

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU010719\
 Data File : VU029076.D
 Acq On : 07 Jan 2019 23:05
 Operator : MD/SY
 Sample : K1051-12
 Misc : 6.32g/10mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE9Y0

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\SOMULM122018WMA.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	1.395	62	69	85	rVB	82921	99670	14.56%	1.643%
2	1.640	141	145	154	rVB	56405	57125	8.34%	0.942%
3	2.222	316	326	340	rVB	144305	221910	32.41%	3.658%
4	2.324	356	358	360	rBV2	310	174	0.03%	0.003%
5	2.344	360	364	372	rVV6	653	976	0.14%	0.016%
6	2.431	387	391	392	rBV	355	157	0.02%	0.003%
7	2.550	420	428	430	rBV2	785	837	0.12%	0.014%
8	2.759	489	493	496	rBV	202	124	0.02%	0.002%
9	2.826	502	514	529	rVV2	3032	6703	0.98%	0.110%
10	3.013	568	572	574	rBV	169	97	0.01%	0.002%
11	3.083	591	594	596	rBV	166	92	0.01%	0.002%
12	3.160	615	618	619	rBV	161	114	0.02%	0.002%
13	3.251	642	646	649	rBV	253	131	0.02%	0.002%
14	3.279	652	655	657	rVV2	173	102	0.01%	0.002%
15	3.296	657	660	664	rVV2	208	165	0.02%	0.003%
16	3.318	664	667	672	rVB	261	183	0.03%	0.003%
17	3.347	672	676	682	rBV	217	285	0.04%	0.005%
18	3.485	716	719	722	rVB2	197	143	0.02%	0.002%
19	3.900	845	848	851	rVB2	215	150	0.02%	0.002%
20	3.922	851	855	858	rBV	139	120	0.02%	0.002%
21	4.003	877	880	881	rBV	160	93	0.01%	0.002%
22	4.032	885	889	894	rBV2	183	141	0.02%	0.002%
23	4.112	909	914	916	rBV	217	173	0.03%	0.003%
24	4.199	927	941	982	rBV2	49071	163389	23.86%	2.693%
25	4.514	1036	1039	1042	rVB	178	101	0.01%	0.002%
26	4.566	1053	1055	1060	rVV2	191	186	0.03%	0.003%
27	4.640	1060	1078	1111	rVV	109295	261812	38.24%	4.315%
28	4.752	1111	1113	1117	rVB2	172	121	0.02%	0.002%
29	4.890	1153	1156	1158	rBV	252	116	0.02%	0.002%
30	4.942	1169	1172	1176	rBV	224	110	0.02%	0.002%
31	4.993	1182	1188	1194	rVB2	211	233	0.03%	0.004%
32	5.029	1195	1199	1202	rBV2	190	151	0.02%	0.002%
33	5.215	1255	1257	1263	rVB2	161	111	0.02%	0.002%
34	5.324	1270	1291	1315	rBV2	250059	684711	100.00%	11.285%

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 Title : VOC Analysis

35	5.537	1354	1357	1359	rBV	250	125	0.02%	0.002%
36	5.572	1365	1368	1371	rBV	196	117	0.02%	0.002%
37	5.614	1376	1381	1383	rBV2	543	366	0.05%	0.006%
38	5.652	1392	1393	1397	rVB2	230	102	0.01%	0.002%
39	5.736	1417	1419	1424	rVB2	244	192	0.03%	0.003%
40	5.791	1434	1436	1443	rBV	171	113	0.02%	0.002%
41	5.877	1450	1463	1490	rBV	255143	525852	76.80%	8.667%
42	6.176	1543	1556	1574	rBV	178660	352109	51.42%	5.803%
43	6.328	1588	1603	1629	rVB	150902	318501	46.52%	5.250%
44	6.450	1639	1641	1647	rVB2	304	179	0.03%	0.003%
45	6.482	1648	1651	1655	rBV2	156	131	0.02%	0.002%
46	6.710	1719	1722	1725	rVV2	163	105	0.02%	0.002%
47	6.893	1773	1779	1781	rBV2	733	648	0.09%	0.011%
48	7.051	1824	1828	1835	rBV2	239	350	0.05%	0.006%
49	7.083	1835	1838	1842	rVB2	201	153	0.02%	0.003%
50	7.106	1842	1845	1848	rBV	172	131	0.02%	0.002%
51	7.225	1870	1882	1908	rBV	80633	155196	22.67%	2.558%
52	7.488	1957	1964	1971	rBV3	517	725	0.11%	0.012%
53	7.562	1974	1987	2005	rBV	299478	545483	79.67%	8.991%
54	7.803	2056	2062	2066	rBV3	389	583	0.09%	0.010%
55	7.848	2066	2076	2099	rVB	52577	103213	15.07%	1.701%
56	8.028	2128	2132	2134	rBV2	153	97	0.01%	0.002%
57	8.131	2161	2164	2167	rBV	126	92	0.01%	0.002%
58	8.209	2184	2188	2193	rVB	124	122	0.02%	0.002%
59	8.327	2212	2225	2251	rBV	188785	379892	55.48%	6.261%
60	8.633	2315	2320	2326	rBV3	631	812	0.12%	0.013%
61	8.672	2328	2332	2335	rVV2	215	157	0.02%	0.003%
62	8.852	2383	2388	2392	rVV2	334	387	0.06%	0.006%
63	9.089	2450	2462	2500	rBV	359079	665106	97.14%	10.962%
64	9.237	2505	2508	2510	rVB	211	129	0.02%	0.002%
65	9.347	2540	2542	2548	rVB	180	101	0.01%	0.002%
66	9.379	2548	2552	2554	rBV2	222	169	0.02%	0.003%
67	9.430	2566	2568	2576	rVB	319	225	0.03%	0.004%
68	9.472	2579	2581	2583	rVV	198	103	0.02%	0.002%
69	9.546	2600	2604	2608	rBV	395	457	0.07%	0.008%
70	9.855	2697	2700	2701	rBV	190	104	0.02%	0.002%
71	9.932	2721	2724	2726	rVV2	146	91	0.01%	0.001%

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 Title : VOC Analysis

72	9.980	2736	2739	2744	rVB2	224	216	0.03%	0.004%
73	10.009	2744	2748	2751	rBV	227	133	0.02%	0.002%
74	10.041	2756	2758	2761	rVB2	236	127	0.02%	0.002%
75	10.131	2783	2786	2788	rBV2	183	116	0.02%	0.002%
76	10.147	2789	2791	2795	rVB2	188	131	0.02%	0.002%
77	10.167	2795	2797	2800	rBV	170	123	0.02%	0.002%
78	10.205	2807	2809	2813	rVB	222	106	0.02%	0.002%
79	10.228	2813	2816	2818	rBV2	191	113	0.02%	0.002%
80	10.292	2831	2836	2839	rBV	178	181	0.03%	0.003%
81	10.437	2868	2881	2905	rVB	246516	396519	57.91%	6.535%
82	10.520	2905	2907	2910	rVB	289	180	0.03%	0.003%
83	10.578	2923	2925	2927	rBV	151	108	0.02%	0.002%
84	10.684	2953	2958	2960	rBV	191	180	0.03%	0.003%
85	10.726	2968	2971	2973	rBV2	227	150	0.02%	0.002%
86	10.948	3038	3040	3042	rBV	226	121	0.02%	0.002%
87	11.073	3076	3079	3082	rBV	289	252	0.04%	0.004%
88	11.170	3106	3109	3115	rVB2	241	257	0.04%	0.004%
89	11.244	3128	3132	3135	rBV2	220	236	0.03%	0.004%
90	11.269	3138	3140	3142	rVB	268	101	0.01%	0.002%
91	11.337	3159	3161	3167	rVB	193	132	0.02%	0.002%
92	11.398	3176	3180	3182	rBV2	284	233	0.03%	0.004%
93	11.485	3195	3207	3227	rBV	383472	607947	88.79%	10.020%
94	11.861	3307	3324	3343	rBV	314020	505170	73.78%	8.326%
95	12.311	3460	3464	3468	rVB2	250	259	0.04%	0.004%
96	12.347	3473	3475	3479	rBV2	297	212	0.03%	0.003%
97	12.404	3490	3493	3495	rBV	189	99	0.01%	0.002%
98	12.803	3615	3617	3620	rBV	230	132	0.02%	0.002%
99	12.845	3626	3630	3632	rBV3	275	210	0.03%	0.003%
100	13.054	3690	3695	3697	rBV	379	343	0.05%	0.006%

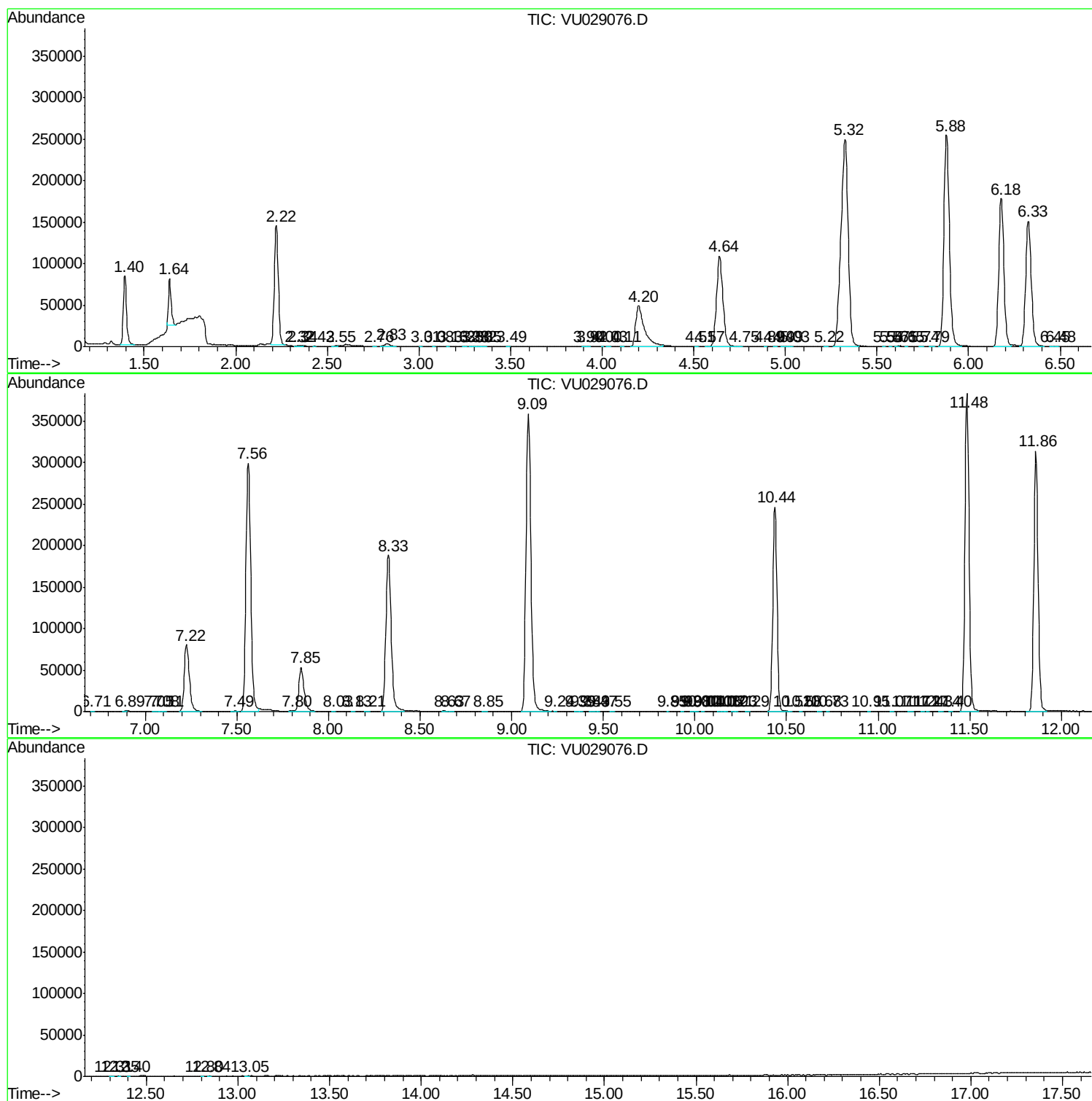
Sum of corrected areas: 6067211

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

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



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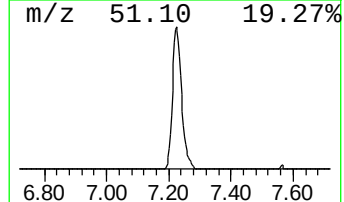
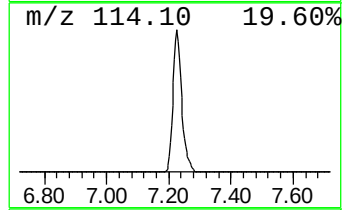
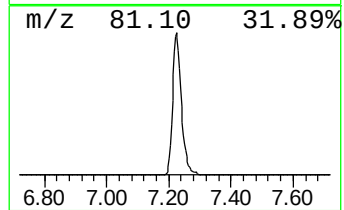
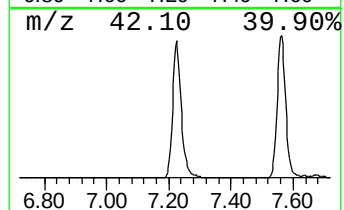
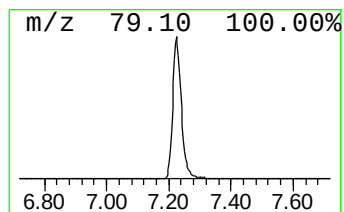
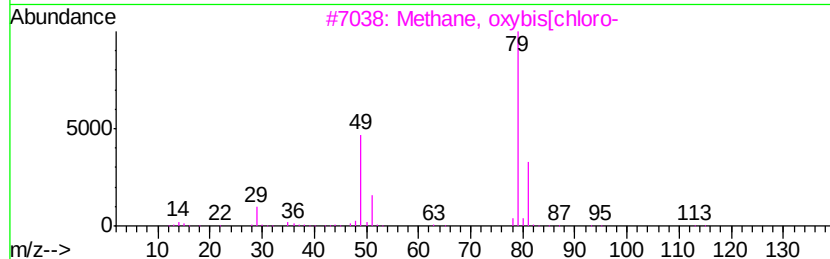
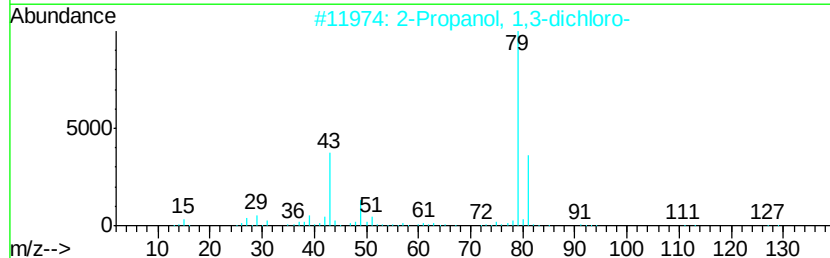
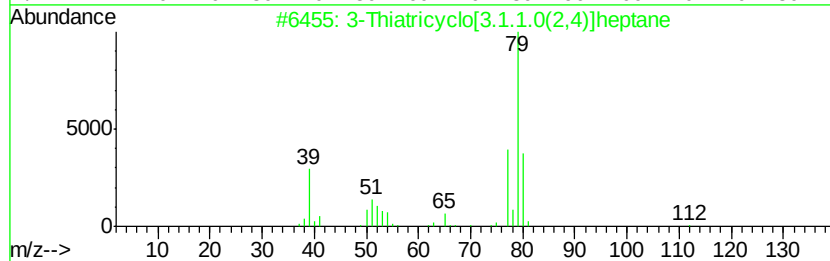
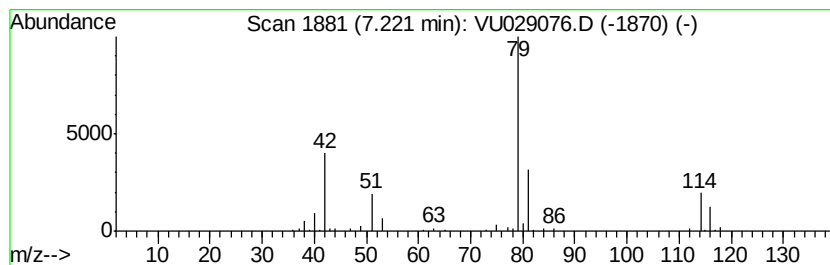
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	14.76 ug/L	155196	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	32
2		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	25
3		Methane, oxvbis[chloro-	114	C2H4Cl2O	000542-88-1	25
4		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	23
5		1,3-Cyclohexadiene	80	C6H8	000592-57-4	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	7.22	14.8	ug/L	155196	1	5.88	525852	50.0