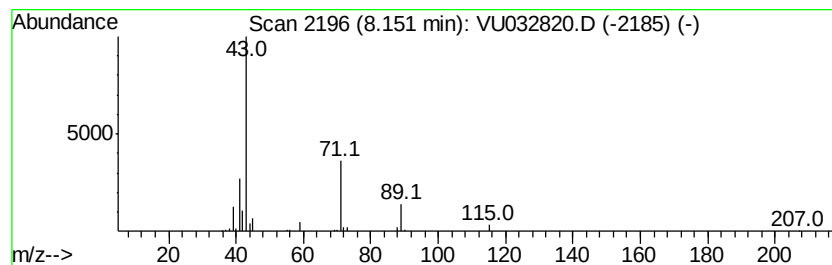
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Quant Title : VOC Analysis

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	6.58 ug/L	95222	Chlorobenzene-d5	9.08

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-, 1-met...	130	C7H14O2	000617-50-5	72
4		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	56



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032820.D
Acq On : 18 Jun 2019 13:37
Operator : JC/SP
Sample : K3363-21
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR2

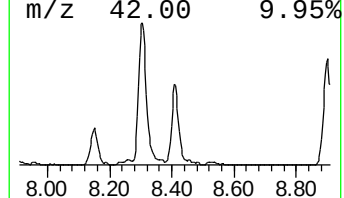
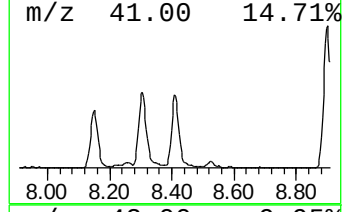
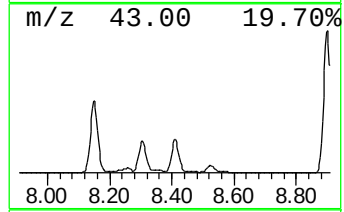
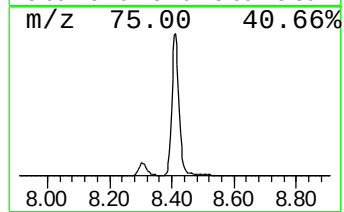
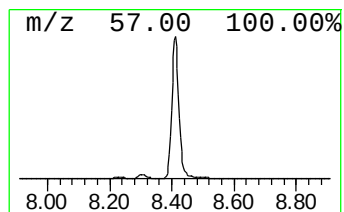
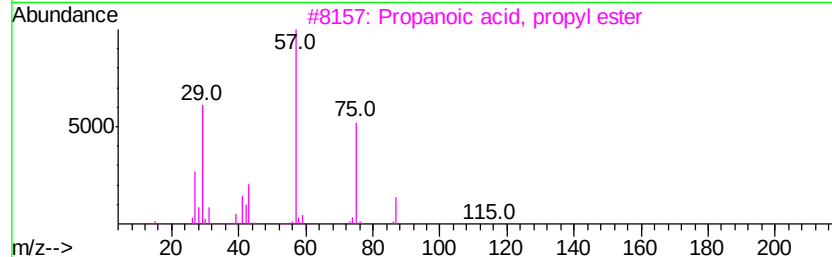
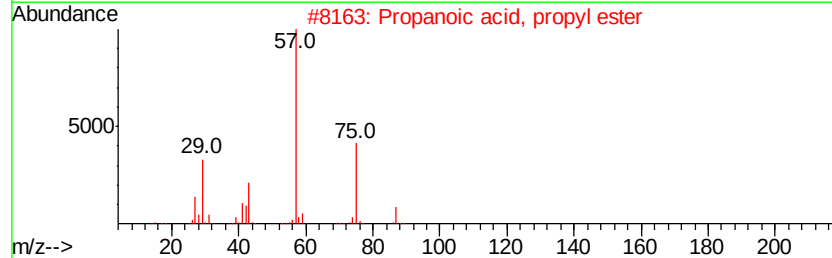
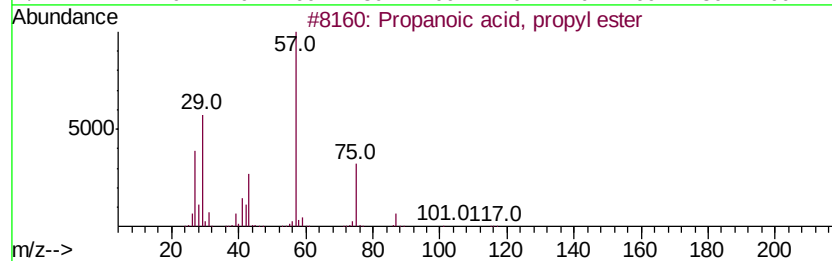
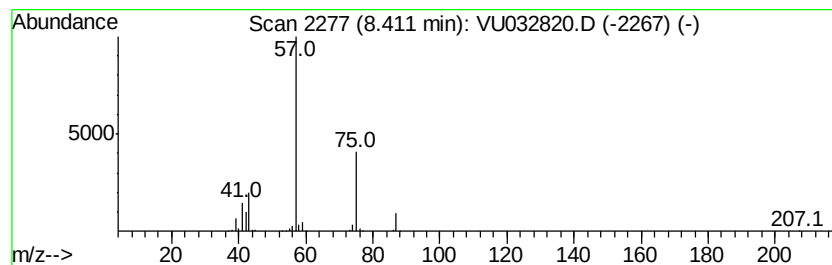
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	13.84 ug/L	200459	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	39



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032820.D
Acq On : 18 Jun 2019 13:37
Operator : JC/SP
Sample : K3363-21
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

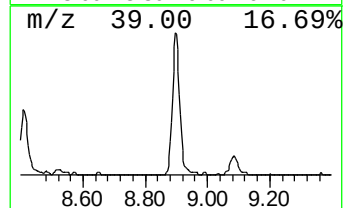
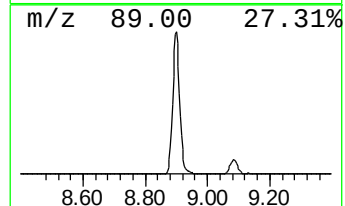
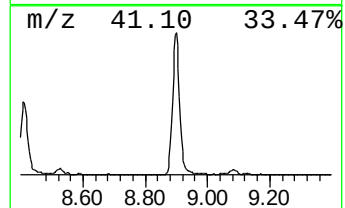
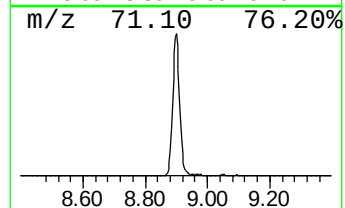
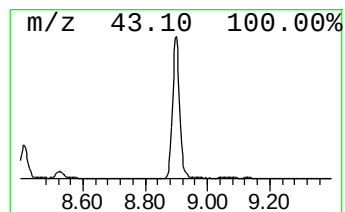
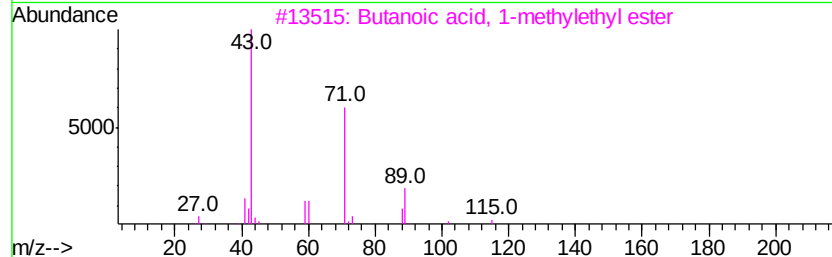
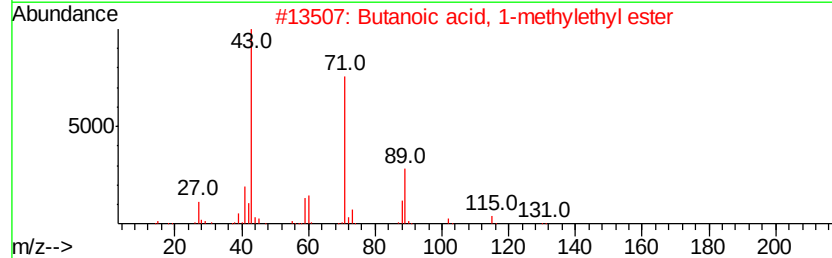
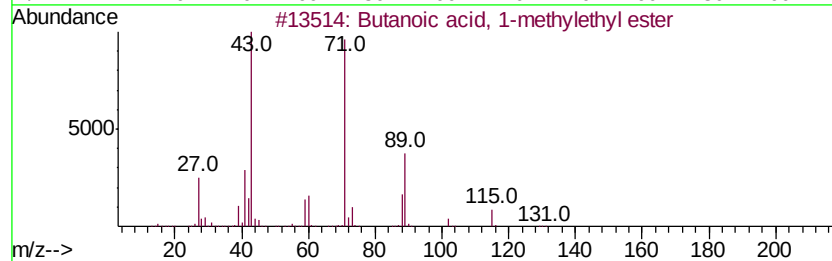
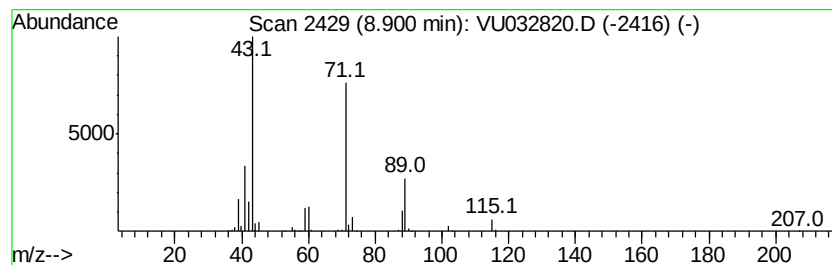
Instrument :
MSVOA_U
ClientSampleId :
C0JR2

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 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.90	18.74 ug/L	271405	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-, pentyl...	158	C9H18O2	002445-72-9	64	
5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	64	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
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Operator : JC/SP
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JR2

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.70	60.1	ug/L	686085	1	5.88	570714	50.0
Propanoic acid, 1...	7.41	15.1	ug/L	172706	1	5.88	570714	50.0
Propanoic acid, 2...	8.15	6.6	ug/L	95222	2	9.08	724060	50.0
Propanoic acid, p...	8.41	13.8	ug/L	200459	2	9.08	724060	50.0
Butanoic acid, 1-...	8.90	18.7	ug/L	271405	2	9.08	724060	50.0