

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112122\
 Data File : VU052037.D
 Acq On : 22 Nov 2022 12:10
 Operator : JC/MD
 Sample : N5679-04ME
 Misc : 5.18g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 53 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COKZ6ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
 Title : VOC Analysis

Signal : TIC: VU052037.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	102	rVB	167361	271655	14.95%	1.871%
2	2.540	362	373	394	rVB	363169	588739	32.41%	4.055%
3	3.173	557	570	592	rBV	85289	196823	10.83%	1.356%
4	3.630	709	712	715	rBV2	277	189	0.01%	0.001%
5	3.665	720	723	724	rBV2	612	347	0.02%	0.002%
6	3.748	746	749	753	rBV2	383	314	0.02%	0.002%
7	3.848	778	780	783	rVV	197	134	0.01%	0.001%
8	4.028	833	836	840	rVB2	277	182	0.01%	0.001%
9	4.247	901	904	908	rBV2	297	200	0.01%	0.001%
10	4.305	920	922	923	rBV2	194	86	0.00%	0.001%
11	4.321	926	927	932	rVV2	227	159	0.01%	0.001%
12	4.395	944	950	952	rBV	218	220	0.01%	0.002%
13	4.459	967	970	973	rBB	316	177	0.01%	0.001%
14	4.485	975	978	981	rBV2	207	166	0.01%	0.001%
15	4.546	993	997	999	rBV	388	274	0.02%	0.002%
16	4.626	1011	1022	1072	rBV2	117383	416309	22.92%	2.867%
17	5.057	1140	1156	1188	rBV	316339	707968	38.97%	4.876%
18	5.437	1272	1274	1276	rBV2	144	90	0.00%	0.001%
19	5.498	1290	1293	1297	rBV2	281	176	0.01%	0.001%
20	5.575	1315	1317	1320	rVB2	276	160	0.01%	0.001%
21	5.597	1320	1324	1326	rBV	213	166	0.01%	0.001%
22	5.633	1332	1335	1339	rVB	382	269	0.01%	0.002%
23	5.716	1339	1361	1383	rBV2	707909	1816589	100.00%	12.512%
24	5.977	1432	1442	1455	rBV6	3171	7418	0.41%	0.051%
25	6.076	1472	1473	1474	rBV6	230	76	0.00%	0.001%
26	6.118	1482	1486	1490	rVB3	531	313	0.02%	0.002%
27	6.147	1493	1495	1497	rBV	390	194	0.01%	0.001%
28	6.244	1510	1525	1561	rBV	578680	1151823	63.41%	7.933%
29	6.469	1592	1595	1596	rBV	303	153	0.01%	0.001%
30	6.536	1603	1616	1628	rBV7	18222	39221	2.16%	0.270%
31	6.684	1650	1662	1693	rVB	410437	820847	45.19%	5.654%
32	6.835	1707	1709	1716	rVB4	822	833	0.05%	0.006%
33	6.867	1716	1719	1721	rBV2	456	285	0.02%	0.002%
34	6.954	1744	1746	1748	rBV2	190	72	0.00%	0.000%
35	6.973	1749	1752	1754	rBV2	217	136	0.01%	0.001%
36	6.990	1754	1757	1760	rVV2	425	308	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
 Title : VOC Analysis

37	7.035	1769	1771	1772	rBV2	183	95	0.01%	0.001%
38	7.080	1780	1785	1788	rBV2	271	236	0.01%	0.002%
39	7.112	1793	1795	1797	rBV2	330	155	0.01%	0.001%
40	7.150	1804	1807	1808	rBV	194	109	0.01%	0.001%
41	7.199	1812	1822	1842	rVB9	4479	13323	0.73%	0.092%
42	7.295	1848	1852	1855	rBV2	257	249	0.01%	0.002%
43	7.311	1855	1857	1858	rVV	299	131	0.01%	0.001%
44	7.337	1862	1865	1868	rVB2	243	149	0.01%	0.001%
45	7.350	1868	1869	1871	rBV	230	127	0.01%	0.001%
46	7.424	1889	1892	1893	rBV	134	72	0.00%	0.000%
47	7.436	1893	1896	1898	rVV2	250	149	0.01%	0.001%
48	7.498	1909	1915	1917	rBV	305	271	0.01%	0.002%
49	7.514	1917	1920	1922	rBV2	234	185	0.01%	0.001%
50	7.562	1923	1935	1963	rVV	198655	379344	20.88%	2.613%
51	7.797	1998	2008	2010	rBV6	4367	7372	0.41%	0.051%
52	7.896	2025	2039	2059	rBV	791845	1456330	80.17%	10.031%
53	8.099	2099	2102	2108	rVB3	619	735	0.04%	0.005%
54	8.179	2108	2127	2149	rBV	129287	261724	14.41%	1.803%
55	8.327	2171	2173	2174	rBV2	356	147	0.01%	0.001%
56	8.446	2205	2210	2212	rBV2	392	332	0.02%	0.002%
57	8.497	2224	2226	2227	rBV	280	118	0.01%	0.001%
58	8.549	2233	2242	2252	rVB3	8652	14359	0.79%	0.099%
59	8.645	2258	2272	2311	rBV	472695	976275	53.74%	6.724%
60	9.047	2395	2397	2398	rBV	164	78	0.00%	0.001%
61	9.076	2403	2406	2407	rBV	173	80	0.00%	0.001%
62	9.163	2431	2433	2436	rBV	206	112	0.01%	0.001%
63	9.205	2443	2446	2454	rVB2	383	352	0.02%	0.002%
64	9.285	2469	2471	2477	rVB2	357	271	0.01%	0.002%
65	9.324	2480	2483	2485	rBV	179	120	0.01%	0.001%
66	9.420	2497	2513	2539	rBV	805032	1492468	82.16%	10.279%
67	9.642	2580	2582	2584	rBV	388	191	0.01%	0.001%
68	9.694	2589	2598	2609	rVB3	5723	9504	0.52%	0.065%
69	9.774	2620	2623	2626	rVB	299	179	0.01%	0.001%
70	9.796	2626	2630	2633	rBV2	191	175	0.01%	0.001%
71	9.874	2650	2654	2657	rBB	387	272	0.01%	0.002%
72	9.890	2657	2659	2662	rBV2	180	121	0.01%	0.001%
73	10.002	2691	2694	2699	rBV2	290	195	0.01%	0.001%
74	10.118	2718	2730	2731	rBV4	5616	7919	0.44%	0.055%
75	10.247	2767	2770	2771	rBV	247	138	0.01%	0.001%
76	10.321	2790	2793	2795	rBV	261	174	0.01%	0.001%

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Integrator: RTE

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77	10.488	2837	2845	2852	rBV2	4146	6135	0.34%	0.042%
78	10.552	2864	2865	2868	rBV	198	124	0.01%	0.001%
79	10.571	2869	2871	2876	rVB2	366	231	0.01%	0.002%
80	10.600	2878	2880	2881	rBV2	302	163	0.01%	0.001%
81	10.758	2916	2929	2958	rBV	680362	1100943	60.60%	7.583%
82	11.108	3034	3038	3040	rBV3	1176	877	0.05%	0.006%
83	11.314	3099	3102	3105	rBV	408	312	0.02%	0.002%
84	11.369	3115	3119	3125	rVB2	650	657	0.04%	0.005%
85	11.411	3125	3132	3137	rBV3	937	1275	0.07%	0.009%
86	11.472	3148	3151	3154	rBV2	518	280	0.02%	0.002%
87	11.549	3173	3175	3179	rVB	329	184	0.01%	0.001%
88	11.571	3179	3182	3183	rBV	307	178	0.01%	0.001%
89	11.751	3235	3238	3243	rVB3	912	793	0.04%	0.005%
90	11.812	3244	3257	3286	rBV	808662	1301238	71.63%	8.962%
91	12.092	3340	3344	3346	rBV2	392	293	0.02%	0.002%
92	12.108	3346	3349	3353	rBV2	454	373	0.02%	0.003%
93	12.192	3361	3375	3396	rBV	806512	1315356	72.41%	9.060%
94	12.713	3534	3537	3538	rBV	340	207	0.01%	0.001%
95	12.954	3609	3612	3614	rBV	414	285	0.02%	0.002%
96	13.221	3686	3695	3709	rBV3	20242	32566	1.79%	0.224%
97	13.410	3751	3754	3756	rBV2	444	296	0.02%	0.002%
98	13.481	3771	3776	3778	rBV3	452	452	0.02%	0.003%
99	13.841	3879	3888	3902	rBV3	12447	20816	1.15%	0.143%
100	14.330	4029	4040	4061	rVB2	50969	87536	4.82%	0.603%

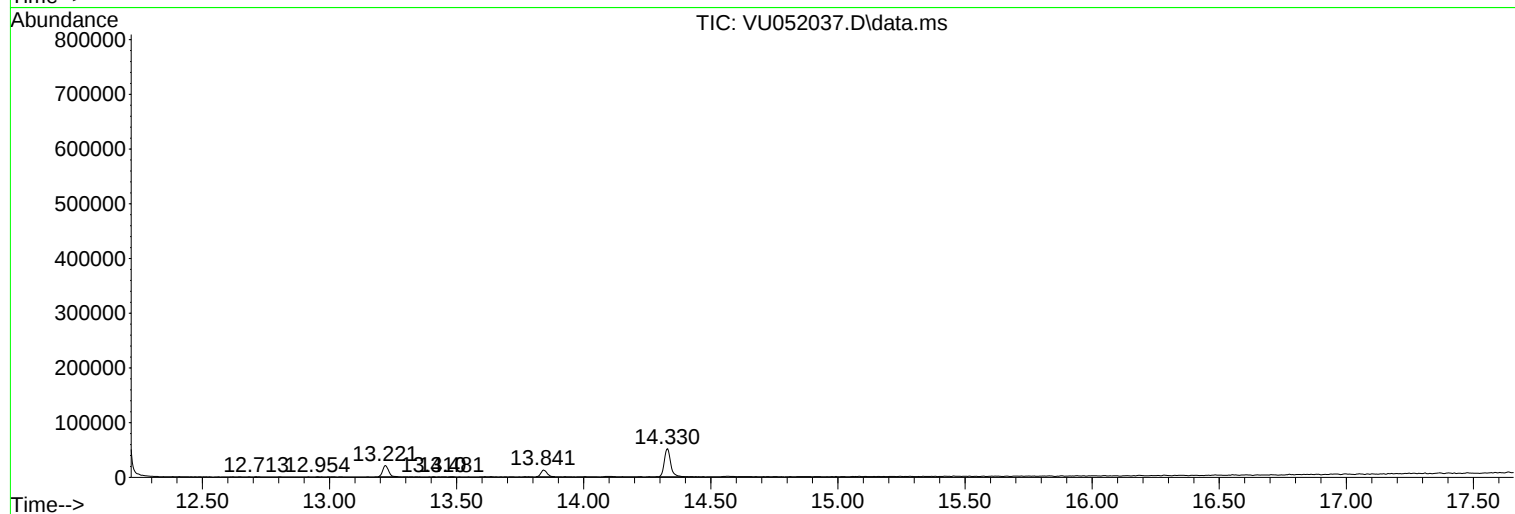
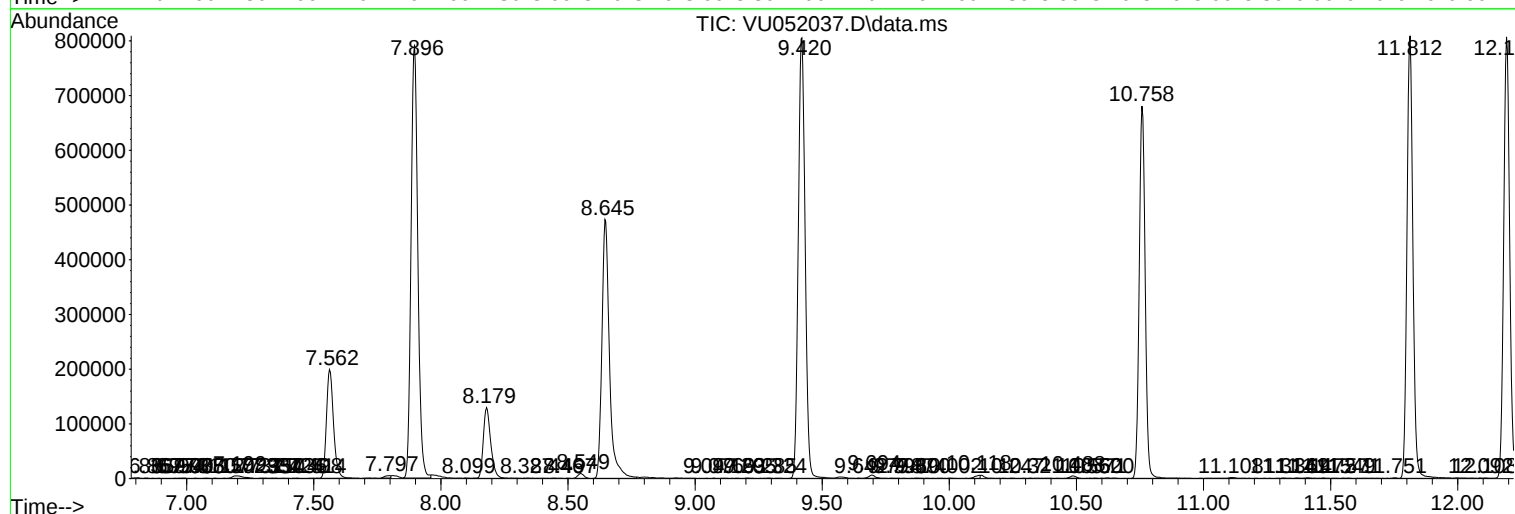
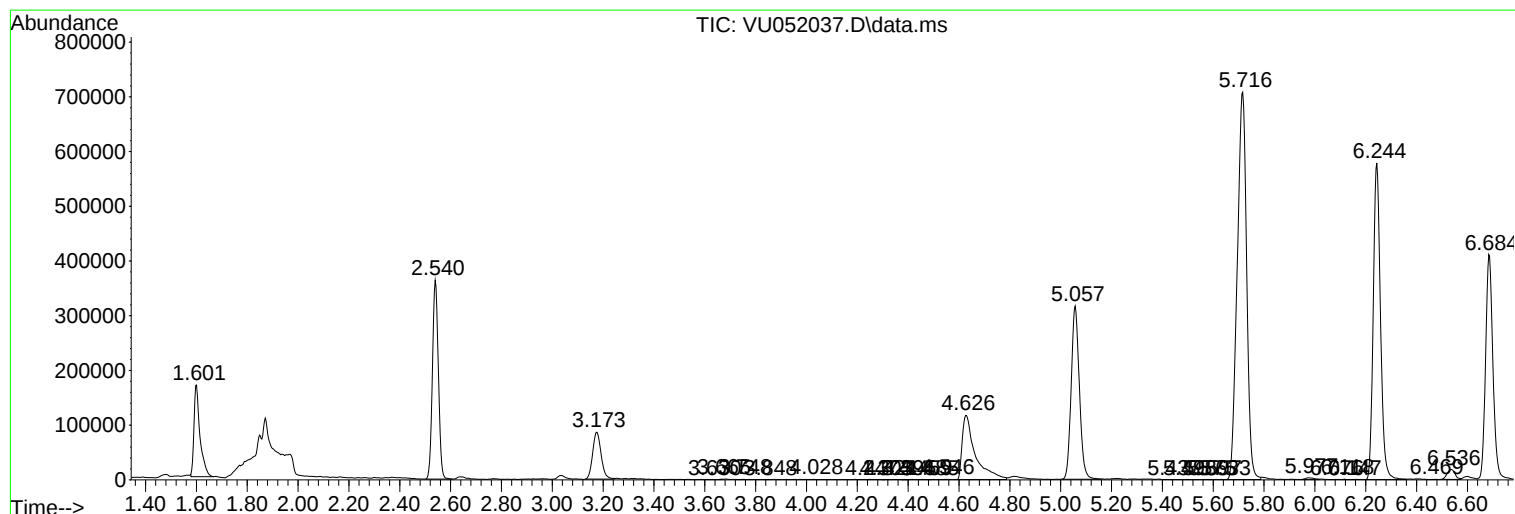
Sum of corrected areas: 14518977

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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