

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
 Data File : VX025680.D
 Acq On : 09 Dec 2021 23:23
 Operator : JC/MD
 Sample : M5004-07ME
 Misc : 6.61g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGKW6ME

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: VX025680.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	54	rVB	61548	59690	15.36%	1.956%
2	1.660	90	94	100	rBV	46557	56139	14.44%	1.840%
3	2.307	194	200	210	rBV	90832	145651	37.48%	4.774%
4	2.428	218	220	221	rVB	352	168	0.04%	0.006%
5	2.630	251	253	256	rBV	306	274	0.07%	0.009%
6	2.721	267	268	269	rBV	287	200	0.05%	0.007%
7	2.800	275	281	285	rBV3	897	1810	0.47%	0.059%
8	2.947	298	305	315	rVB	4530	10309	2.65%	0.338%
9	3.062	321	324	325	rBV	254	307	0.08%	0.010%
10	3.514	395	398	399	rBV	319	275	0.07%	0.009%
11	3.611	411	414	416	rBV2	350	357	0.09%	0.012%
12	3.873	455	457	458	rBV2	234	205	0.05%	0.007%
13	4.105	494	495	496	rBV	260	169	0.04%	0.006%
14	4.227	511	515	520	rVB2	260	355	0.09%	0.012%
15	4.318	528	530	533	rVB	308	309	0.08%	0.010%
16	4.349	533	535	537	rBV	303	333	0.09%	0.011%
17	4.459	544	553	569	rBV	26775	77580	19.96%	2.543%
18	4.654	584	585	587	rBV	206	205	0.05%	0.007%
19	4.733	596	598	601	rBV	208	176	0.05%	0.006%
20	4.769	601	604	606	rVB	416	374	0.10%	0.012%
21	4.800	606	609	610	rBV2	312	266	0.07%	0.009%
22	4.885	620	623	626	rBV	265	353	0.09%	0.012%
23	5.062	640	652	670	rBV	49888	155440	40.00%	5.095%
24	5.221	676	678	679	rBV	298	203	0.05%	0.007%
25	5.404	706	708	710	rBV	289	307	0.08%	0.010%
26	5.605	737	741	744	rBV	267	451	0.12%	0.015%
27	5.739	760	763	764	rVB	224	221	0.06%	0.007%
28	5.781	768	770	775	rVB2	307	416	0.11%	0.014%
29	5.824	775	777	779	rBV	261	290	0.07%	0.010%
30	5.873	783	785	788	rBV2	201	266	0.07%	0.009%
31	5.970	790	801	818	rBV2	129812	388646	100.00%	12.738%
32	6.385	867	869	871	rVB	343	267	0.07%	0.009%
33	6.763	922	931	944	rBV	107891	256395	65.97%	8.403%
34	7.117	983	989	995	rBV3	2352	4840	1.25%	0.159%
35	7.312	1012	1021	1034	rBV	78036	172008	44.26%	5.638%
36	7.549	1058	1060	1065	rBV2	177	250	0.06%	0.008%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
 Title : VOC Analysis

37	7.696	1082	1084	1086	rBV	202	173	0.04%	0.006%
38	8.025	1136	1138	1139	rBV	184	182	0.05%	0.006%
39	8.324	1181	1187	1196	rBV	56595	91693	23.59%	3.005%
40	8.537	1219	1222	1224	rVV	272	276	0.07%	0.009%
41	8.574	1226	1228	1230	rBV2	202	226	0.06%	0.007%
42	8.604	1230	1233	1234	rVV	336	323	0.08%	0.011%
43	8.653	1234	1241	1248	rVV	209351	325675	83.80%	10.674%
44	8.720	1249	1252	1259	rVB	2809	4518	1.16%	0.148%
45	8.842	1268	1272	1273	rBV	311	379	0.10%	0.012%
46	8.860	1273	1275	1277	rBV2	239	277	0.07%	0.009%
47	8.952	1285	1290	1298	rBV	39345	55903	14.38%	1.832%
48	9.232	1334	1336	1337	rBV	221	182	0.05%	0.006%
49	9.275	1339	1343	1347	rVB4	1964	2940	0.76%	0.096%
50	9.384	1356	1361	1372	rBV	115430	169800	43.69%	5.565%
51	9.683	1408	1410	1413	rBV2	296	426	0.11%	0.014%
52	9.884	1441	1443	1447	rVB	306	269	0.07%	0.009%
53	10.055	1465	1471	1486	rBV	230797	310580	79.91%	10.179%
54	10.244	1501	1502	1506	rVB	384	399	0.10%	0.013%
55	10.397	1525	1527	1530	rBV	270	196	0.05%	0.006%
56	10.549	1550	1552	1554	rBV2	183	193	0.05%	0.006%
57	10.677	1570	1573	1575	rBV	360	392	0.10%	0.013%
58	10.909	1610	1611	1613	rBV	289	199	0.05%	0.007%
59	11.098	1640	1642	1643	rBV	328	279	0.07%	0.009%
60	11.122	1643	1646	1650	rVV2	1611	1753	0.45%	0.057%
61	11.195	1653	1658	1670	rVB	142276	181462	46.69%	5.947%
62	11.280	1670	1672	1674	rBV	549	578	0.15%	0.019%
63	11.433	1695	1697	1699	rBV	376	277	0.07%	0.009%
64	11.476	1702	1704	1706	rVB	288	240	0.06%	0.008%
65	11.500	1706	1708	1710	rBV	195	194	0.05%	0.006%
66	11.567	1717	1719	1721	rBV2	216	242	0.06%	0.008%
67	11.591	1721	1723	1724	rBV	399	224	0.06%	0.007%
68	11.750	1746	1749	1751	rBV3	800	860	0.22%	0.028%
69	11.841	1762	1764	1766	rVB2	380	367	0.09%	0.012%
70	11.927	1776	1778	1783	rVB3	613	821	0.21%	0.027%
71	12.024	1789	1794	1805	rVV	225853	285698	73.51%	9.364%
72	12.152	1808	1815	1818	rVV2	1172	1992	0.51%	0.065%
73	12.323	1837	1843	1850	rVB	209879	266909	68.68%	8.748%
74	12.427	1857	1860	1864	rVB3	506	719	0.19%	0.024%
75	12.457	1864	1865	1867	rBV	296	305	0.08%	0.010%
76	12.500	1870	1872	1876	rVV2	276	322	0.08%	0.011%

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Integrator: RTE

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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

77	12.640	1894	1895	1896	rBV	478	291	0.07%	0.010%
78	12.658	1896	1898	1903	rVV	536	662	0.17%	0.022%
79	12.701	1903	1905	1908	rVB	367	219	0.06%	0.007%
80	12.817	1922	1924	1927	rBV2	275	330	0.08%	0.011%
81	12.841	1927	1928	1930	rVV	391	229	0.06%	0.008%
82	13.359	2011	2013	2015	rVB	367	203	0.05%	0.007%
83	13.512	2036	2038	2041	rVB2	379	339	0.09%	0.011%
84	13.579	2047	2049	2050	rVB	322	173	0.04%	0.006%
85	13.597	2050	2052	2054	rBV	248	295	0.08%	0.010%
86	13.902	2100	2102	2105	rBV2	336	352	0.09%	0.012%
87	13.945	2107	2109	2111	rVB	260	182	0.05%	0.006%
88	14.060	2126	2128	2129	rBV2	291	202	0.05%	0.007%
89	14.359	2173	2177	2180	rBV2	325	537	0.14%	0.018%
90	14.548	2206	2208	2209	rVV	312	217	0.06%	0.007%
91	14.603	2215	2217	2218	rBV	216	172	0.04%	0.006%
92	15.146	2303	2306	2308	rBV2	256	368	0.09%	0.012%
93	15.444	2353	2355	2356	rVB	406	204	0.05%	0.007%
94	15.603	2379	2381	2384	rBV2	243	179	0.05%	0.006%
95	15.731	2400	2402	2405	rVB2	314	303	0.08%	0.010%
96	16.389	2509	2510	2513	rBV	354	362	0.09%	0.012%
97	16.499	2525	2528	2530	rBV2	318	443	0.11%	0.015%
98	16.554	2536	2537	2540	rBV3	274	315	0.08%	0.010%
99	16.603	2543	2545	2547	rBV2	315	310	0.08%	0.010%
100	16.761	2569	2571	2572	rBV	333	255	0.07%	0.008%

Sum of corrected areas: 3051090

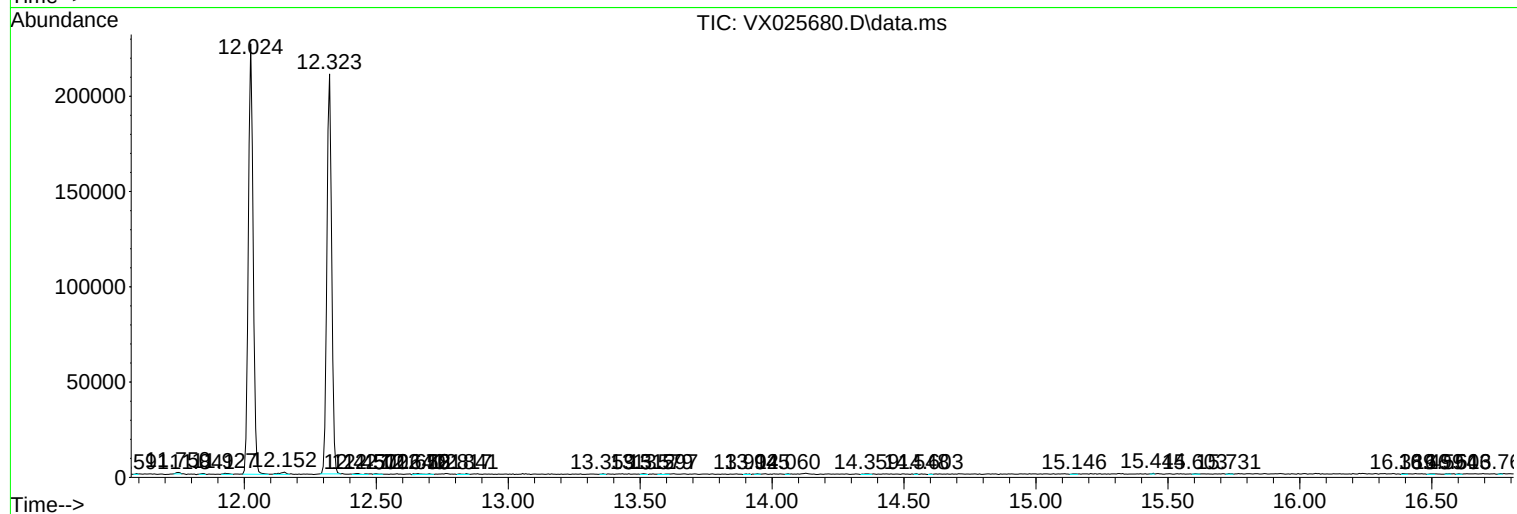
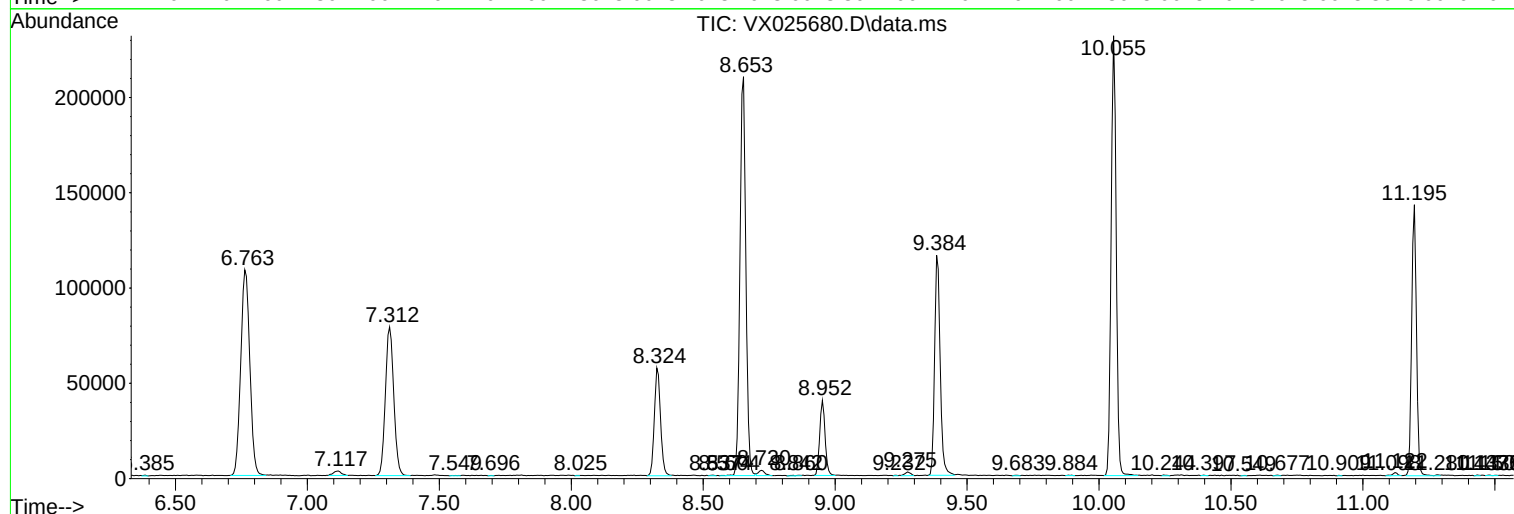
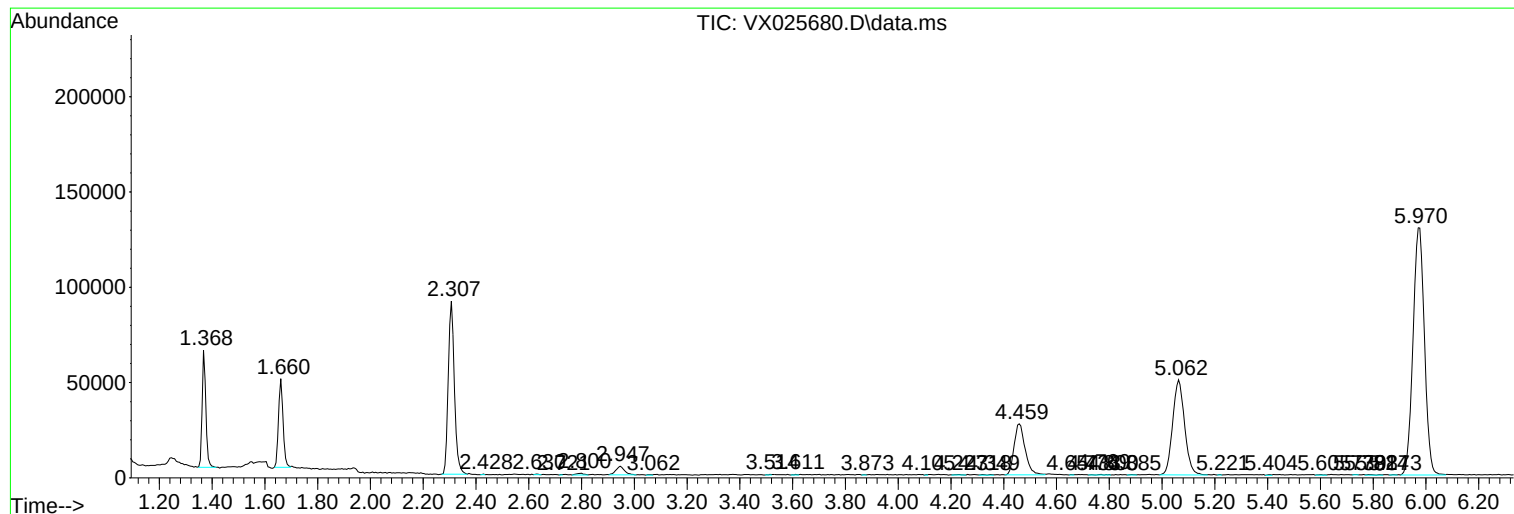
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Instrument :
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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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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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