

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU052718\
 Data File : VU024212.D
 Acq On : 28 May 2018 01:32
 Operator : MD/SY
 Sample : J3091-19
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 33 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM052518WMA.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	0.709	33	37	42	rVV2	153	194	0.00%	0.001%
2	0.796	60	64	70	rVB	199	205	0.00%	0.001%
3	1.089	148	155	171	rBV	155945	182809	3.33%	1.295%
4	1.182	179	184	190	rBV3	6243	6082	0.11%	0.043%
5	1.294	214	219	227	rVB	8279	8488	0.15%	0.060%
6	1.400	245	252	265	rBV	149963	160027	2.91%	1.133%
7	1.671	328	336	354	rVB	114779	151669	2.76%	1.074%
8	1.883	395	402	412	rVB	15257	20445	0.37%	0.145%
9	2.272	512	523	532	rBV	245538	372531	6.78%	2.638%
10	2.323	533	539	556	rVB	36310	59883	1.09%	0.424%
11	2.449	565	578	591	rBV	21098	44427	0.81%	0.315%
12	2.609	624	628	634	rVV4	512	666	0.01%	0.005%
13	2.635	634	636	639	rVB	352	188	0.00%	0.001%
14	2.670	644	647	652	rVB2	382	255	0.00%	0.002%
15	2.703	652	657	658	rBV3	527	422	0.01%	0.003%
16	2.838	687	699	717	rBV	8989	18878	0.34%	0.134%
17	2.982	740	744	747	rBV2	316	279	0.01%	0.002%
18	3.124	783	788	791	rVB	186	212	0.00%	0.002%
19	3.178	800	805	806	rBV2	733	525	0.01%	0.004%
20	3.249	823	827	832	rBV2	205	200	0.00%	0.001%
21	3.381	863	868	872	rVB3	405	445	0.01%	0.003%
22	3.519	908	911	914	rVB2	205	167	0.00%	0.001%
23	3.545	914	919	922	rBV	272	222	0.00%	0.002%
24	3.613	936	940	943	rBV	200	188	0.00%	0.001%
25	3.690	960	964	966	rBV2	173	173	0.00%	0.001%
26	3.780	989	992	997	rVB2	188	210	0.00%	0.001%
27	3.995	1052	1059	1063	rVB2	207	286	0.01%	0.002%
28	4.043	1070	1074	1078	rBV	177	187	0.00%	0.001%
29	4.178	1097	1116	1161	rBV	94719	286222	5.21%	2.027%
30	4.384	1168	1180	1210	rVB	27345	67032	1.22%	0.475%
31	4.519	1219	1222	1226	rVB2	268	174	0.00%	0.001%
32	4.651	1246	1263	1286	rBV	181061	425778	7.75%	3.015%
33	4.879	1329	1334	1336	rBV2	323	294	0.01%	0.002%
34	4.921	1343	1347	1351	rVV2	222	149	0.00%	0.001%

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 Title : VOC Analysis

35	4.992	1365	1369	1375	rVB2	394	363	0.01%	0.003%
36	5.034	1378	1382	1389	rVB2	249	231	0.00%	0.002%
37	5.146	1415	1417	1422	rVB2	354	272	0.00%	0.002%
38	5.204	1431	1435	1439	rBV2	190	163	0.00%	0.001%
39	5.342	1454	1478	1525	rBV2	360766	1100332	20.03%	7.792%
40	5.667	1576	1579	1582	rVV3	234	187	0.00%	0.001%
41	5.805	1616	1622	1625	rBV3	279	356	0.01%	0.003%
42	5.889	1633	1648	1689	rBV	346190	710835	12.94%	5.034%
43	6.188	1725	1741	1774	rBV	2805443	5494198	100.00%	38.909%
44	6.333	1776	1786	1821	rVB	253135	529410	9.64%	3.749%
45	6.574	1859	1861	1866	rVB3	260	169	0.00%	0.001%
46	6.600	1866	1869	1876	rVB	381	414	0.01%	0.003%
47	6.712	1901	1904	1908	rVB2	258	195	0.00%	0.001%
48	6.767	1915	1921	1923	rBV	208	203	0.00%	0.001%
49	6.783	1923	1926	1929	rBV2	261	240	0.00%	0.002%
50	6.828	1933	1940	1950	rVB5	1320	2364	0.04%	0.017%
51	6.886	1956	1958	1961	rVB2	272	148	0.00%	0.001%
52	6.992	1989	1991	1998	rVB2	206	189	0.00%	0.001%
53	7.230	2051	2065	2083	rBV	116962	212177	3.86%	1.503%
54	7.397	2110	2117	2123	rVV4	2106	2826	0.05%	0.020%
55	7.442	2129	2131	2134	rVB3	253	161	0.00%	0.001%
56	7.461	2134	2137	2141	rBV3	497	499	0.01%	0.004%
57	7.522	2152	2156	2157	rBV2	371	216	0.00%	0.002%
58	7.567	2157	2170	2205	rVV	451662	830256	15.11%	5.880%
59	7.770	2230	2233	2241	rVB4	693	895	0.02%	0.006%
60	7.854	2247	2259	2282	rBV	79819	137529	2.50%	0.974%
61	7.982	2296	2299	2304	rVB3	495	476	0.01%	0.003%
62	8.008	2304	2307	2312	rBV3	328	273	0.00%	0.002%
63	8.030	2312	2314	2318	rBV	340	178	0.00%	0.001%
64	8.185	2349	2362	2367	rBV4	2785	4810	0.09%	0.034%
65	8.233	2367	2377	2391	rVB	26446	45909	0.84%	0.325%
66	8.313	2391	2402	2439	rBV	298945	532273	9.69%	3.769%
67	8.487	2454	2456	2460	rVB2	560	295	0.01%	0.002%
68	8.651	2500	2507	2509	rBV	297	296	0.01%	0.002%
69	8.722	2526	2529	2533	rVB2	191	175	0.00%	0.001%
70	8.850	2565	2569	2576	rBV2	500	583	0.01%	0.004%
71	9.095	2632	2645	2690	rBV	491087	846470	15.41%	5.995%

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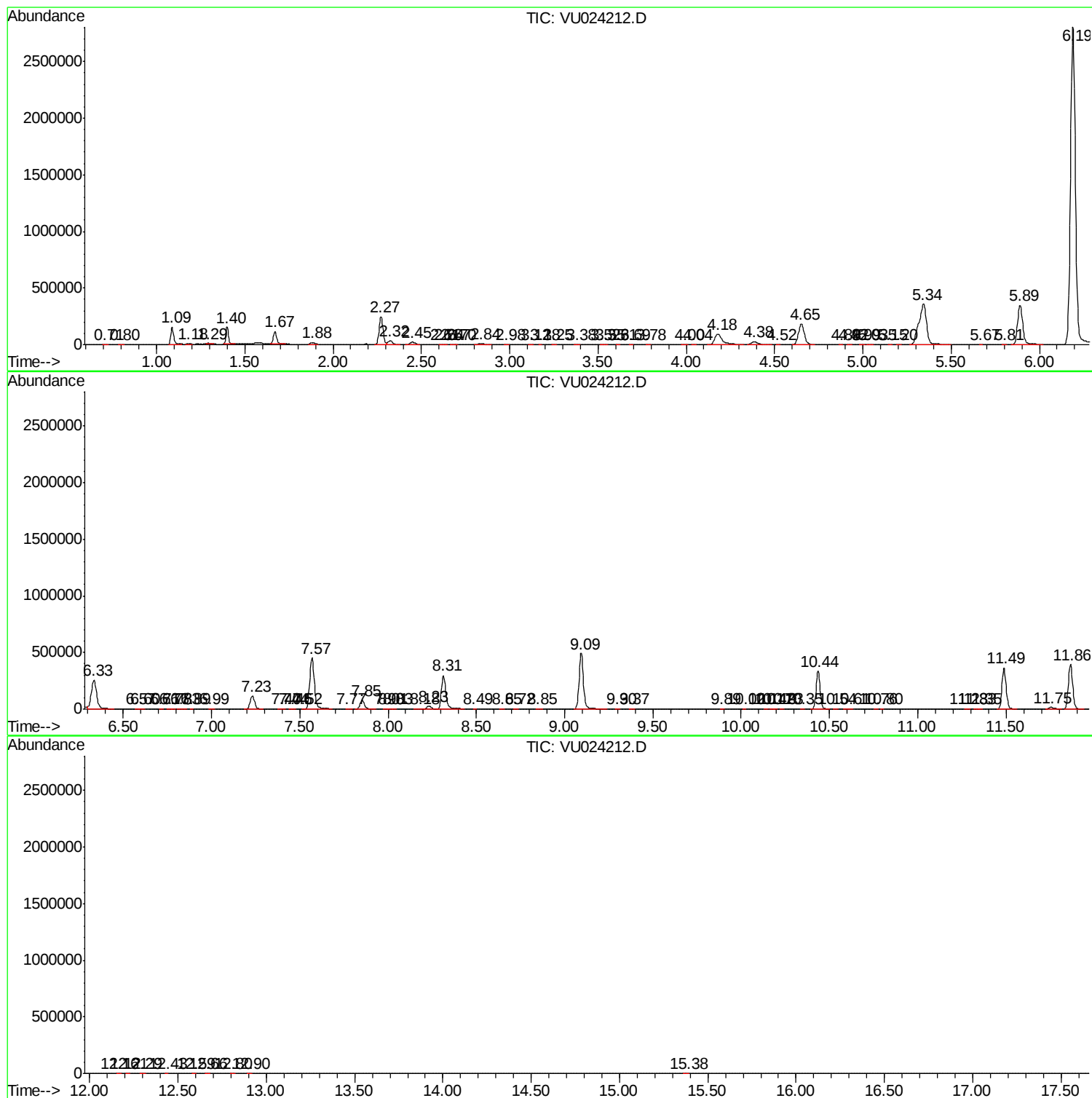
72	9.300	2704	2709	2712	rBV3	294	276	0.01%	0.002%
73	9.371	2728	2731	2738	rBV2	425	510	0.01%	0.004%
74	9.889	2889	2892	2897	rBV	235	252	0.00%	0.002%
75	10.017	2929	2932	2934	rBV	238	180	0.00%	0.001%
76	10.140	2967	2970	2974	rVB2	279	208	0.00%	0.001%
77	10.175	2977	2981	2984	rVB2	278	220	0.00%	0.002%
78	10.194	2984	2987	2989	rBV	336	231	0.00%	0.002%
79	10.233	2995	2999	3002	rBV	455	403	0.01%	0.003%
80	10.345	3031	3034	3038	rVB	348	251	0.00%	0.002%
81	10.435	3049	3062	3081	rBV	333448	540889	9.84%	3.830%
82	10.535	3089	3093	3096	rBV2	478	416	0.01%	0.003%
83	10.612	3107	3117	3123	rBV2	3199	5005	0.09%	0.035%
84	10.763	3160	3164	3167	rBV2	204	214	0.00%	0.002%
85	10.799	3172	3175	3177	rBV2	265	197	0.00%	0.001%
86	11.278	3320	3324	3330	rBV2	269	383	0.01%	0.003%
87	11.326	3336	3339	3345	rBV2	586	522	0.01%	0.004%
88	11.355	3345	3348	3351	rBV2	248	179	0.00%	0.001%
89	11.487	3377	3389	3412	rBV	363807	601743	10.95%	4.261%
90	11.754	3462	3472	3491	rBV3	15013	33123	0.60%	0.235%
91	11.863	3495	3506	3530	rVB	393136	665496	12.11%	4.713%
92	12.159	3596	3598	3604	rVB2	329	266	0.00%	0.002%
93	12.213	3612	3615	3618	rBV2	386	247	0.00%	0.002%
94	12.291	3637	3639	3647	rVB3	367	378	0.01%	0.003%
95	12.432	3680	3683	3685	rBV	205	166	0.00%	0.001%
96	12.590	3729	3732	3735	rBV	292	194	0.00%	0.001%
97	12.660	3752	3754	3759	rVV2	245	192	0.00%	0.001%
98	12.802	3795	3798	3804	rBV2	323	355	0.01%	0.003%
99	12.902	3825	3829	3834	rVB	999	784	0.01%	0.006%
100	15.381	4593	4600	4603	rBV2	621	892	0.02%	0.006%

Sum of corrected areas: 14120650

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Quant Title : VOC Analysis

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



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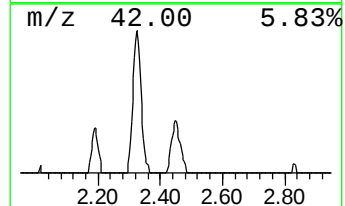
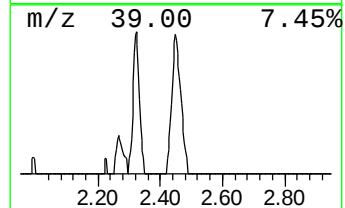
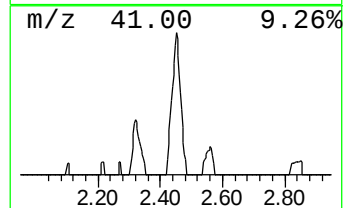
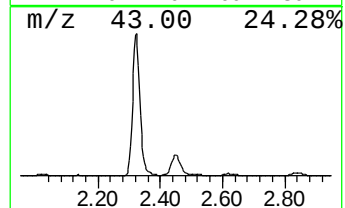
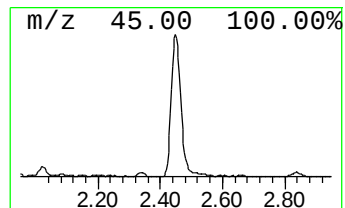
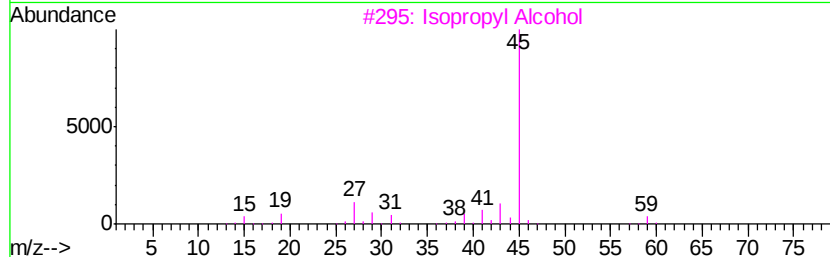
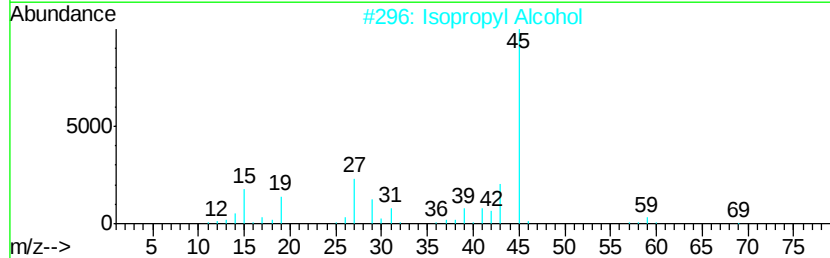
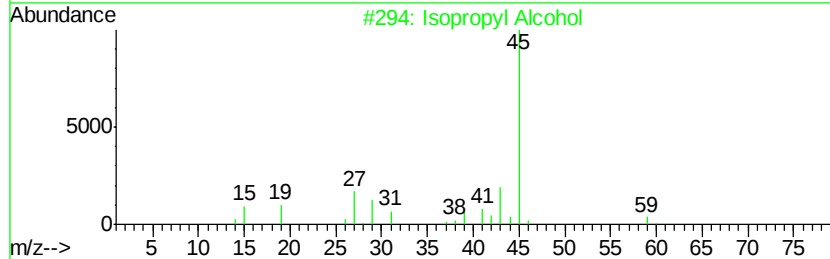
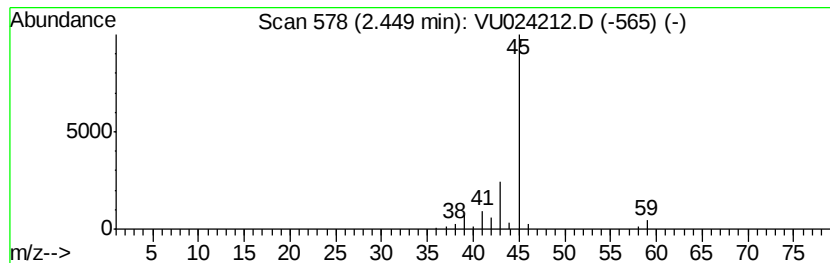
Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM052518WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	3.12 ug/L	44427	1,4-Difluorobenzene	5.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	43
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4



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ALS Vial : 33 Sample Multiplier: 1

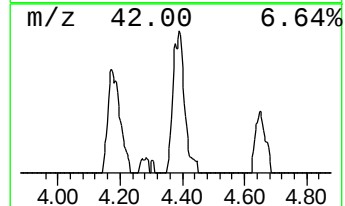
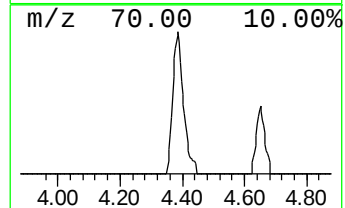
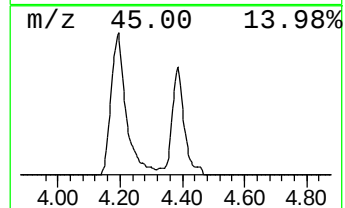
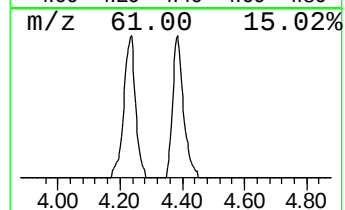
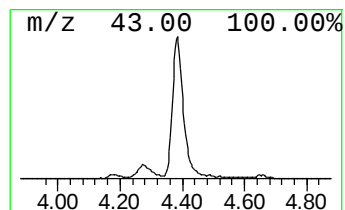
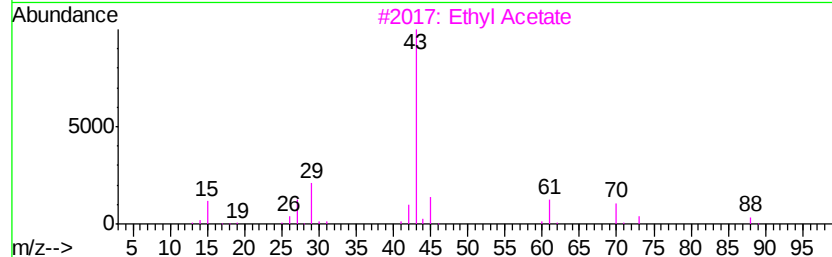
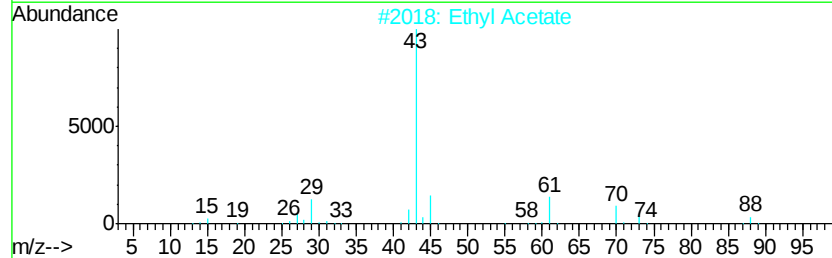
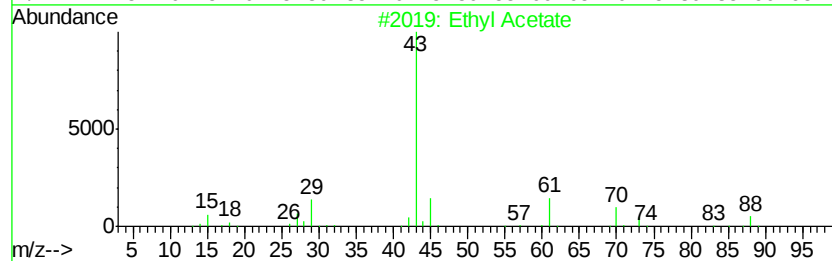
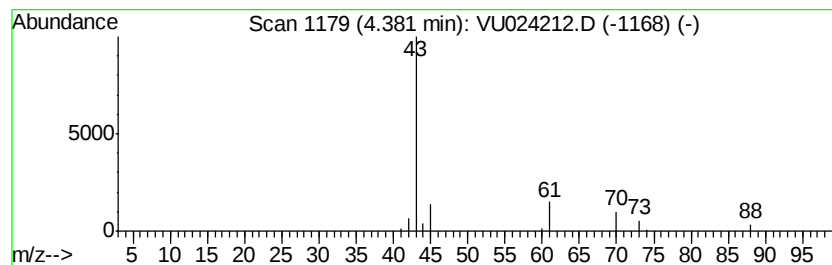
Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM052518WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Ethyl Acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	4.72 ug/L	67032	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2		Ethyl Acetate	88	C4H8O2	000141-78-6	90
3		Ethyl Acetate	88	C4H8O2	000141-78-6	90
4		Ethyl Acetate	88	C4H8O2	000141-78-6	83
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	9



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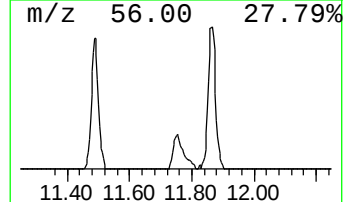
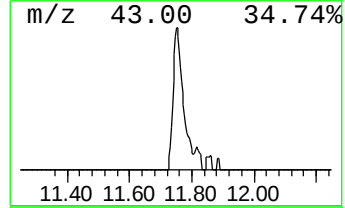
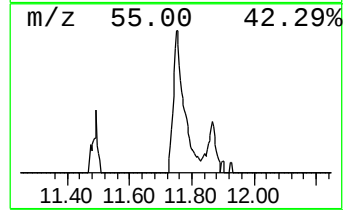
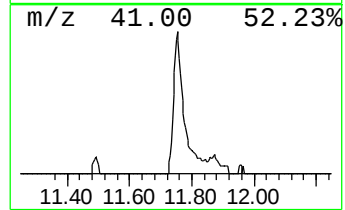
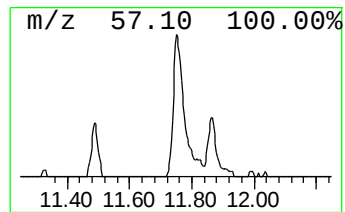
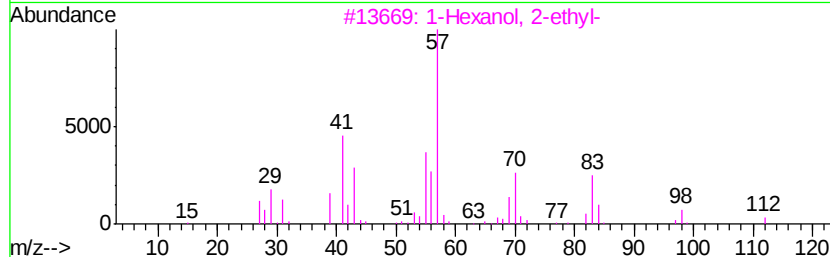
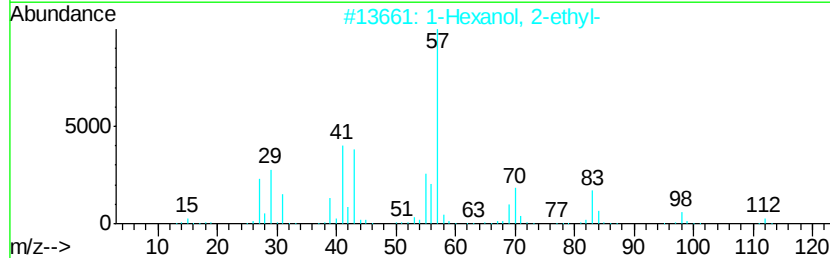
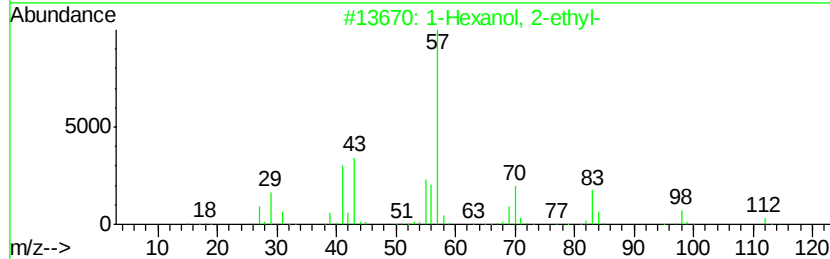
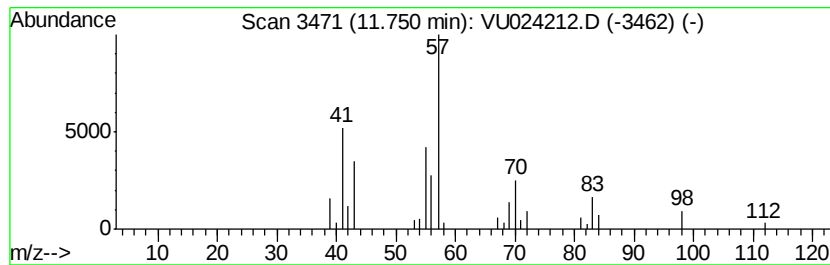
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Quant Title : VOC Analysis

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.75 ug/L	33123	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
5		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	2.45	3.1	ug/L	44427	1	5.89	710835	50.0
Ethyl Acetate	4.38	4.7	ug/L	67032	1	5.89	710835	50.0
1-Hexanol, 2-ethyl-	11.75	2.8	ug/L	33123	3	11.49	601743	50.0