

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
 Data File : VX026070.D
 Acq On : 27 Dec 2021 18:27
 Operator : JC/MD
 Sample : M5174-01ME
 Misc : 4.61g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GBC12ME

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\SFAMXML122321WMA.M
 Title : VOC Analysis

Signal : TIC: VX026070.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	54	rVB	95223	112276	13.34%	1.849%
2	1.666	92	95	103	rVB	58850	82904	9.85%	1.365%
3	2.288	191	197	206	rBV	185222	291653	34.66%	4.804%
4	2.648	253	256	258	rBV3	347	495	0.06%	0.008%
5	2.721	263	268	274	rBV3	1396	2716	0.32%	0.045%
6	2.788	274	279	285	rVB4	2564	5254	0.62%	0.087%
7	2.849	285	289	290	rBV3	312	429	0.05%	0.007%
8	2.947	299	305	310	rBV4	842	2066	0.25%	0.034%
9	3.075	324	326	330	rBV2	298	435	0.05%	0.007%
10	3.123	333	334	336	rBV2	226	195	0.02%	0.003%
11	3.196	343	346	351	rVB2	301	303	0.04%	0.005%
12	3.282	357	360	362	rBV2	186	194	0.02%	0.003%
13	3.526	399	400	402	rBV2	194	176	0.02%	0.003%
14	3.605	410	413	414	rVB2	318	319	0.04%	0.005%
15	3.623	414	416	419	rBV2	204	234	0.03%	0.004%
16	3.660	419	422	425	rVB2	433	423	0.05%	0.007%
17	3.757	435	438	439	rBV	205	256	0.03%	0.004%
18	4.111	493	496	498	rBV	195	211	0.03%	0.003%
19	4.160	503	504	507	rBV2	225	184	0.02%	0.003%
20	4.294	524	526	529	rVB2	254	308	0.04%	0.005%
21	4.489	548	558	576	rBV	34132	153823	18.28%	2.534%
22	4.824	611	613	614	rBV	396	234	0.03%	0.004%
23	4.861	618	619	621	rBV2	342	264	0.03%	0.004%
24	5.068	637	653	672	rBV	99612	319914	38.02%	5.269%
25	5.330	692	696	700	rBV2	135	195	0.02%	0.003%
26	5.470	717	719	721	rBV	166	205	0.02%	0.003%
27	5.617	742	743	747	rBV2	210	235	0.03%	0.004%
28	5.684	752	754	756	rVB	264	204	0.02%	0.003%
29	5.970	788	801	817	rBV3	298460	841425	100.00%	13.859%
30	6.184	834	836	838	rBV2	292	256	0.03%	0.004%
31	6.245	844	846	848	rBV2	258	225	0.03%	0.004%
32	6.287	851	853	856	rVB	265	201	0.02%	0.003%
33	6.330	858	860	863	rBV	246	281	0.03%	0.005%
34	6.361	863	865	867	rBV3	418	503	0.06%	0.008%
35	6.763	921	931	945	rBV	181081	440985	52.41%	7.263%
36	6.946	959	961	963	rVB2	274	197	0.02%	0.003%

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 Title : VOC Analysis

37	7.049	976	978	980	rBV2	236	272	0.03%	0.004%
38	7.110	982	988	996	rVB3	3364	7928	0.94%	0.131%
39	7.214	999	1005	1007	rBV3	872	1278	0.15%	0.021%
40	7.312	1012	1021	1040	rVB	166369	375409	44.62%	6.183%
41	7.440	1040	1042	1045	rVB	366	363	0.04%	0.006%
42	7.482	1045	1049	1050	rBV	702	791	0.09%	0.013%
43	7.604	1067	1069	1070	rVB	289	191	0.02%	0.003%
44	7.720	1087	1088	1090	rBV	300	255	0.03%	0.004%
45	7.757	1093	1094	1096	rBV	321	192	0.02%	0.003%
46	7.787	1096	1099	1100	rVB	272	223	0.03%	0.004%
47	8.019	1135	1137	1143	rVB2	271	304	0.04%	0.005%
48	8.110	1149	1152	1153	rBV	303	251	0.03%	0.004%
49	8.250	1170	1175	1181	rBV4	3685	6412	0.76%	0.106%
50	8.330	1181	1188	1198	rVB	94097	157945	18.77%	2.601%
51	8.464	1208	1210	1213	rBV2	270	328	0.04%	0.005%
52	8.488	1213	1214	1216	rBV	359	259	0.03%	0.004%
53	8.561	1223	1226	1228	rBV2	241	218	0.03%	0.004%
54	8.653	1234	1241	1248	rBV	408211	660116	78.45%	10.873%
55	8.909	1280	1283	1284	rBV2	331	268	0.03%	0.004%
56	8.952	1285	1290	1302	rVV	58287	94630	11.25%	1.559%
57	9.202	1329	1331	1334	rBV	191	210	0.02%	0.003%
58	9.275	1339	1343	1348	rBV3	6629	11194	1.33%	0.184%
59	9.342	1349	1354	1357	rVV3	3884	8540	1.01%	0.141%
60	9.415	1358	1366	1378	rVB	158405	366382	43.54%	6.035%
61	9.622	1396	1400	1402	rVB3	782	956	0.11%	0.016%
62	9.714	1412	1415	1421	rVB2	687	1150	0.14%	0.019%
63	9.787	1424	1427	1428	rBV	334	283	0.03%	0.005%
64	9.890	1442	1444	1445	rBV	313	272	0.03%	0.004%
65	9.933	1449	1451	1453	rVV	284	252	0.03%	0.004%
66	10.000	1461	1462	1465	rBV3	254	290	0.03%	0.005%
67	10.055	1465	1471	1483	rVV	343942	528066	62.76%	8.698%
68	10.201	1491	1495	1498	rVB3	524	767	0.09%	0.013%
69	10.305	1507	1512	1518	rBV3	1842	3188	0.38%	0.053%
70	10.439	1531	1534	1535	rBV	261	236	0.03%	0.004%
71	10.567	1552	1555	1556	rBV	237	293	0.03%	0.005%
72	10.585	1556	1558	1561	rVB2	578	676	0.08%	0.011%
73	10.628	1563	1565	1566	rBV	269	224	0.03%	0.004%
74	10.652	1566	1569	1573	rBV4	553	852	0.10%	0.014%
75	10.756	1580	1586	1587	rBV2	480	752	0.09%	0.012%
76	10.774	1587	1589	1595	rVB5	840	1216	0.14%	0.020%

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 Title : VOC Analysis

77	10.854	1599	1602	1605	rBV4	470	733	0.09%	0.012%
78	11.030	1629	1631	1633	rVB3	305	227	0.03%	0.004%
79	11.079	1637	1639	1641	rBV3	375	363	0.04%	0.006%
80	11.122	1641	1646	1650	rVB2	6109	7693	0.91%	0.127%
81	11.201	1653	1659	1668	rBV	268407	369960	43.97%	6.094%
82	11.323	1675	1679	1684	rVB3	7682	12333	1.47%	0.203%
83	11.396	1687	1691	1694	rBV3	804	1112	0.13%	0.018%
84	11.482	1701	1705	1709	rBV4	3123	4097	0.49%	0.067%
85	11.549	1714	1716	1719	rVB2	772	636	0.08%	0.010%
86	11.634	1727	1730	1734	rVB2	1079	1332	0.16%	0.022%
87	11.689	1734	1739	1741	rBV4	1358	2114	0.25%	0.035%
88	11.713	1741	1743	1746	rVV3	1809	2360	0.28%	0.039%
89	11.750	1746	1749	1757	rVB3	5802	9417	1.12%	0.155%
90	11.841	1759	1764	1769	rBV6	1963	3621	0.43%	0.060%
91	11.933	1776	1779	1783	rVB3	2945	3500	0.42%	0.058%
92	12.024	1789	1794	1800	rBV	423870	535145	63.60%	8.814%
93	12.152	1812	1815	1824	rVB5	6024	11804	1.40%	0.194%
94	12.323	1838	1843	1850	rVB	454680	573583	68.17%	9.447%
95	12.427	1856	1860	1864	rBV2	4068	5194	0.62%	0.086%
96	12.768	1913	1916	1919	rVB	3358	3837	0.46%	0.063%
97	12.920	1931	1941	1945	rBV8	2429	6896	0.82%	0.114%
98	13.384	2013	2017	2019	rBV4	2061	2671	0.32%	0.044%
99	13.847	2089	2093	2096	rBV5	2042	3005	0.36%	0.049%
100	15.420	2348	2351	2358	rVB3	11116	16123	1.92%	0.266%

Sum of corrected areas: 6071366

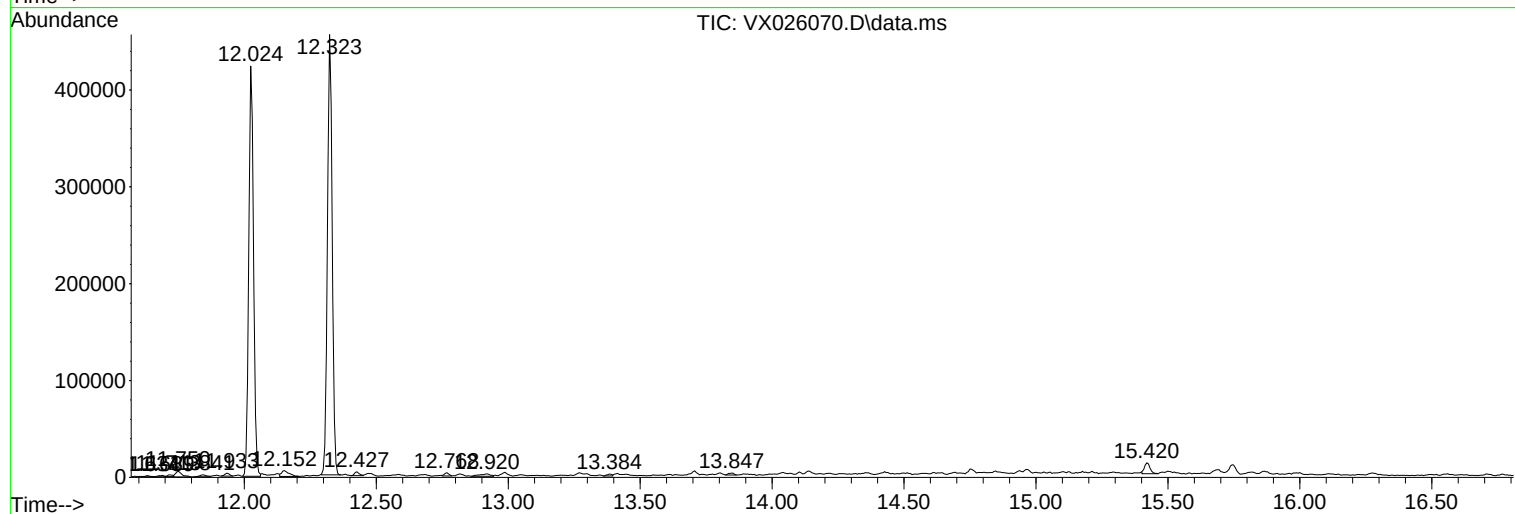
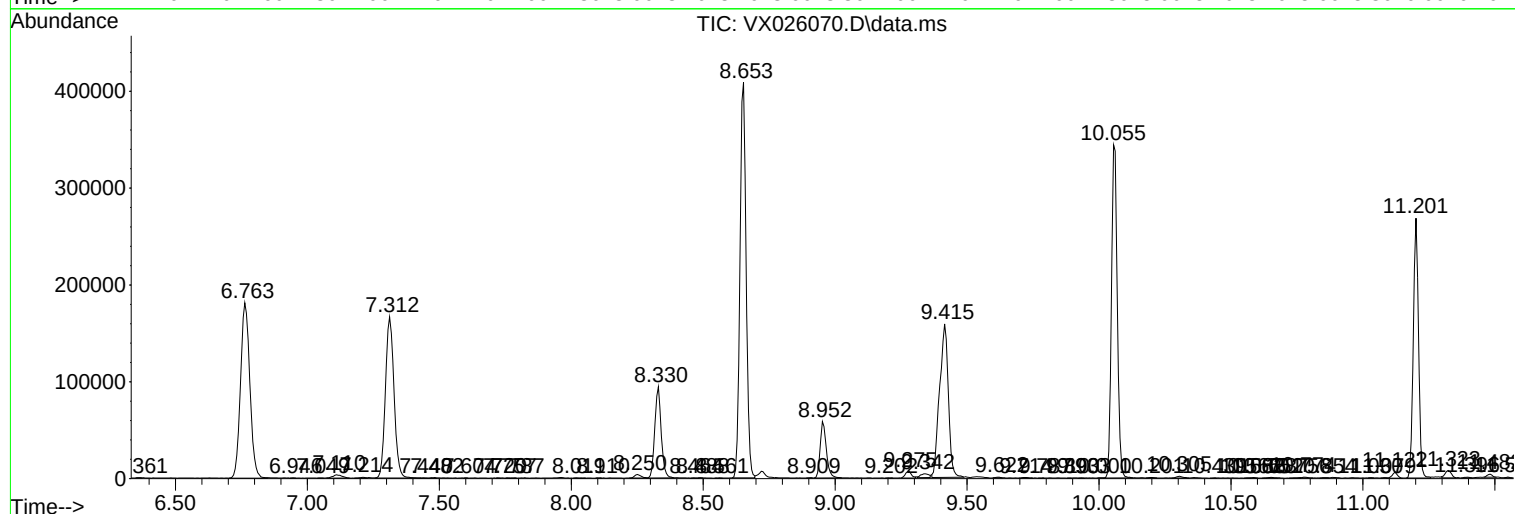
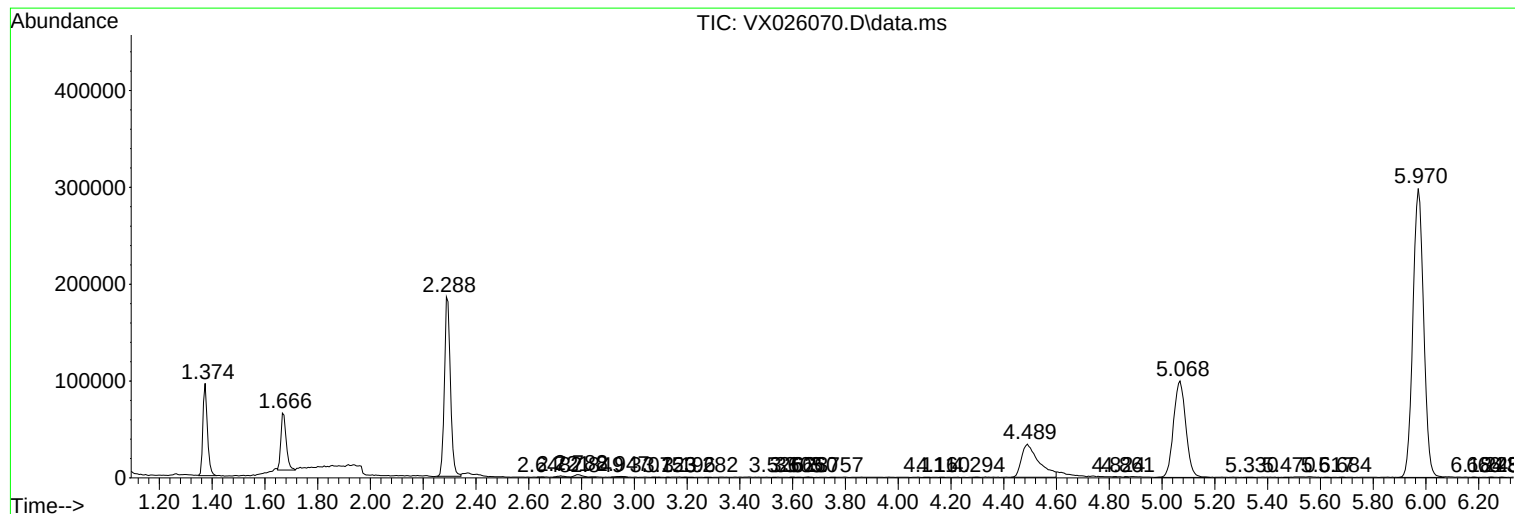
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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\SFAMXML122321WMA.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