

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU052118\
 Data File : VU023965.D
 Acq On : 21 May 2018 11:45
 Operator : MD/SY
 Sample : VU0521MBL01
 Misc : 5.00µL/5.0mL/100µL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 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\SOMULM051218WMA.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	0.609	3	6	11	rBV	188	183	0.01%	0.002%
2	0.667	19	24	29	rVB	179	202	0.01%	0.002%
3	0.693	29	32	35	rBV2	175	107	0.01%	0.001%
4	0.748	46	49	52	rVV2	166	133	0.01%	0.001%
5	0.799	57	65	70	rBV2	193	323	0.02%	0.003%
6	0.870	83	87	89	rBV	266	186	0.01%	0.002%
7	0.892	89	94	98	rBV2	211	259	0.02%	0.002%
8	0.915	98	101	103	rBV	168	98	0.01%	0.001%
9	0.982	119	122	125	rBV2	150	106	0.01%	0.001%
10	1.088	136	155	180	rBV	1364475	1549490	100.00%	14.336%
11	1.182	181	184	192	rVB	5531	5450	0.35%	0.050%
12	1.400	245	252	265	rBV	151329	159161	10.27%	1.473%
13	1.680	331	339	355	rVB	127438	159286	10.28%	1.474%
14	2.272	512	523	536	rBV	258945	390485	25.20%	3.613%
15	2.397	558	562	565	rBV2	275	249	0.02%	0.002%
16	2.474	581	586	590	rBV3	454	479	0.03%	0.004%
17	2.532	602	604	607	rBV	158	81	0.01%	0.001%
18	2.580	617	619	621	rBV	125	84	0.01%	0.001%
19	2.609	625	628	629	rBV	199	115	0.01%	0.001%
20	2.674	645	648	649	rBV	131	79	0.01%	0.001%
21	2.703	649	657	665	rVB3	1530	2287	0.15%	0.021%
22	2.841	690	700	711	rBV2	1667	3473	0.22%	0.032%
23	2.979	741	743	749	rVB3	372	256	0.02%	0.002%
24	3.072	770	772	777	rVB2	194	180	0.01%	0.002%
25	3.098	778	780	782	rBV2	189	115	0.01%	0.001%
26	3.130	789	790	795	rBV2	109	106	0.01%	0.001%
27	3.185	800	807	811	rVV2	305	341	0.02%	0.003%
28	3.227	818	820	823	rBV	139	90	0.01%	0.001%
29	3.275	830	835	838	rBV	178	230	0.01%	0.002%
30	3.349	854	858	860	rBV	110	116	0.01%	0.001%
31	3.368	862	864	866	rBV	167	122	0.01%	0.001%
32	3.445	886	888	892	rVB	203	91	0.01%	0.001%
33	3.474	892	897	900	rBV2	236	202	0.01%	0.002%
34	3.503	904	906	911	rVB	228	144	0.01%	0.001%

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 Title : VOC Analysis

35	3.539	911	917	919	rBV2	212	238	0.02%	0.002%
36	3.641	947	949	954	rVV2	165	170	0.01%	0.002%
37	3.706	965	969	970	rBV	236	148	0.01%	0.001%
38	3.741	976	980	984	rBV	154	152	0.01%	0.001%
39	3.821	999	1005	1008	rVB2	191	249	0.02%	0.002%
40	3.850	1008	1014	1018	rBV2	240	215	0.01%	0.002%
41	3.873	1018	1021	1023	rBV2	201	157	0.01%	0.001%
42	3.928	1036	1038	1041	rVB	159	91	0.01%	0.001%
43	3.947	1041	1044	1048	rBV2	202	180	0.01%	0.002%
44	3.966	1048	1050	1054	rBV	171	118	0.01%	0.001%
45	4.053	1068	1077	1079	rBV	259	400	0.03%	0.004%
46	4.072	1079	1083	1089	rBV2	625	731	0.05%	0.007%
47	4.178	1102	1116	1150	rBV	121404	324350	20.93%	3.001%
48	4.651	1246	1263	1286	rBV	198636	470611	30.37%	4.354%
49	4.860	1325	1328	1329	rBV	254	148	0.01%	0.001%
50	4.886	1331	1336	1338	rBV3	449	500	0.03%	0.005%
51	4.928	1346	1349	1352	rBV	149	104	0.01%	0.001%
52	4.976	1361	1364	1367	rBV	310	162	0.01%	0.001%
53	4.995	1367	1370	1373	rBV2	315	256	0.02%	0.002%
54	5.098	1397	1402	1404	rBV	208	177	0.01%	0.002%
55	5.130	1408	1412	1414	rBV2	137	96	0.01%	0.001%
56	5.149	1414	1418	1419	rBV2	133	89	0.01%	0.001%
57	5.243	1441	1447	1449	rBV2	222	269	0.02%	0.002%
58	5.342	1454	1478	1524	rBV2	389567	1196097	77.19%	11.066%
59	5.667	1576	1579	1580	rBV	310	174	0.01%	0.002%
60	5.889	1633	1648	1692	rBV	339806	707663	45.67%	6.547%
61	6.188	1733	1741	1749	rVB6	1947	3704	0.24%	0.034%
62	6.217	1749	1750	1754	rVV2	226	121	0.01%	0.001%
63	6.236	1754	1756	1758	rVB2	335	148	0.01%	0.001%
64	6.336	1771	1787	1817	rBV	283086	573197	36.99%	5.303%
65	6.603	1867	1870	1873	rBV	150	92	0.01%	0.001%
66	6.616	1873	1874	1881	rBV2	143	128	0.01%	0.001%
67	6.670	1888	1891	1894	rVB2	241	138	0.01%	0.001%
68	6.690	1894	1897	1899	rBV	206	133	0.01%	0.001%
69	6.725	1905	1908	1910	rBV2	202	116	0.01%	0.001%
70	6.741	1910	1913	1915	rBV2	148	92	0.01%	0.001%
71	6.776	1921	1924	1927	rBV2	110	82	0.01%	0.001%

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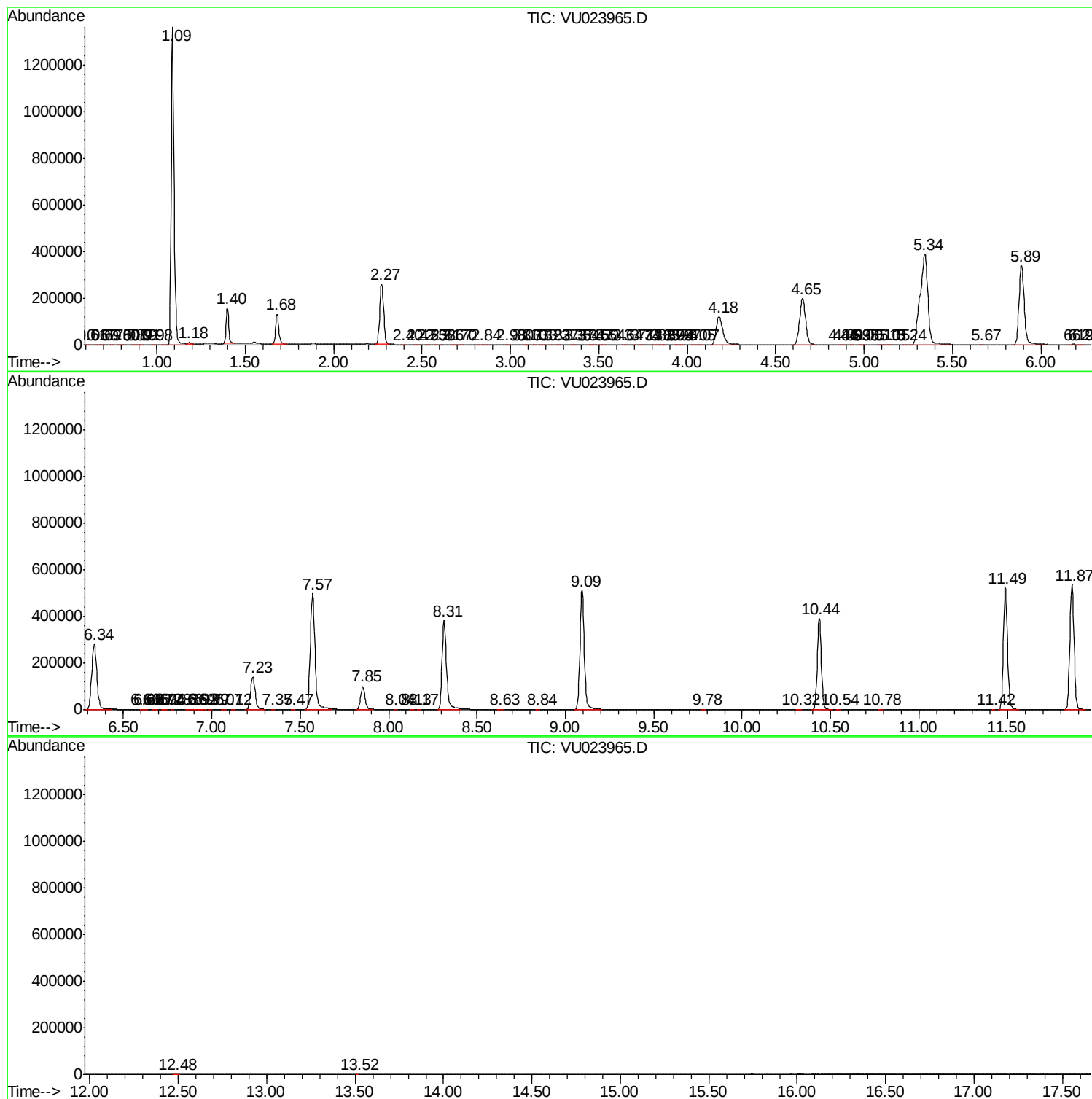
72	6.863	1947	1951	1963	rVB3	970	1599	0.10%	0.015%
73	6.921	1963	1969	1970	rBV	214	200	0.01%	0.002%
74	6.931	1970	1972	1975	rVB2	198	107	0.01%	0.001%
75	6.963	1975	1982	1983	rBV	249	292	0.02%	0.003%
76	6.985	1988	1989	1994	rVB	126	107	0.01%	0.001%
77	7.066	2010	2014	2018	rBV2	211	221	0.01%	0.002%
78	7.120	2028	2031	2035	rBV	150	145	0.01%	0.001%
79	7.233	2053	2066	2087	rBV	141381	258381	16.68%	2.391%
80	7.345	2099	2101	2104	rVB2	269	88	0.01%	0.001%
81	7.468	2133	2139	2140	rBV2	339	272	0.02%	0.003%
82	7.571	2157	2171	2204	rBV	498154	922799	59.56%	8.538%
83	7.853	2247	2259	2276	rBV	101331	173163	11.18%	1.602%
84	8.040	2314	2317	2319	rBV	194	105	0.01%	0.001%
85	8.130	2343	2345	2349	rBV2	132	85	0.01%	0.001%
86	8.175	2354	2359	2361	rBV2	254	226	0.01%	0.002%
87	8.313	2390	2402	2432	rBV	382541	668734	43.16%	6.187%
88	8.635	2495	2502	2506	rBV4	530	709	0.05%	0.007%
89	8.844	2563	2567	2570	rBV2	223	186	0.01%	0.002%
90	9.095	2631	2645	2680	rBV	511245	882478	56.95%	8.165%
91	9.779	2855	2858	2861	rBV2	280	229	0.01%	0.002%
92	10.320	3021	3026	3031	rVB4	998	1176	0.08%	0.011%
93	10.435	3049	3062	3085	rBV	389803	625194	40.35%	5.784%
94	10.541	3092	3095	3099	rBV	214	197	0.01%	0.002%
95	10.783	3166	3170	3173	rBV2	275	244	0.02%	0.002%
96	11.422	3366	3369	3371	rBV2	317	224	0.01%	0.002%
97	11.487	3377	3389	3414	rBV	522244	836815	54.01%	7.742%
98	11.866	3493	3507	3529	rBV	534701	877669	56.64%	8.120%
99	12.483	3695	3699	3706	rVB2	577	725	0.05%	0.007%
100	13.516	4017	4020	4021	rBV3	477	314	0.02%	0.003%

Sum of corrected areas: 10808489

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Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM051218WMA.M
Quant Title : VOC Analysis

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



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TIC Library : C:\DATABASE\NIST11.L
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No Library Search Compounds Detected

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--
					# RT Resp Conc