

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
 Data File : VX025676.D
 Acq On : 09 Dec 2021 21:50
 Operator : JC/MD
 Sample : M5004-03 20X
 Misc : 5.35g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGKW2

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_X\Method\SFAMXML112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025676.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	56	rVB	62892	62378	15.68%	1.991%
2	1.660	90	94	103	rBV	45636	57402	14.43%	1.832%
3	2.307	194	200	210	rBV	96089	152106	38.25%	4.856%
4	2.709	262	266	271	rBV	293	570	0.14%	0.018%
5	2.794	276	280	284	rVB4	1039	1613	0.41%	0.051%
6	2.947	297	305	313	rVB2	2664	6487	1.63%	0.207%
7	3.099	328	330	332	rBV	241	192	0.05%	0.006%
8	3.136	335	336	338	rBV	331	215	0.05%	0.007%
9	3.312	361	365	367	rBV2	181	214	0.05%	0.007%
10	3.489	393	394	397	rBV2	255	306	0.08%	0.010%
11	3.934	465	467	468	rBV	283	211	0.05%	0.007%
12	4.081	489	491	494	rVB	339	321	0.08%	0.010%
13	4.459	544	553	569	rBV	28774	80657	20.28%	2.575%
14	4.739	596	599	603	rBV	161	277	0.07%	0.009%
15	4.891	621	624	625	rBV2	350	328	0.08%	0.010%
16	4.904	625	626	628	rBV	266	211	0.05%	0.007%
17	5.062	641	652	671	rVB	54015	162520	40.86%	5.188%
18	5.245	681	682	686	rBV2	262	196	0.05%	0.006%
19	5.294	686	690	692	rBV2	251	268	0.07%	0.009%
20	5.318	692	694	696	rVB	273	204	0.05%	0.007%
21	5.343	696	698	700	rBV2	204	237	0.06%	0.008%
22	5.477	718	720	723	rVB	282	237	0.06%	0.008%
23	5.611	740	742	744	rBV	199	204	0.05%	0.007%
24	5.641	744	747	748	rVB	203	183	0.05%	0.006%
25	5.757	764	766	768	rBV	262	181	0.05%	0.006%
26	5.855	778	782	783	rVB	295	261	0.07%	0.008%
27	5.885	785	787	788	rVB	316	192	0.05%	0.006%
28	5.971	788	801	816	rBV2	132708	397703	100.00%	12.695%
29	6.342	861	862	863	rBV	437	217	0.05%	0.007%
30	6.458	879	881	883	rVB2	352	184	0.05%	0.006%
31	6.477	883	884	887	rBV	209	214	0.05%	0.007%
32	6.605	902	905	907	rBV	333	440	0.11%	0.014%
33	6.763	922	931	946	rBV	108613	261102	65.65%	8.335%
34	7.111	983	988	994	rVB4	2371	5351	1.35%	0.171%
35	7.159	994	996	997	rBV	259	248	0.06%	0.008%
36	7.312	1013	1021	1033	rVB	80915	174609	43.90%	5.574%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
 Title : VOC Analysis

37	7.476	1046	1048	1052	rVB2	398	334	0.08%	0.011%
38	7.525	1054	1056	1058	rBV	329	305	0.08%	0.010%
39	7.592	1064	1067	1069	rBV	214	320	0.08%	0.010%
40	7.671	1078	1080	1081	rBV	305	255	0.06%	0.008%
41	8.092	1147	1149	1150	rBV	241	207	0.05%	0.007%
42	8.220	1168	1170	1171	rBV2	251	227	0.06%	0.007%
43	8.324	1181	1187	1197	rVV	56653	93876	23.60%	2.997%
44	8.574	1225	1228	1232	rBV	145	228	0.06%	0.007%
45	8.653	1234	1241	1248	rBV	212241	335817	84.44%	10.720%
46	8.720	1249	1252	1258	rVV	3288	4540	1.14%	0.145%
47	8.769	1258	1260	1261	rVB	377	208	0.05%	0.007%
48	8.885	1277	1279	1281	rVB	318	275	0.07%	0.009%
49	8.909	1281	1283	1285	rBV	378	430	0.11%	0.014%
50	8.952	1285	1290	1299	rVB	39564	57660	14.50%	1.841%
51	9.068	1307	1309	1311	rVB2	228	210	0.05%	0.007%
52	9.122	1316	1318	1319	rBV2	268	225	0.06%	0.007%
53	9.275	1339	1343	1348	rVV3	2746	4129	1.04%	0.132%
54	9.385	1356	1361	1376	rVV	124174	181676	45.68%	5.799%
55	9.506	1380	1381	1383	rBV	307	220	0.06%	0.007%
56	9.567	1390	1391	1393	rBV	257	210	0.05%	0.007%
57	9.610	1395	1398	1402	rBV	276	416	0.10%	0.013%
58	9.763	1421	1423	1427	rBV2	377	440	0.11%	0.014%
59	9.897	1444	1445	1447	rBV	293	214	0.05%	0.007%
60	10.055	1465	1471	1482	rBV	230989	314309	79.03%	10.033%
61	10.269	1504	1506	1509	rVB	318	283	0.07%	0.009%
62	10.305	1509	1512	1515	rBV2	452	577	0.15%	0.018%
63	10.439	1532	1534	1535	rBV	259	188	0.05%	0.006%
64	10.805	1591	1594	1595	rVB2	253	207	0.05%	0.007%
65	10.988	1622	1624	1626	rVB	319	180	0.05%	0.006%
66	11.122	1642	1646	1650	rVB3	1372	1950	0.49%	0.062%
67	11.195	1653	1658	1667	rVB	146893	185030	46.52%	5.907%
68	11.482	1703	1705	1709	rVB	345	314	0.08%	0.010%
69	11.555	1714	1717	1719	rBV	404	368	0.09%	0.012%
70	11.750	1745	1749	1752	rVB4	1348	1725	0.43%	0.055%
71	11.841	1762	1764	1765	rBV2	264	238	0.06%	0.008%
72	11.933	1777	1779	1782	rVB2	500	491	0.12%	0.016%
73	12.024	1789	1794	1801	rBV	232153	288565	72.56%	9.212%
74	12.122	1808	1810	1813	rBV2	511	705	0.18%	0.023%
75	12.152	1813	1815	1818	rVB	1303	1234	0.31%	0.039%
76	12.323	1835	1843	1853	rBV	214018	278692	70.08%	8.896%

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77	12.421	1858	1859	1863	rVV2	408	531	0.13%	0.017%
78	12.488	1868	1870	1873	rBV2	318	270	0.07%	0.009%
79	12.701	1902	1905	1907	rBV	255	333	0.08%	0.011%
80	12.762	1912	1915	1918	rVV2	397	463	0.12%	0.015%
81	12.799	1918	1921	1924	rVV2	219	270	0.07%	0.009%
82	12.829	1924	1926	1928	rVV	323	234	0.06%	0.007%
83	12.860	1929	1931	1932	rVB2	325	186	0.05%	0.006%
84	13.024	1955	1958	1960	rBV	152	208	0.05%	0.007%
85	13.268	1996	1998	2001	rBV	193	213	0.05%	0.007%
86	13.500	2034	2036	2039	rVB2	306	365	0.09%	0.012%
87	13.536	2039	2042	2045	rVB2	282	422	0.11%	0.013%
88	13.573	2045	2048	2050	rBV	299	275	0.07%	0.009%
89	13.744	2074	2076	2079	rVB	342	245	0.06%	0.008%
90	13.829	2089	2090	2093	rBV2	341	385	0.10%	0.012%
91	13.884	2097	2099	2100	rBV2	248	244	0.06%	0.008%
92	14.609	2217	2218	2221	rBV	279	259	0.07%	0.008%
93	14.652	2223	2225	2226	rVV	292	190	0.05%	0.006%
94	14.945	2271	2273	2274	rBV	310	206	0.05%	0.007%
95	15.792	2411	2412	2415	rBV2	356	402	0.10%	0.013%
96	15.981	2441	2443	2448	rVB3	318	397	0.10%	0.013%
97	16.292	2493	2494	2496	rVB	421	180	0.05%	0.006%
98	16.426	2514	2516	2518	rBV2	274	241	0.06%	0.008%
99	16.505	2528	2529	2531	rBV	331	221	0.06%	0.007%
100	16.767	2571	2572	2574	rVB	329	184	0.05%	0.006%

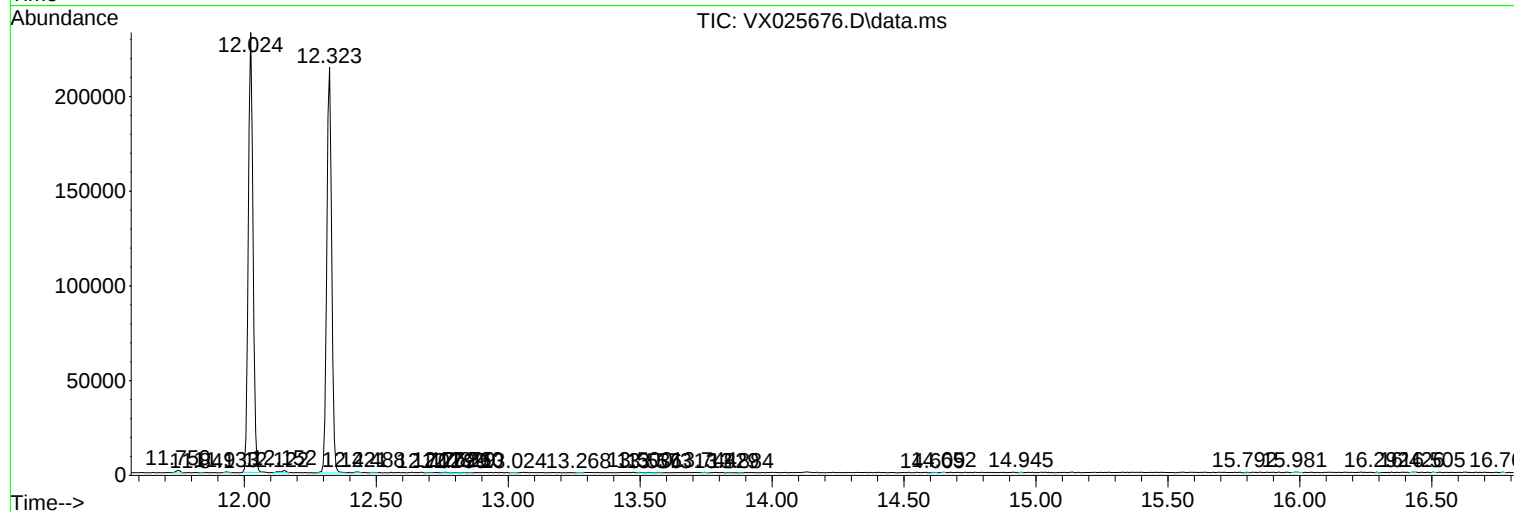
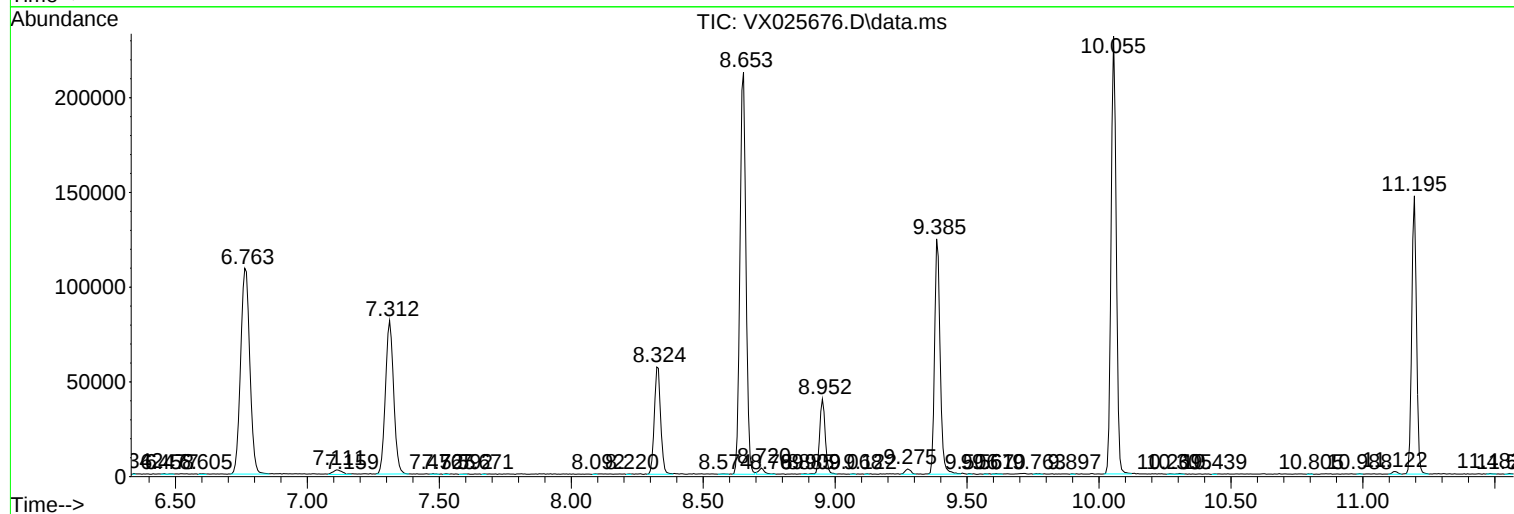
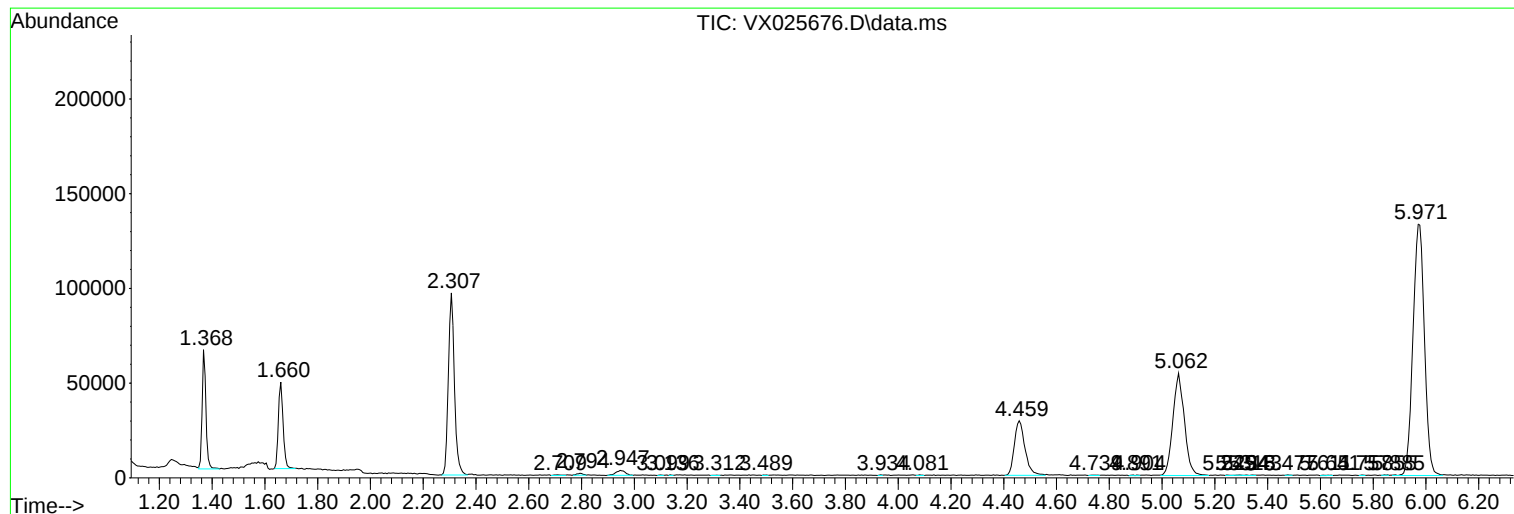
Sum of corrected areas: 3132641

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.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