

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050818\
 Data File : VU023739.D
 Acq On : 08 May 2018 16:05
 Operator : MD/SY
 Sample : J2661-06
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 15 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\SOMULM050818WMA.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	0.683	25	29	37	rVB2	244	273	0.002%	0.0002%
2	0.725	37	42	43	rBV2	134	111	0.001%	0.0001%
3	0.812	66	69	76	rVB2	219	199	0.001%	0.0002%
4	0.876	83	89	91	rVV2	121	121	0.001%	0.0001%
5	0.957	107	114	117	rBV	96	118	0.001%	0.0001%
6	1.088	136	155	179	rBV	1238088	1404556	100.00%	11.867%
7	1.182	181	184	192	rVB2	6245	5966	0.42%	0.0050%
8	1.400	245	252	274	rVB	197414	208915	14.87%	1.765%
9	1.680	331	339	359	rVB	140399	175637	12.50%	1.484%
10	2.272	512	523	537	rBV	319109	480383	34.20%	4.059%
11	2.416	565	568	571	rVB2	309	198	0.001%	0.0002%
12	2.452	571	579	582	rVV5	675	955	0.07%	0.0008%
13	2.481	583	588	595	rVB2	1081	1537	0.11%	0.0013%
14	2.523	598	601	604	rVB2	290	186	0.001%	0.0002%
15	2.577	614	618	622	rVB	259	197	0.001%	0.0002%
16	2.609	623	628	630	rBV	377	362	0.003%	0.0003%
17	2.667	643	646	651	rVB2	278	233	0.002%	0.0002%
18	2.706	651	658	663	rBV2	788	1039	0.007%	0.0009%
19	2.735	663	667	671	rVB2	179	139	0.001%	0.0001%
20	2.760	671	675	681	rBV2	356	317	0.002%	0.0003%
21	2.844	681	701	711	rBV3	1299	3337	0.24%	0.0028%
22	2.915	718	723	726	rBV	180	157	0.001%	0.0001%
23	2.953	732	735	737	rBV2	174	118	0.001%	0.0001%
24	2.986	742	745	746	rBV2	307	171	0.001%	0.0001%
25	3.040	756	762	769	rVB2	196	233	0.002%	0.0002%
26	3.104	779	782	787	rBV2	134	144	0.001%	0.0001%
27	3.146	792	795	799	rVB2	217	140	0.001%	0.0001%
28	3.172	799	803	806	rBV2	199	140	0.001%	0.0001%
29	3.204	810	813	819	rVB2	224	221	0.002%	0.0002%
30	3.252	826	828	831	rVB2	184	108	0.001%	0.0001%
31	3.452	882	890	892	rBV2	182	241	0.002%	0.0002%
32	3.545	911	919	922	rBV	173	223	0.002%	0.0002%
33	3.651	949	952	959	rVB2	101	116	0.001%	0.0001%
34	3.735	975	978	983	rVB2	193	157	0.001%	0.0001%

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 Title : VOC Analysis

35	3.989	1051	1057	1060	rBV2	149	133	0.01%	0.001%
36	4.047	1072	1075	1080	rBV	108	120	0.01%	0.001%
37	4.182	1101	1117	1150	rBV2	130430	344519	24.53%	2.911%
38	4.391	1179	1182	1187	rBV4	398	399	0.03%	0.003%
39	4.413	1187	1189	1196	rVB3	551	516	0.04%	0.004%
40	4.484	1209	1211	1217	rVB3	381	319	0.02%	0.003%
41	4.513	1217	1220	1224	rBV2	298	290	0.02%	0.002%
42	4.584	1238	1242	1246	rBV2	448	369	0.03%	0.003%
43	4.651	1246	1263	1288	rVV	216133	509629	36.28%	4.306%
44	4.847	1321	1324	1328	rVB2	150	113	0.01%	0.001%
45	4.892	1328	1338	1346	rVB4	767	1318	0.09%	0.011%
46	4.989	1365	1368	1372	rVV2	336	233	0.02%	0.002%
47	5.043	1382	1385	1390	rVB2	148	116	0.01%	0.001%
48	5.085	1390	1398	1399	rBV	140	182	0.01%	0.002%
49	5.346	1453	1479	1509	rBV2	453684	1346050	95.83%	11.373%
50	5.667	1576	1579	1581	rBV3	367	208	0.01%	0.002%
51	5.696	1585	1588	1592	rVV2	205	118	0.01%	0.001%
52	5.751	1602	1605	1610	rVB2	178	207	0.01%	0.002%
53	5.889	1634	1648	1673	rBV	396033	795496	56.64%	6.721%
54	6.185	1731	1740	1748	rBV6	1729	3244	0.23%	0.027%
55	6.230	1751	1754	1759	rVB2	332	265	0.02%	0.002%
56	6.336	1772	1787	1820	rBV	295799	612496	43.61%	5.175%
57	6.587	1862	1865	1868	rBV	177	130	0.01%	0.001%
58	6.641	1878	1882	1888	rVB2	138	165	0.01%	0.001%
59	6.725	1905	1908	1915	rVB2	180	205	0.01%	0.002%
60	6.863	1949	1951	1952	rBV	320	136	0.01%	0.001%
61	6.934	1970	1973	1976	rBV2	160	115	0.01%	0.001%
62	6.953	1976	1979	1985	rVV2	147	174	0.01%	0.001%
63	7.005	1992	1995	1998	rBV2	174	148	0.01%	0.001%
64	7.034	2001	2004	2007	rVV	159	126	0.01%	0.001%
65	7.053	2007	2010	2015	rVV	144	124	0.01%	0.001%
66	7.085	2016	2020	2023	rVV	166	137	0.01%	0.001%
67	7.159	2035	2043	2045	rBV2	146	189	0.01%	0.002%
68	7.233	2052	2066	2094	rBV	160686	290783	20.70%	2.457%
69	7.397	2114	2117	2120	rVB2	258	166	0.01%	0.001%
70	7.419	2120	2124	2127	rBV2	223	211	0.02%	0.002%
71	7.481	2140	2143	2153	rVB2	170	224	0.02%	0.002%

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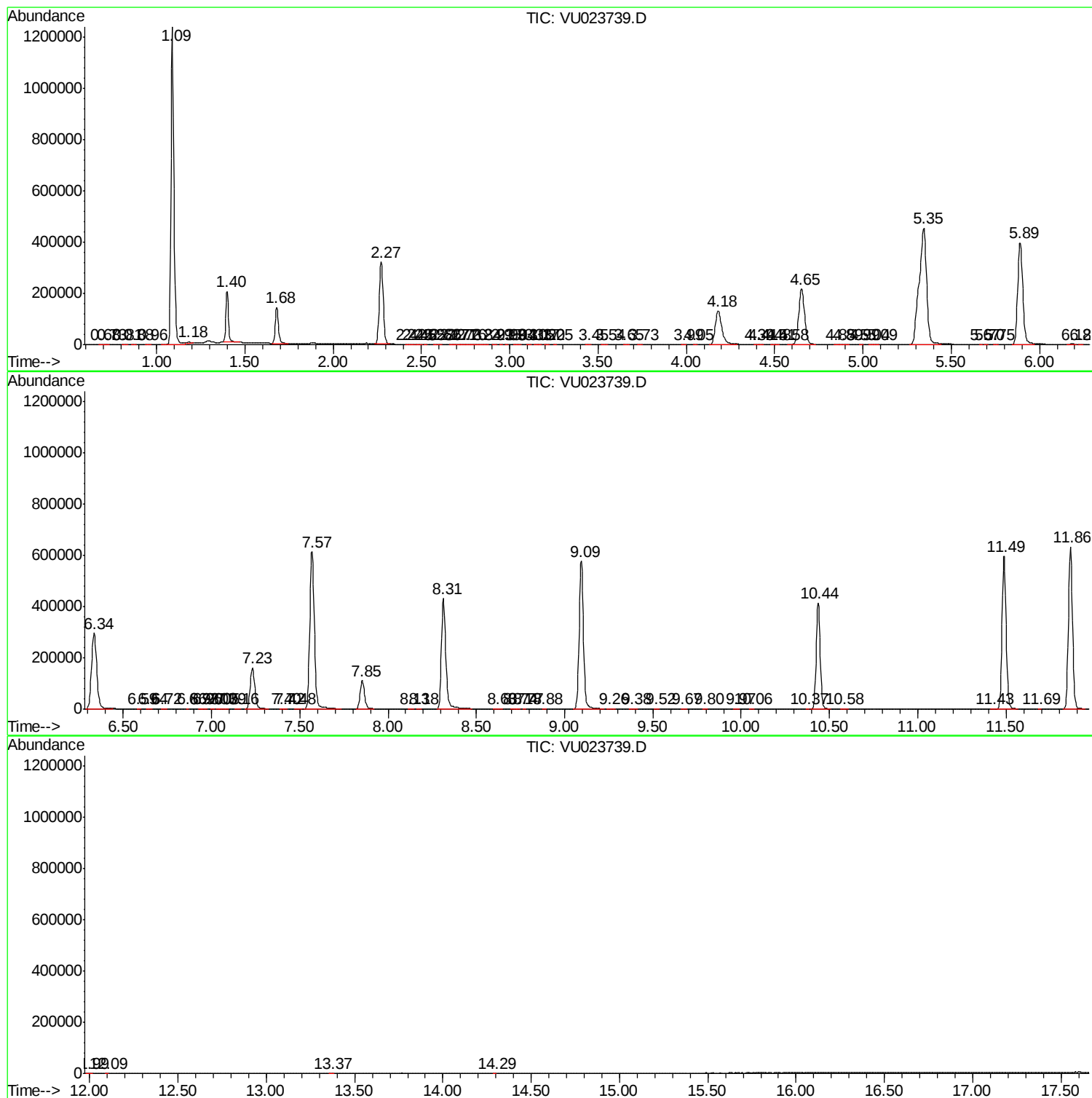
72	7.571	2156	2171	2222	rBV	612029	1096153	78.04%	9.262%
73	7.853	2248	2259	2279	rBV	111770	191909	13.66%	1.621%
74	8.127	2340	2344	2349	rBV2	229	301	0.02%	0.003%
75	8.181	2355	2361	2363	rBV3	245	310	0.02%	0.003%
76	8.313	2390	2402	2452	rVV	430399	749902	53.39%	6.336%
77	8.625	2490	2499	2506	rBV5	600	1294	0.09%	0.011%
78	8.712	2521	2526	2531	rVB2	235	235	0.02%	0.002%
79	8.738	2531	2534	2537	rBV2	124	114	0.01%	0.001%
80	8.770	2541	2544	2547	rVB	186	119	0.01%	0.001%
81	8.882	2576	2579	2582	rBV2	230	140	0.01%	0.001%
82	9.095	2631	2645	2684	rBV	575651	982267	69.93%	8.299%
83	9.255	2689	2695	2705	rVB3	702	1198	0.09%	0.010%
84	9.384	2729	2735	2743	rVV3	945	1266	0.09%	0.011%
85	9.519	2773	2777	2782	rBV	269	234	0.02%	0.002%
86	9.670	2821	2824	2830	rBV2	197	179	0.01%	0.002%
87	9.796	2859	2863	2867	rBV2	285	273	0.02%	0.002%
88	9.972	2913	2918	2923	rBV2	225	259	0.02%	0.002%
89	10.059	2940	2945	2948	rBV2	198	199	0.01%	0.002%
90	10.374	3040	3043	3045	rBV2	172	132	0.01%	0.001%
91	10.435	3049	3062	3083	rVV	413634	654116	46.57%	5.527%
92	10.577	3102	3106	3114	rBV2	700	865	0.06%	0.007%
93	11.426	3366	3370	3377	rVB2	591	778	0.06%	0.007%
94	11.487	3377	3389	3414	rBV	595216	951900	67.77%	8.043%
95	11.689	3449	3452	3455	rVB2	256	174	0.01%	0.001%
96	11.863	3493	3506	3532	rBV	631351	1002885	71.40%	8.474%
97	11.988	3541	3545	3553	rVB4	651	637	0.05%	0.005%
98	12.094	3575	3578	3581	rBV2	226	154	0.01%	0.001%
99	13.368	3969	3974	3978	rBV2	641	698	0.05%	0.006%
100	14.294	4258	4262	4264	rBV	321	315	0.02%	0.003%

Sum of corrected areas: 11835327

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ALS Vial : 15 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050818WMA.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
