

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090322\
 Data File : VU050623.D
 Acq On : 03 Sep 2022 19:31
 Operator : SY/MD
 Sample : N4362-02MERE
 Misc : 5.47g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0FB5MERE

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\SFAMULM090222WMA.M
 Title : VOC Analysis

Signal : TIC: VU050623.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	72	79	89	rBV	202861	294726	9.19%	1.449%
2	2.533	359	371	389	rBV	625954	1017662	31.73%	5.004%
3	3.176	558	571	595	rBV2	32316	95506	2.98%	0.470%
4	3.491	667	669	673	rBV3	344	189	0.01%	0.001%
5	3.510	673	675	679	rBV2	361	240	0.01%	0.001%
6	3.584	695	698	701	rBV3	232	196	0.01%	0.001%
7	3.697	731	733	737	rVB2	293	152	0.00%	0.001%
8	3.819	766	771	772	rBV	84	81	0.00%	0.000%
9	3.841	776	778	781	rVB	166	79	0.00%	0.000%
10	3.861	781	784	785	rBV	216	128	0.00%	0.001%
11	3.896	793	795	796	rVB	150	57	0.00%	0.000%
12	3.932	803	806	808	rBV	218	157	0.00%	0.001%
13	3.973	816	819	824	rBV	303	203	0.01%	0.001%
14	4.031	835	837	838	rBV	164	56	0.00%	0.000%
15	4.073	846	850	854	rBV2	209	176	0.01%	0.001%
16	4.166	874	879	882	rBV2	214	229	0.01%	0.001%
17	4.198	887	889	893	rVB2	343	240	0.01%	0.001%
18	4.221	893	896	901	rBV2	388	345	0.01%	0.002%
19	4.243	901	903	905	rBV2	124	64	0.00%	0.000%
20	4.263	905	909	911	rBV2	146	130	0.00%	0.001%
21	4.333	927	931	934	rBV2	250	187	0.01%	0.001%
22	4.366	938	941	944	rBV2	191	117	0.00%	0.001%
23	4.430	959	961	963	rBV	128	67	0.00%	0.000%
24	4.446	963	966	973	rVV2	294	286	0.01%	0.001%
25	4.497	979	982	988	rBV2	201	229	0.01%	0.001%
26	4.526	988	991	995	rVB	346	266	0.01%	0.001%
27	4.552	995	999	1002	rVB2	174	161	0.01%	0.001%
28	4.571	1002	1005	1009	rBV2	349	287	0.01%	0.001%
29	4.645	1013	1028	1105	rBV	222856	945724	29.48%	4.650%
30	5.060	1139	1157	1190	rBV	535342	1258617	39.24%	6.189%
31	5.237	1210	1212	1213	rBV	326	112	0.00%	0.001%
32	5.372	1243	1254	1261	rBV7	1022	1807	0.06%	0.009%
33	5.501	1291	1294	1295	rBV	227	108	0.00%	0.001%
34	5.517	1297	1299	1304	rVB2	490	264	0.01%	0.001%
35	5.552	1308	1310	1313	rVB2	262	115	0.00%	0.001%
36	5.607	1321	1327	1329	rBV	331	331	0.01%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
 Title : VOC Analysis

37	5.716	1340	1361	1392	rBV2	1257406	3207728	100.00%	15.772%
38	5.980	1431	1443	1465	rBV5	13937	36290	1.13%	0.178%
39	6.176	1495	1504	1505	rBV4	1296	1491	0.05%	0.007%
40	6.247	1512	1526	1553	rBV	463871	943920	29.43%	4.641%
41	6.526	1603	1613	1628	rBV9	7622	17095	0.53%	0.084%
42	6.610	1628	1639	1648	rVV4	6068	12869	0.40%	0.063%
43	6.690	1649	1664	1692	rVV	724301	1485744	46.32%	7.305%
44	6.880	1721	1723	1727	rVB4	477	343	0.01%	0.002%
45	6.902	1727	1730	1732	rBV	301	200	0.01%	0.001%
46	6.915	1732	1734	1736	rVB	363	150	0.00%	0.001%
47	6.941	1738	1742	1743	rBV2	675	489	0.02%	0.002%
48	7.063	1777	1780	1782	rBV	283	182	0.01%	0.001%
49	7.115	1794	1796	1797	rBV	286	115	0.00%	0.001%
50	7.192	1816	1820	1822	rBV3	2059	1797	0.06%	0.009%
51	7.353	1869	1870	1876	rVB2	415	213	0.01%	0.001%
52	7.446	1896	1899	1902	rVB2	297	185	0.01%	0.001%
53	7.465	1902	1905	1907	rBV	79	62	0.00%	0.000%
54	7.500	1911	1916	1917	rBV2	328	243	0.01%	0.001%
55	7.568	1922	1937	1967	rBV	282630	561341	17.50%	2.760%
56	7.896	2025	2039	2061	rBV	1385213	2520062	78.56%	12.391%
57	8.182	2115	2128	2151	rBV	184039	374330	11.67%	1.841%
58	8.484	2220	2222	2223	rBV	308	112	0.00%	0.001%
59	8.520	2230	2233	2235	rBV	331	178	0.01%	0.001%
60	8.552	2235	2243	2252	rVB3	9168	14352	0.45%	0.071%
61	8.661	2259	2277	2314	rBV2	639114	1825963	56.92%	8.978%
62	8.925	2356	2359	2363	rBV5	1012	1011	0.03%	0.005%
63	8.960	2368	2370	2373	rBV2	399	314	0.01%	0.002%
64	9.108	2414	2416	2418	rBV2	357	198	0.01%	0.001%
65	9.221	2449	2451	2454	rBV2	468	298	0.01%	0.001%
66	9.333	2480	2486	2487	rBV2	587	484	0.02%	0.002%
67	9.420	2499	2513	2533	rBV	594050	1137059	35.45%	5.591%
68	9.639	2578	2581	2582	rBV2	412	200	0.01%	0.001%
69	9.674	2590	2592	2593	rBV	387	201	0.01%	0.001%
70	9.854	2646	2648	2649	rBV	152	52	0.00%	0.000%
71	9.951	2676	2678	2680	rBV2	187	124	0.00%	0.001%
72	9.970	2681	2684	2688	rVV2	603	580	0.02%	0.003%
73	10.070	2712	2715	2718	rBV	339	243	0.01%	0.001%
74	10.102	2721	2725	2729	rVV2	881	1033	0.03%	0.005%
75	10.137	2733	2736	2739	rBV2	430	289	0.01%	0.001%
76	10.372	2807	2809	2814	rVB2	428	324	0.01%	0.002%

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77	10.397	2815	2817	2821	rBV2	318	201	0.01%	0.001%
78	10.655	2896	2897	2899	rBV	164	76	0.00%	0.000%
79	10.764	2917	2931	2958	rBV	1037802	1747288	54.47%	8.591%
80	11.060	3019	3023	3026	rBV2	438	356	0.01%	0.002%
81	11.086	3026	3031	3034	rBV4	805	758	0.02%	0.004%
82	11.114	3034	3040	3048	rVB5	3261	4458	0.14%	0.022%
83	11.417	3129	3134	3135	rBV3	1290	880	0.03%	0.004%
84	11.687	3214	3218	3222	rVB3	445	405	0.01%	0.002%
85	11.815	3245	3258	3274	rBV	544729	864572	26.95%	4.251%
86	12.195	3362	3376	3401	rBV	1210160	1950089	60.79%	9.588%
87	12.452	3454	3456	3459	rBV2	473	324	0.01%	0.002%
88	12.558	3486	3489	3495	rBV3	707	788	0.02%	0.004%
89	12.732	3541	3543	3548	rBV2	503	482	0.02%	0.002%

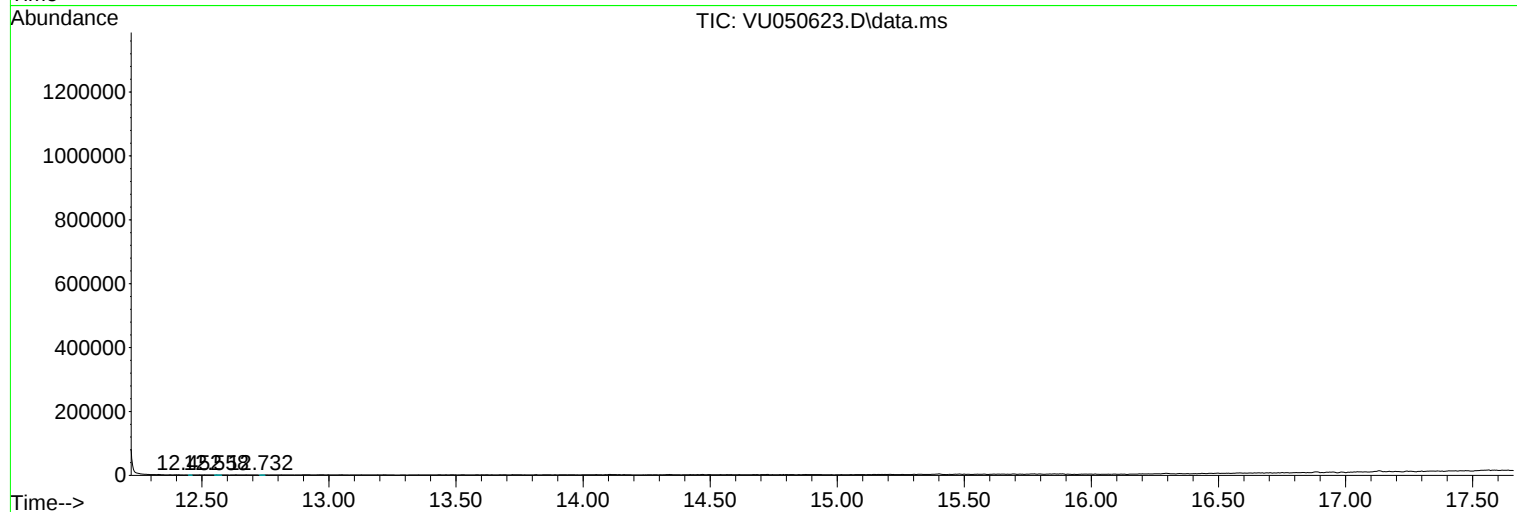
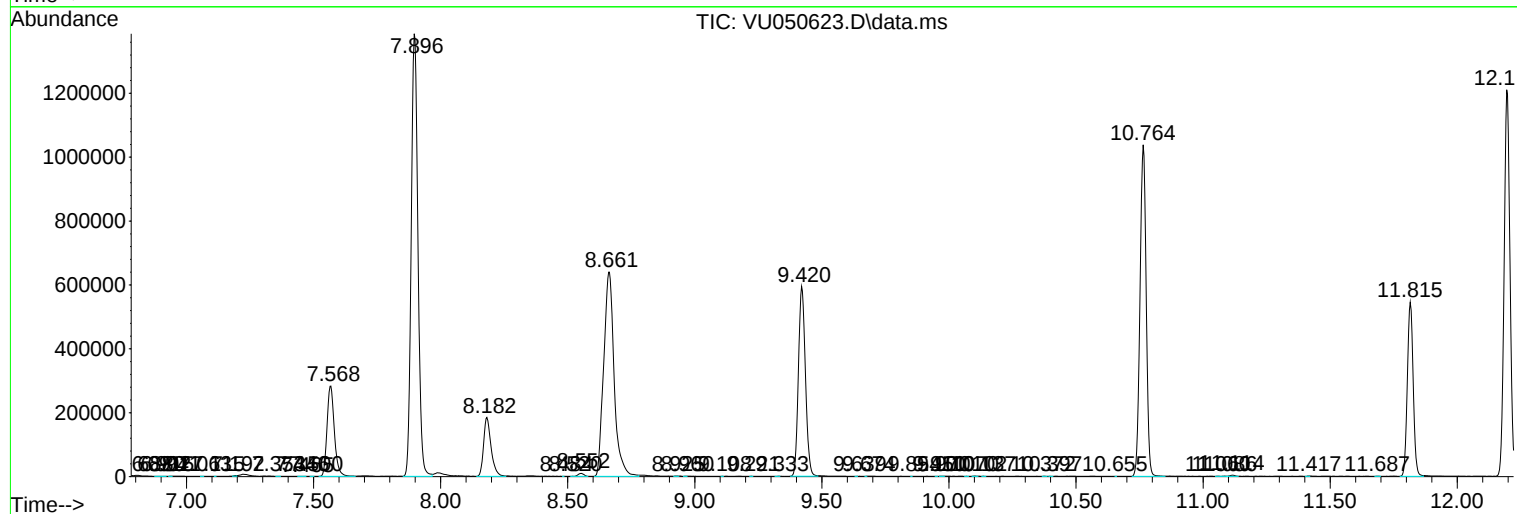
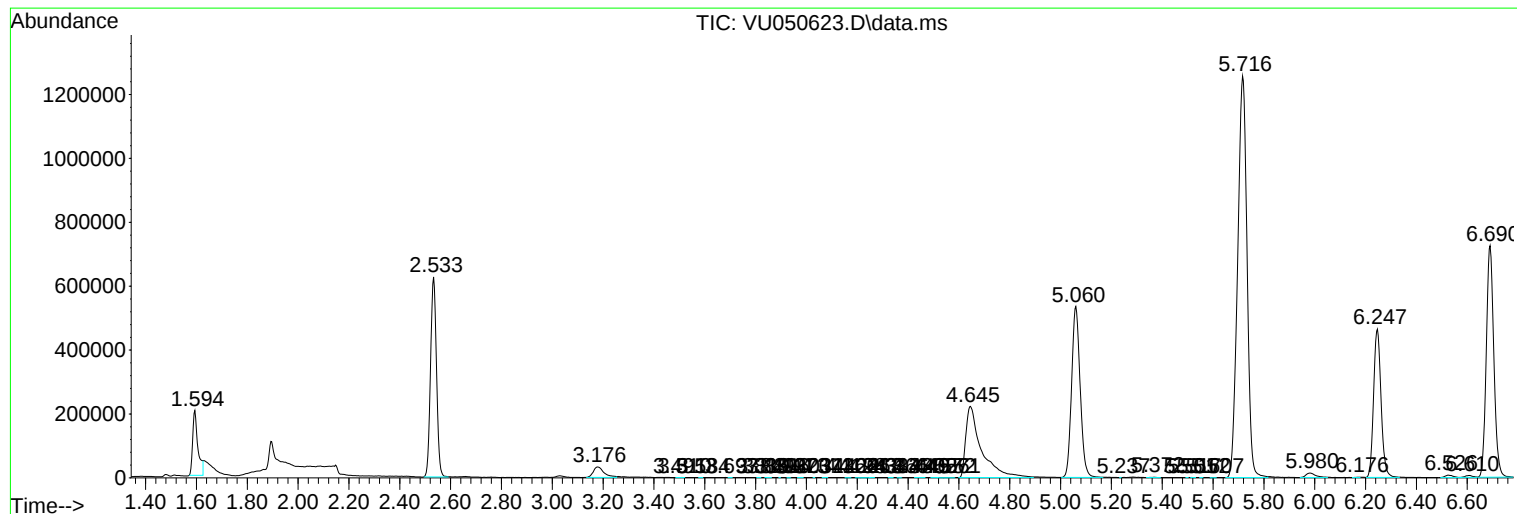
Sum of corrected areas: 20337835

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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



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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
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No Library Search Compounds Detected

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TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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