

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU052118\
 Data File : VU023985.D
 Acq On : 21 May 2018 22:28
 Operator : MD/SY
 Sample : J3031-03
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 25 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	0.616	6	8	12	rVB	152	89	0.01%	0.001%
2	0.641	13	16	20	rVB2	171	144	0.01%	0.002%
3	0.667	20	24	28	rBV2	210	167	0.02%	0.002%
4	0.715	35	39	42	rVB2	159	104	0.01%	0.001%
5	0.792	61	63	64	rBV	138	57	0.01%	0.001%
6	0.809	65	68	73	rVV	237	246	0.02%	0.003%
7	0.844	75	79	82	rVV2	188	162	0.02%	0.002%
8	0.866	83	86	89	rVV2	112	94	0.01%	0.001%
9	0.886	89	92	96	rVB2	244	171	0.02%	0.002%
10	0.905	96	98	99	rBV2	178	83	0.01%	0.001%
11	0.911	99	100	102	rBV	106	45	0.00%	0.000%
12	0.928	102	105	107	rVV2	83	72	0.01%	0.001%
13	0.953	110	113	115	rVB	118	65	0.01%	0.001%
14	0.979	119	121	122	rBV	98	45	0.00%	0.000%
15	1.088	136	155	179	rBV	869175	1019954	97.04%	10.897%
16	1.182	180	184	191	rVB	9223	9741	0.93%	0.104%
17	1.397	244	251	263	rBV	144577	147699	14.05%	1.578%
18	1.677	331	338	357	rVB	107938	139432	13.27%	1.490%
19	2.268	511	522	535	rBV	228574	343406	32.67%	3.669%
20	2.455	573	580	582	rBV4	1064	1320	0.13%	0.014%
21	2.616	626	630	640	rBV2	602	934	0.09%	0.010%
22	2.667	644	646	651	rVV2	313	253	0.02%	0.003%
23	2.702	651	657	663	rVB3	917	1253	0.12%	0.013%
24	2.738	663	668	671	rBV2	261	244	0.02%	0.003%
25	2.792	681	685	687	rBV2	236	186	0.02%	0.002%
26	2.844	691	701	707	rVV2	756	1540	0.15%	0.016%
27	2.915	720	723	725	rBV	111	74	0.01%	0.001%
28	2.989	744	746	748	rBV	167	85	0.01%	0.001%
29	3.111	783	784	788	rBV2	138	110	0.01%	0.001%
30	3.223	816	819	823	rBV2	180	197	0.02%	0.002%
31	3.246	823	826	827	rBV	172	83	0.01%	0.001%
32	3.288	837	839	841	rBV	121	63	0.01%	0.001%
33	3.300	841	843	846	rVB	137	82	0.01%	0.001%
34	3.362	858	862	868	rBV2	205	231	0.02%	0.002%

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 Title : VOC Analysis

35	3.577	928	929	933	rVB	202	124	0.01%	0.001%
36	3.599	933	936	940	rBV2	252	235	0.02%	0.003%
37	3.689	961	964	967	rBV	586	446	0.04%	0.005%
38	3.853	1012	1015	1018	rBV2	183	118	0.01%	0.001%
39	4.120	1095	1098	1099	rBV	138	80	0.01%	0.001%
40	4.181	1103	1117	1151	rBV	113251	302385	28.77%	3.231%
41	4.561	1231	1235	1240	rVB2	361	357	0.03%	0.004%
42	4.587	1242	1243	1246	rVB	219	85	0.01%	0.001%
43	4.651	1246	1263	1292	rBV	180231	422868	40.23%	4.518%
44	4.837	1317	1321	1323	rBV2	176	143	0.01%	0.002%
45	4.882	1330	1335	1338	rBV4	886	972	0.09%	0.010%
46	4.985	1363	1367	1370	rBV3	277	229	0.02%	0.002%
47	5.249	1446	1449	1452	rBV	143	77	0.01%	0.001%
48	5.345	1453	1479	1509	rBV2	348863	1051108	100.00%	11.230%
49	5.667	1578	1579	1582	rBV	134	65	0.01%	0.001%
50	5.757	1604	1607	1610	rVB	258	167	0.02%	0.002%
51	5.786	1613	1616	1617	rBV	100	59	0.01%	0.001%
52	5.889	1633	1648	1682	rBV	317088	650357	61.87%	6.948%
53	6.181	1733	1739	1742	rBV5	794	952	0.09%	0.010%
54	6.217	1747	1750	1752	rVB4	256	127	0.01%	0.001%
55	6.336	1772	1787	1812	rBV	246128	500125	47.58%	5.343%
56	6.503	1837	1839	1840	rVB	192	48	0.00%	0.001%
57	6.664	1886	1889	1892	rVB2	217	161	0.02%	0.002%
58	6.705	1896	1902	1903	rBV	212	213	0.02%	0.002%
59	6.770	1917	1922	1924	rBV	165	154	0.01%	0.002%
60	6.792	1926	1929	1934	rVV2	208	218	0.02%	0.002%
61	6.866	1945	1952	1955	rBV2	364	425	0.04%	0.005%
62	6.902	1960	1963	1967	rBV2	148	140	0.01%	0.001%
63	7.111	2026	2028	2030	rBV2	138	71	0.01%	0.001%
64	7.172	2042	2047	2049	rBV2	150	138	0.01%	0.001%
65	7.188	2049	2052	2054	rBV	193	151	0.01%	0.002%
66	7.233	2054	2066	2089	rBV	119752	214711	20.43%	2.294%
67	7.413	2120	2122	2126	rVB	282	160	0.02%	0.002%
68	7.458	2133	2136	2139	rBV	138	117	0.01%	0.001%
69	7.477	2139	2142	2146	rVB	210	200	0.02%	0.002%
70	7.570	2154	2171	2219	rBV	441567	814405	77.48%	8.701%
71	7.853	2248	2259	2280	rBV	85466	146720	13.96%	1.568%

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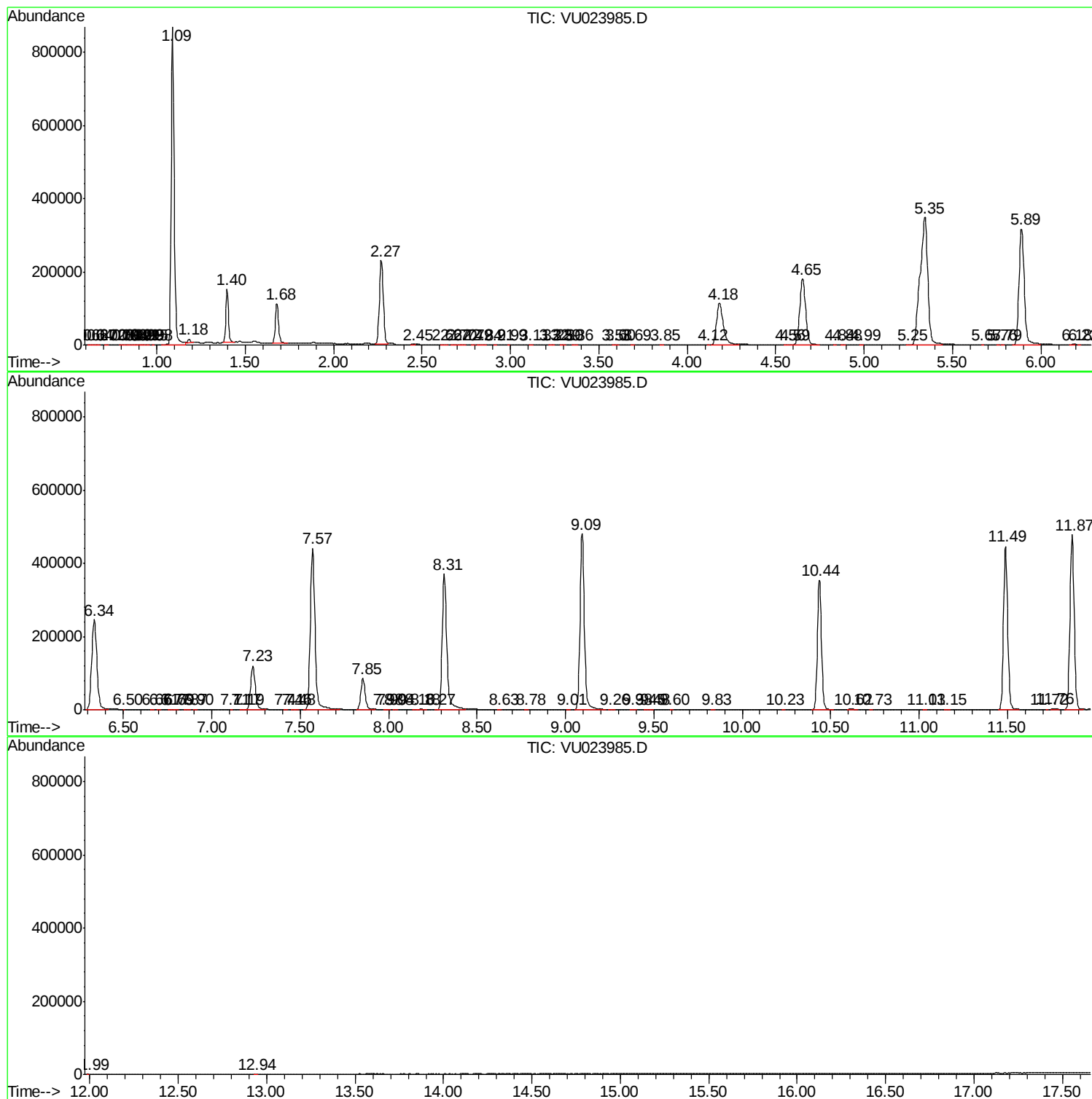
72	7.976	2295	2297	2299	rBV	266	143	0.01%	0.002%
73	7.995	2299	2303	2307	rVB2	452	387	0.04%	0.004%
74	8.037	2312	2316	2320	rBV2	337	303	0.03%	0.003%
75	8.156	2346	2353	2354	rBV2	202	217	0.02%	0.002%
76	8.184	2354	2362	2371	rVB2	1380	1855	0.18%	0.020%
77	8.271	2386	2389	2390	rBV	112	55	0.01%	0.001%
78	8.313	2390	2402	2440	rBV	371215	668816	63.63%	7.146%
79	8.628	2496	2500	2503	rVB2	300	244	0.02%	0.003%
80	8.783	2544	2548	2550	rBV	463	405	0.04%	0.004%
81	9.014	2617	2620	2623	rBV	184	127	0.01%	0.001%
82	9.094	2632	2645	2686	rBV	481151	823365	78.33%	8.797%
83	9.255	2691	2695	2702	rBV2	620	813	0.08%	0.009%
84	9.384	2729	2735	2740	rBV3	750	1005	0.10%	0.011%
85	9.455	2753	2757	2761	rBV2	252	273	0.03%	0.003%
86	9.483	2764	2766	2770	rVB	180	113	0.01%	0.001%
87	9.596	2799	2801	2805	rVB	202	112	0.01%	0.001%
88	9.831	2871	2874	2878	rBV2	246	183	0.02%	0.002%
89	10.233	2996	2999	3002	rBV	266	188	0.02%	0.002%
90	10.435	3049	3062	3087	rBV	354006	572817	54.50%	6.120%
91	10.615	3111	3118	3129	rVB2	1500	2229	0.21%	0.024%
92	10.728	3150	3153	3156	rBV2	214	190	0.02%	0.002%
93	11.030	3244	3247	3250	rBV	245	184	0.02%	0.002%
94	11.152	3282	3285	3291	rBV2	368	392	0.04%	0.004%
95	11.490	3377	3390	3414	rBV	445928	723348	68.82%	7.728%
96	11.725	3460	3463	3464	rBV	215	101	0.01%	0.001%
97	11.760	3469	3474	3484	rVB4	1870	3333	0.32%	0.036%
98	11.866	3493	3507	3527	rBV	477618	780490	74.25%	8.339%
99	11.988	3543	3545	3547	rBV	374	181	0.02%	0.002%
100	12.937	3837	3840	3843	rBV2	399	265	0.03%	0.003%

Sum of corrected areas: 9359676

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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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No Library Search Compounds Detected

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