

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\  
 Data File : VU032828.D  
 Acq On : 18 Jun 2019 16:44  
 Operator : JC/SP  
 Sample : K3363-13  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0JP5

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	5035	4372	0.40%	0.044%
2	1.395	87	95	106	rBV	128236	126873	11.53%	1.267%
3	1.675	174	182	200	rVB	96503	120617	10.96%	1.204%
4	2.267	356	366	377	rVB	206743	306014	27.81%	3.055%
5	2.437	415	419	420	rBV4	1737	1160	0.11%	0.012%
6	2.614	467	474	490	rBV3	2419	4780	0.43%	0.048%
7	2.694	490	499	511	rVV2	7560	12436	1.13%	0.124%
8	2.756	515	518	523	rBV4	219	216	0.02%	0.002%
9	2.817	532	537	538	rBV4	470	384	0.03%	0.004%
10	2.894	558	561	564	rBV3	335	273	0.02%	0.003%
11	3.055	605	611	617	rVB	507	685	0.06%	0.007%
12	3.151	636	641	643	rBV2	378	269	0.02%	0.003%
13	3.196	653	655	659	rVB3	378	257	0.02%	0.003%
14	3.228	659	665	666	rBV	228	229	0.02%	0.002%
15	3.270	673	678	681	rBV3	269	284	0.03%	0.003%
16	3.321	690	694	698	rBV3	510	433	0.04%	0.004%
17	3.408	718	721	724	rBV4	301	221	0.02%	0.002%
18	3.543	761	763	767	rVB3	541	362	0.03%	0.004%
19	3.566	767	770	774	rBV3	495	538	0.05%	0.005%
20	3.637	785	792	795	rBV3	1147	1536	0.14%	0.015%
21	3.694	807	810	814	rBV4	569	360	0.03%	0.004%
22	3.826	849	851	856	rVB	325	221	0.02%	0.002%
23	3.907	874	876	882	rVB3	310	270	0.02%	0.003%
24	3.936	882	885	888	rBV2	432	366	0.03%	0.004%
25	4.026	909	913	917	rBV3	314	297	0.03%	0.003%
26	4.071	924	927	931	rBV3	462	405	0.04%	0.004%
27	4.167	945	957	991	rBV	86723	229281	20.84%	2.289%
28	4.382	1021	1024	1027	rVB3	490	321	0.03%	0.003%
29	4.411	1027	1033	1035	rBV3	340	356	0.03%	0.004%
30	4.456	1043	1047	1050	rBV3	527	519	0.05%	0.005%
31	4.527	1067	1069	1073	rVB2	402	281	0.03%	0.003%
32	4.640	1087	1104	1124	rBV	154920	362982	32.99%	3.624%
33	4.878	1175	1178	1185	rVV3	460	583	0.05%	0.006%
34	4.916	1187	1190	1195	rVB2	372	216	0.02%	0.002%

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Integrator: RTE  
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
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Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM061719WMA.M  
 Title : VOC Analysis

35	4.971	1203	1207	1210	rBV2	399	304	0.03%	0.003%
36	5.048	1229	1231	1234	rVV2	350	246	0.02%	0.002%
37	5.090	1242	1244	1249	rVB2	342	244	0.02%	0.002%
38	5.141	1258	1260	1265	rVB2	374	274	0.02%	0.003%
39	5.170	1265	1269	1272	rBV4	327	249	0.02%	0.002%
40	5.193	1272	1276	1279	rBV2	270	249	0.02%	0.002%
41	5.331	1295	1319	1347	rBV2	314110	920886	83.68%	9.194%
42	5.456	1355	1358	1362	rBV3	528	316	0.03%	0.003%
43	5.550	1378	1387	1400	rVB3	4879	9984	0.91%	0.100%
44	5.881	1476	1490	1516	rBV	286654	564073	51.26%	5.632%
45	6.045	1537	1541	1545	rVB5	395	351	0.03%	0.004%
46	6.132	1562	1568	1571	rBV3	598	536	0.05%	0.005%
47	6.161	1574	1577	1578	rBV2	366	216	0.02%	0.002%
48	6.222	1593	1596	1598	rVV3	444	309	0.03%	0.003%
49	6.325	1613	1628	1648	rVV	210761	418398	38.02%	4.177%
50	6.421	1651	1658	1668	rBV3	5204	9506	0.86%	0.095%
51	6.534	1685	1693	1699	rBV3	2504	4459	0.41%	0.045%
52	6.575	1699	1706	1715	rBV	4951	9071	0.82%	0.091%
53	6.697	1732	1744	1771	rBV	617493	1100443	100.00%	10.987%
54	6.923	1812	1814	1815	rBV2	514	240	0.02%	0.002%
55	7.003	1836	1839	1841	rBV2	324	252	0.02%	0.003%
56	7.029	1845	1847	1853	rVB2	325	281	0.03%	0.003%
57	7.222	1895	1907	1924	rBV	107576	191563	17.41%	1.913%
58	7.299	1929	1931	1936	rVB3	677	601	0.05%	0.006%
59	7.415	1955	1967	1980	rBV	131403	220364	20.03%	2.200%
60	7.559	1999	2012	2029	rBV	433359	755006	68.61%	7.538%
61	7.768	2073	2077	2085	rVB6	1034	1370	0.12%	0.014%
62	7.800	2085	2087	2090	rBV3	424	323	0.03%	0.003%
63	7.842	2090	2100	2123	rVV3	82392	146727	13.33%	1.465%
64	8.064	2167	2169	2173	rVB2	431	280	0.03%	0.003%
65	8.103	2175	2181	2183	rBV2	365	299	0.03%	0.003%
66	8.151	2183	2196	2208	rBV	70424	117155	10.65%	1.170%
67	8.228	2212	2220	2222	rBV3	6939	8777	0.80%	0.088%
68	8.257	2224	2229	2235	rVV2	18268	26531	2.41%	0.265%
69	8.305	2235	2244	2265	rVV	295408	499869	45.42%	4.991%
70	8.411	2266	2277	2295	rVB	408150	635978	57.79%	6.350%
71	8.521	2304	2311	2325	rVB2	17284	28878	2.62%	0.288%

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 Title : VOC Analysis

72	8.720	2370	2373	2376	rBV	248	227	0.02%	0.002%
73	8.900	2414	2429	2450	rBV	296960	470046	42.71%	4.693%
74	9.029	2466	2469	2470	rBV	475	300	0.03%	0.003%
75	9.083	2470	2486	2508	rVV	438348	728094	66.16%	7.270%
76	9.241	2531	2535	2539	rBV3	486	450	0.04%	0.004%
77	9.373	2572	2576	2582	rBV3	789	701	0.06%	0.007%
78	9.604	2638	2648	2662	rBV	5089	9276	0.84%	0.093%
79	9.765	2684	2698	2714	rBV	8790	14640	1.33%	0.146%
80	10.109	2801	2805	2807	rBV3	317	277	0.03%	0.003%
81	10.221	2833	2840	2844	rBV3	327	416	0.04%	0.004%
82	10.273	2852	2856	2862	rVB3	251	218	0.02%	0.002%
83	10.334	2872	2875	2878	rBV3	406	343	0.03%	0.003%
84	10.424	2890	2903	2923	rBV	297403	484420	44.02%	4.837%
85	10.594	2953	2956	2959	rBV2	350	219	0.02%	0.002%
86	10.839	3029	3032	3037	rVB2	319	268	0.02%	0.003%
87	10.922	3055	3058	3063	rVB2	391	355	0.03%	0.004%
88	10.951	3063	3067	3072	rBV2	443	478	0.04%	0.005%
89	11.395	3200	3205	3207	rBV2	328	334	0.03%	0.003%
90	11.479	3218	3231	3249	rBV	457498	725646	65.94%	7.245%
91	11.784	3324	3326	3332	rVB2	543	357	0.03%	0.004%
92	11.855	3334	3348	3370	rBV	437199	722474	65.65%	7.213%
93	12.218	3454	3461	3465	rBV4	338	422	0.04%	0.004%
94	12.308	3485	3489	3492	rBV2	508	461	0.04%	0.005%
95	13.102	3733	3736	3739	rBV2	356	285	0.03%	0.003%
96	13.295	3792	3796	3801	rBV3	432	391	0.04%	0.004%
97	13.321	3802	3804	3807	rVV3	508	304	0.03%	0.003%
98	13.874	3972	3976	3979	rBV3	668	635	0.06%	0.006%
99	13.999	4013	4015	4018	rBV2	375	270	0.02%	0.003%
100	14.430	4146	4149	4152	rBV3	494	365	0.03%	0.004%

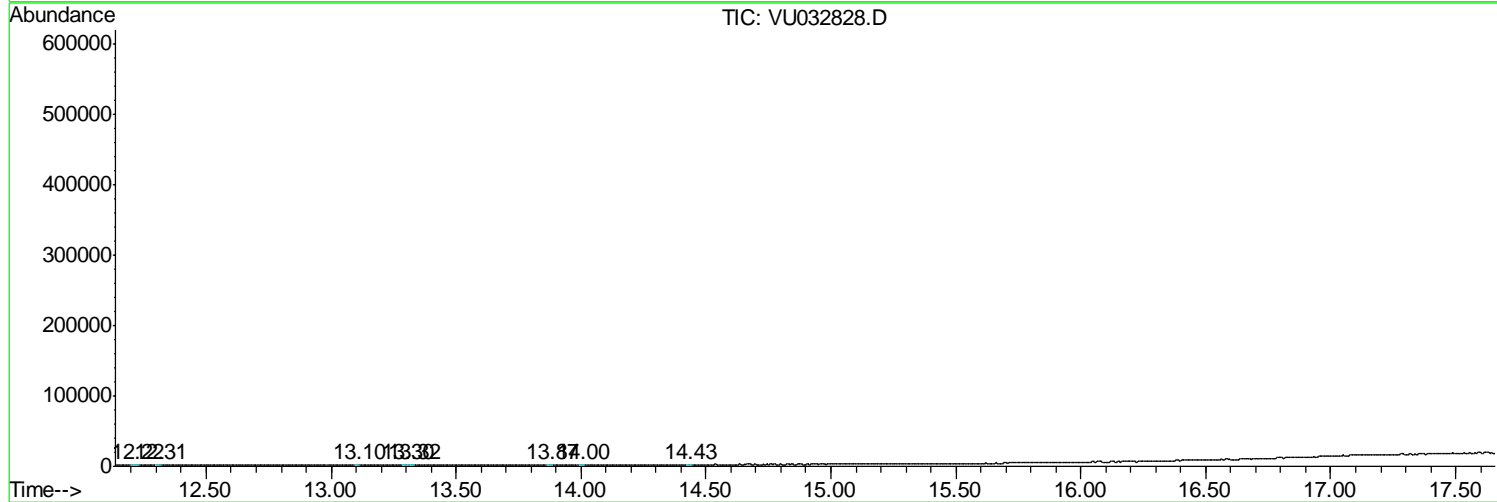
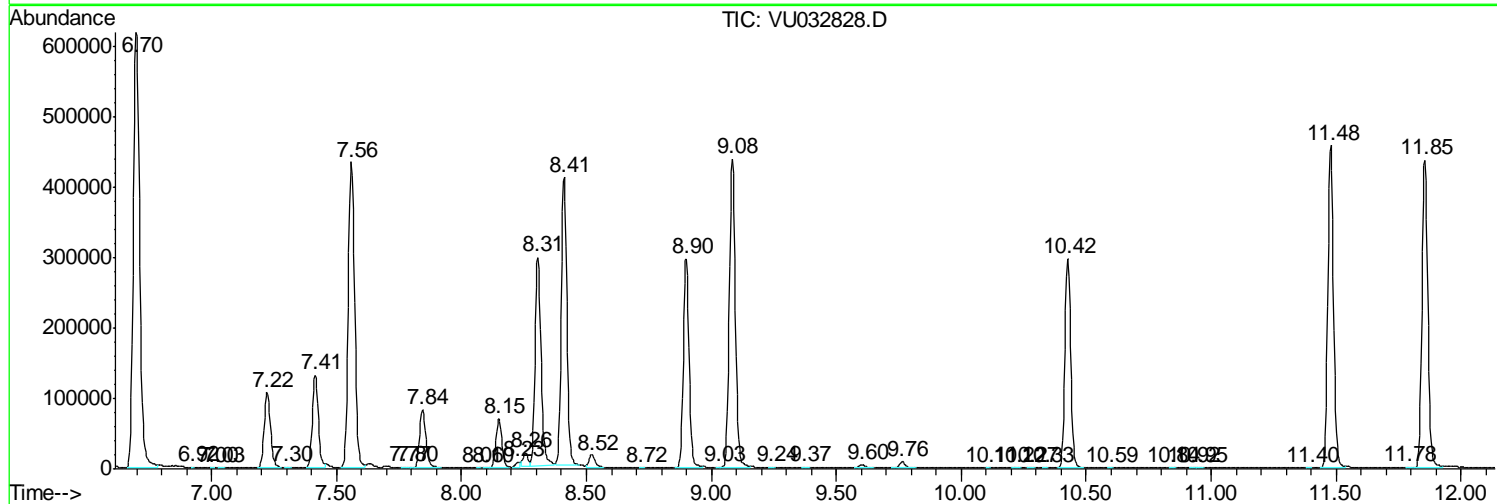
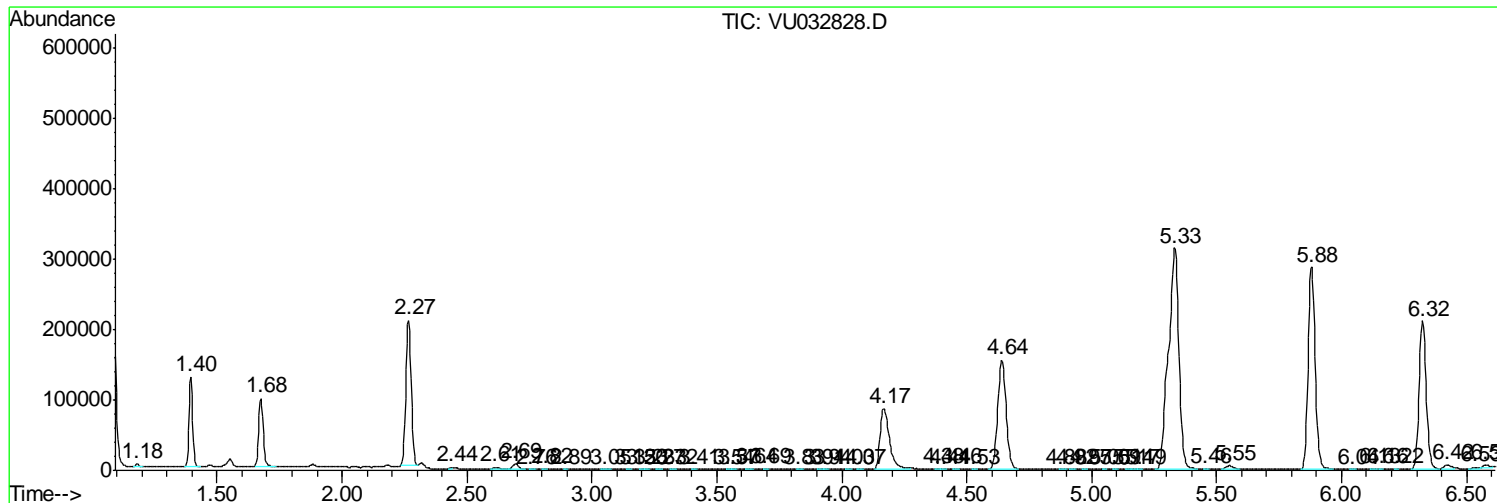
Sum of corrected areas: 10015677

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 ALS Vial : 22 Sample Multiplier: 1

**Instrument :**  
 MSVOA\_U  
**Client Sampled :**  
 C0JP5

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\  
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 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
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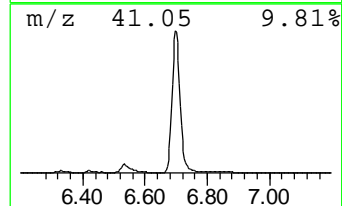
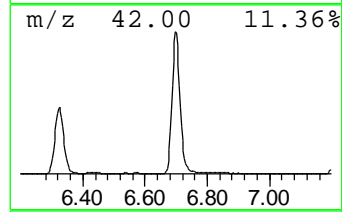
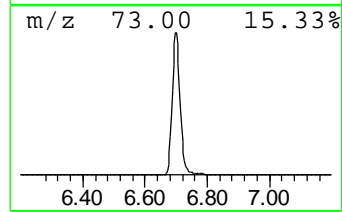
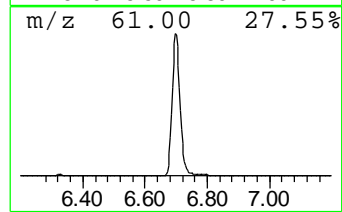
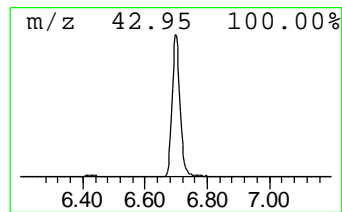
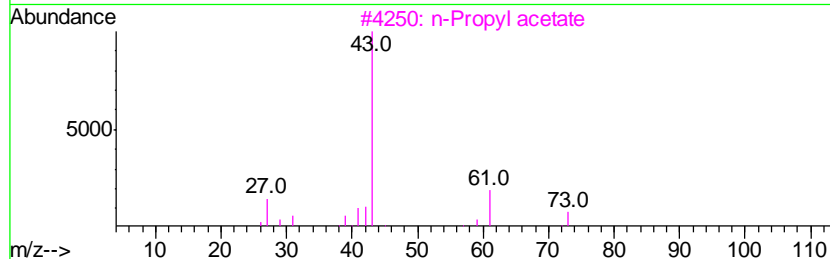
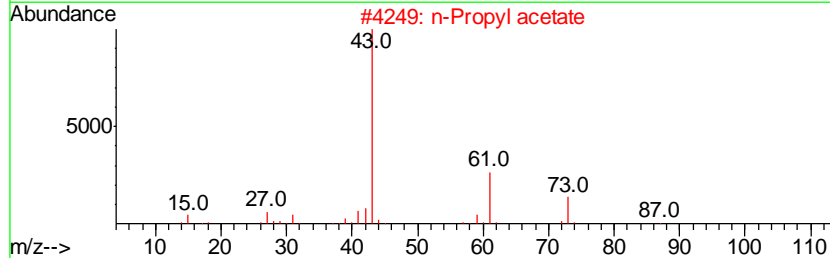
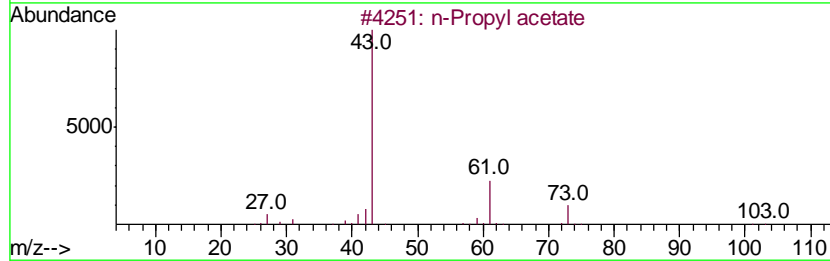
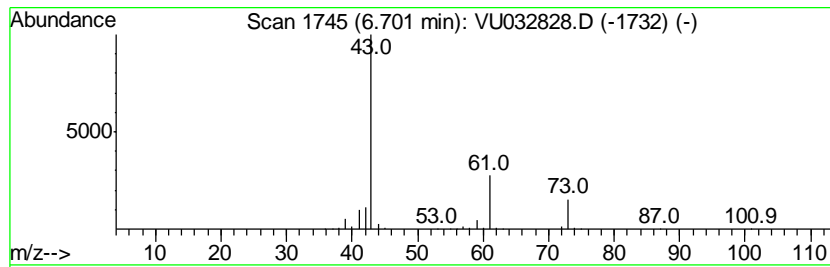
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM061719WMA.M  
 Quant Title : VOC Analysis

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

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 Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	97.54 ug/L	1100440	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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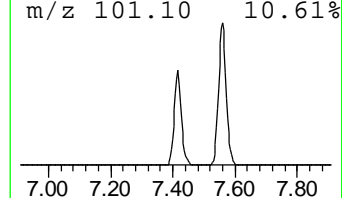
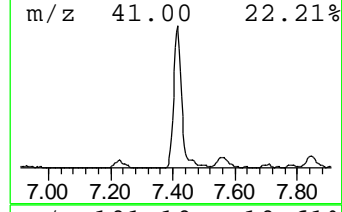
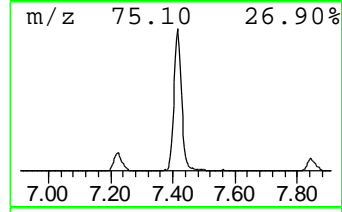
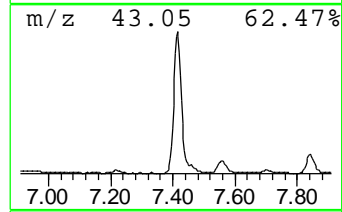
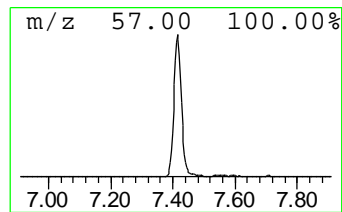
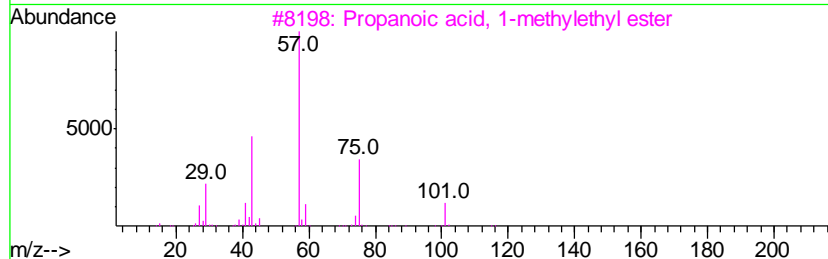
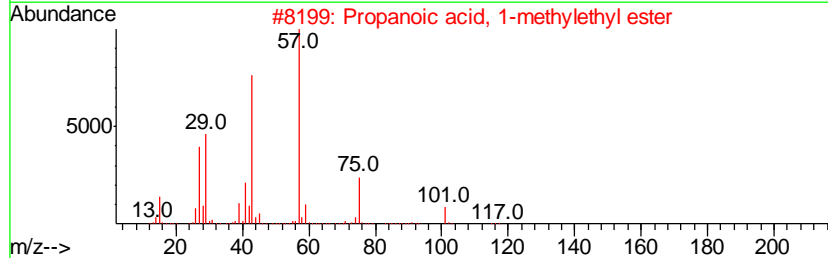
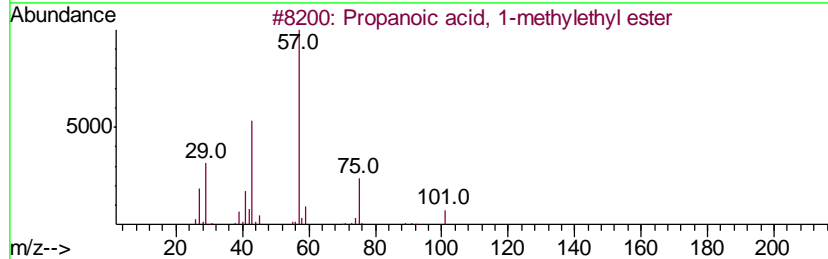
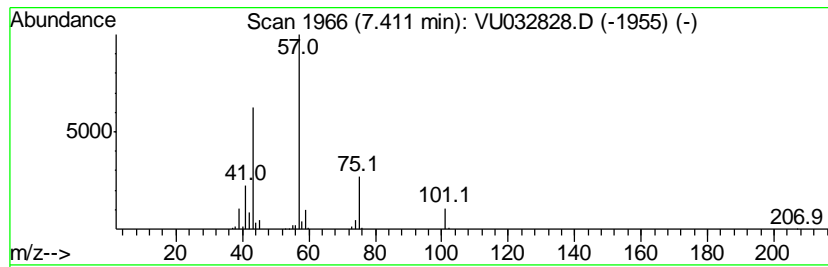
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 Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	19.53 ug/L	220364	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	74
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42
5		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	42



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

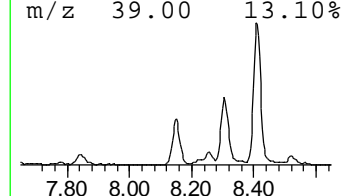
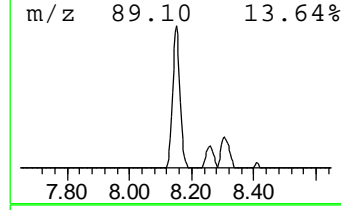
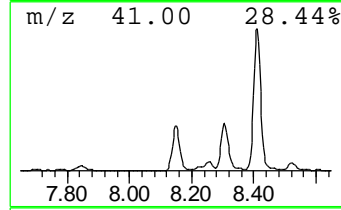
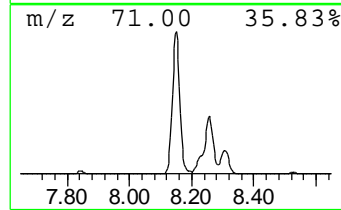
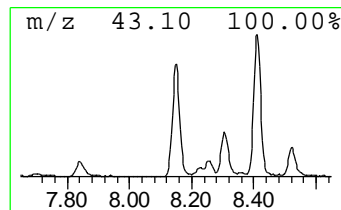
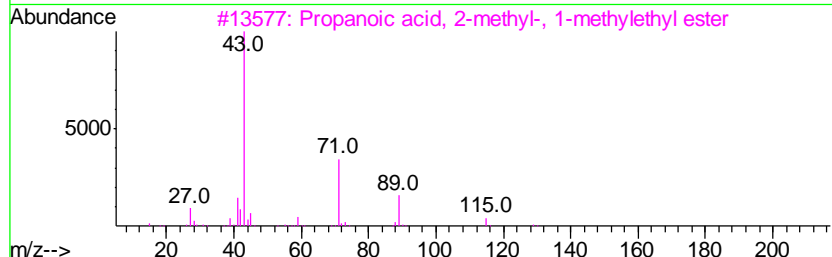
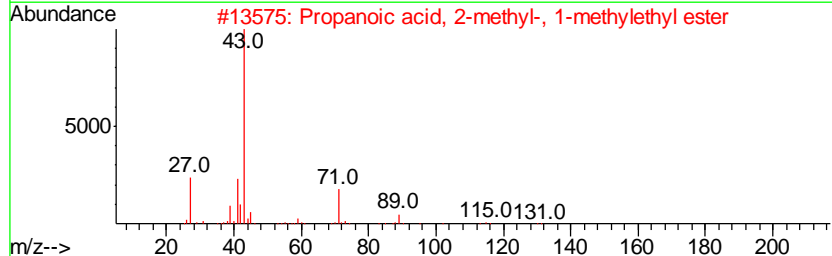
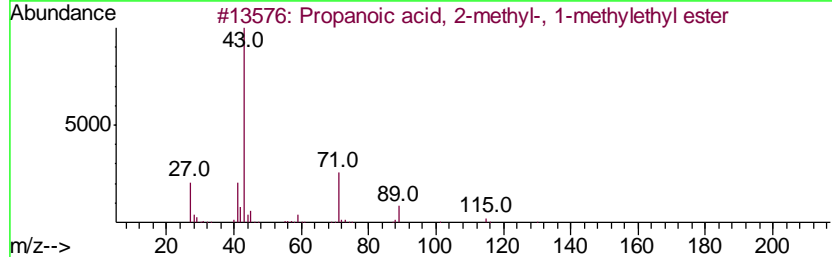
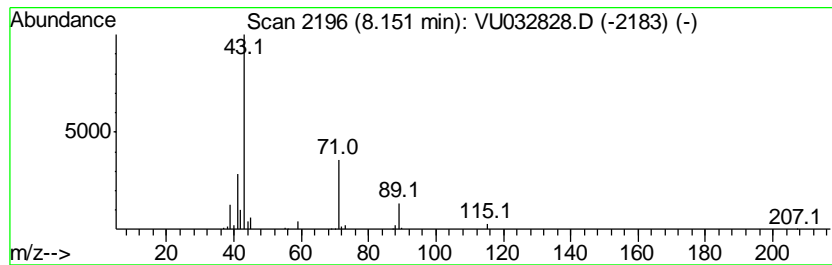
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 TIC Integration Parameters: LSCINT.P

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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	8.05 ug/L	117155	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	83
4		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\  
 Data File : VU032828.D  
 Acq On : 18 Jun 2019 16:44  
 Operator : JC/SP  
 Sample : K3363-13  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampled :  
 C0JP5

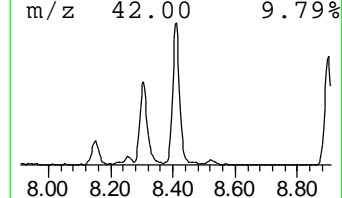
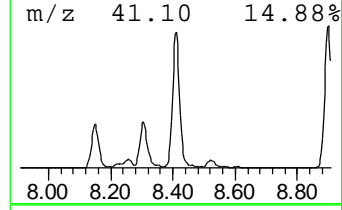
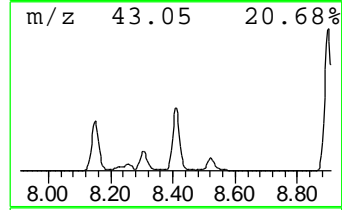
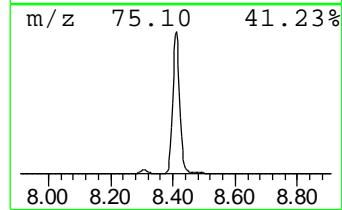
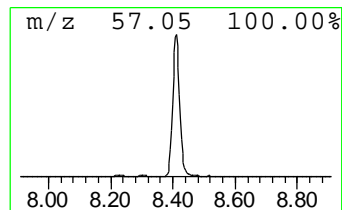
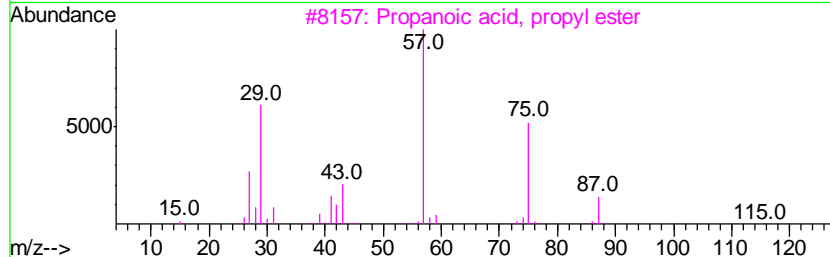
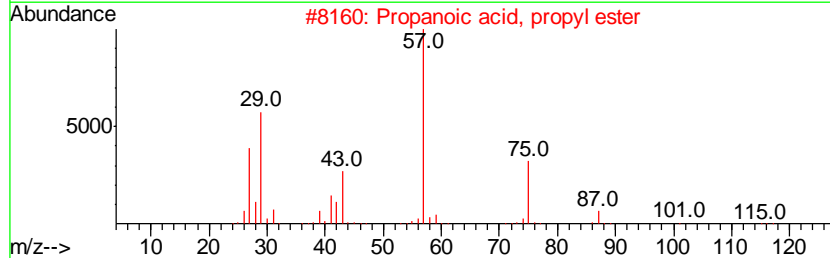
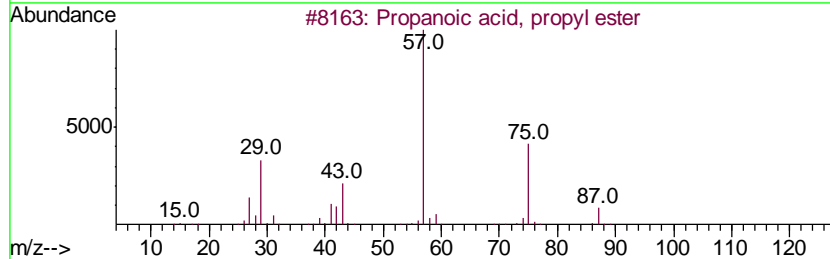
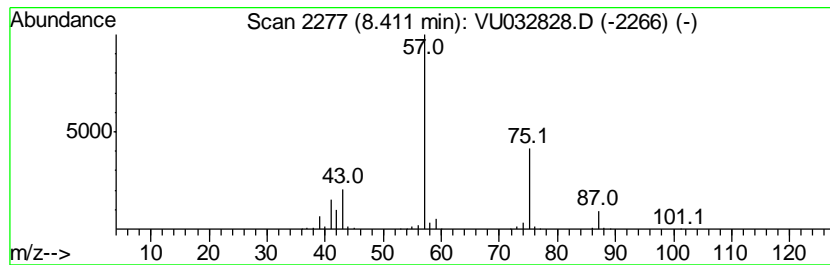
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 Quant Title : VOC Analysis

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

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 Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	43.67 ug/L	635978	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	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\  
 Data File : VU032828.D  
 Acq On : 18 Jun 2019 16:44  
 Operator : JC/SP  
 Sample : K3363-13  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampled :  
 C0JP5

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

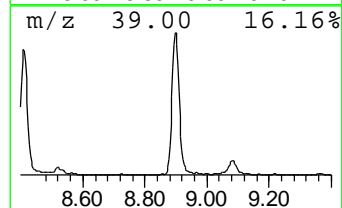
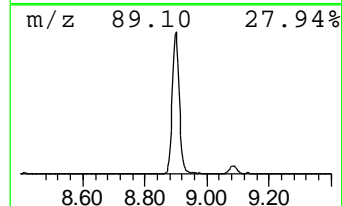
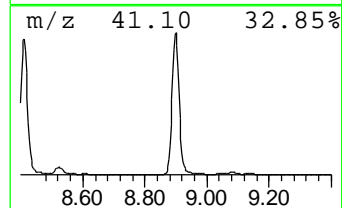
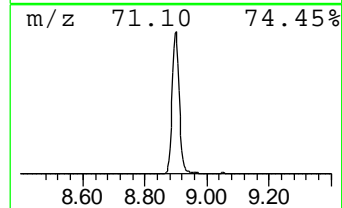
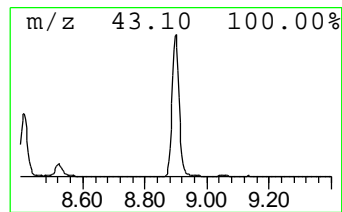
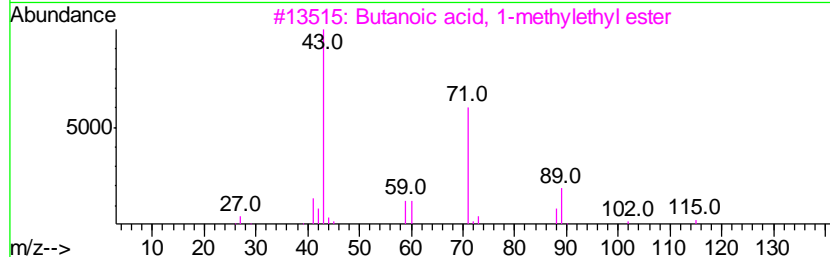
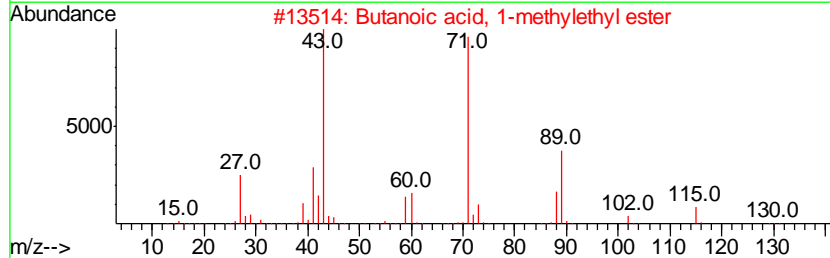
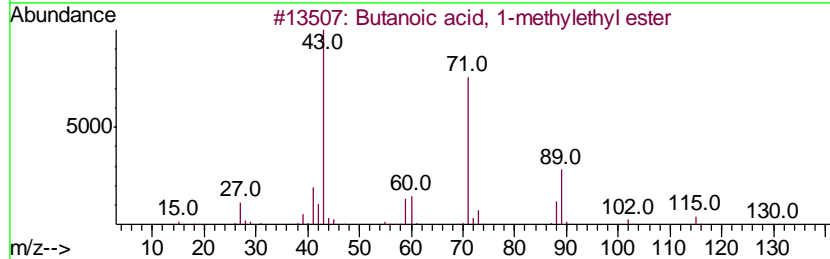
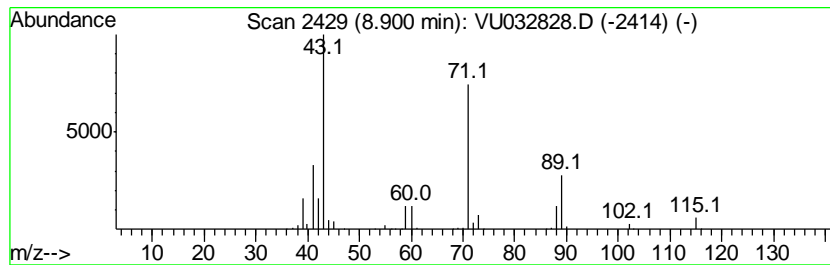
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	32.28 ug/L	470046	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-, propy...	130	C7H14O2	000644-49-5	64
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_U\DATA\VU061819\  
Data File : VU032828.D  
Acq On : 18 Jun 2019 16:44  
Operator : JC/SP  
Sample : K3363-13  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 22 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
C0JP5

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	97.5	ug/L	1100440	1	5.88	564073	50.0
Propanoic acid, 1...	7.41	19.5	ug/L	220364	1	5.88	564073	50.0
Propanoic acid, 2...	8.15	8.1	ug/L	117155	2	9.08	728094	50.0
Propanoic acid, p...	8.41	43.7	ug/L	635978	2	9.08	728094	50.0
Butanoic acid, 1-...	8.90	32.3	ug/L	470046	2	9.08	728094	50.0