

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
 Data File : VX026010.D
 Acq On : 24 Dec 2021 12:16
 Operator : JC/MD
 Sample : VX1224MBL01
 Misc : 5.0g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK659

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\SFAMXLM122321WMA.M
 Title : VOC Analysis

Signal : TIC: VX026010.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	53	rVB	146499	148652	13.73%	1.789%
2	1.666	91	95	107	rVB	104748	137552	12.71%	1.656%
3	2.313	194	201	211	rBV	230270	381107	35.20%	4.587%
4	2.514	232	234	241	rVB3	1355	1975	0.18%	0.024%
5	2.581	243	245	247	rVB	354	272	0.03%	0.003%
6	2.605	247	249	250	rBV	318	287	0.03%	0.003%
7	2.697	262	264	265	rBV	260	227	0.02%	0.003%
8	2.794	275	280	285	rVB4	1796	2804	0.26%	0.034%
9	2.874	288	293	294	rBV3	346	377	0.03%	0.005%
10	3.105	326	331	334	rBV4	620	1023	0.09%	0.012%
11	3.191	342	345	346	rVB	324	267	0.02%	0.003%
12	3.264	353	357	360	rBV2	370	519	0.05%	0.006%
13	3.623	414	416	419	rVV	220	278	0.03%	0.003%
14	4.239	514	517	520	rBV2	245	283	0.03%	0.003%
15	4.453	543	552	565	rBV	79008	236169	21.82%	2.843%
16	4.904	623	626	630	rBV2	254	252	0.02%	0.003%
17	5.056	638	651	671	rBV2	122596	422574	39.03%	5.086%
18	5.239	679	681	683	rBV	348	268	0.02%	0.003%
19	5.379	702	704	705	rBV2	284	243	0.02%	0.003%
20	5.495	716	723	727	rVV4	692	1882	0.17%	0.023%
21	5.971	788	801	816	rBV2	360912	1082593	100.00%	13.031%
22	6.355	862	864	869	rVB2	307	416	0.04%	0.005%
23	6.525	891	892	896	rBV2	242	265	0.02%	0.003%
24	6.757	921	930	949	rVV	245297	593784	54.85%	7.147%
25	6.885	949	951	954	rVV3	297	398	0.04%	0.005%
26	6.928	956	958	960	rVV2	246	260	0.02%	0.003%
27	7.007	969	971	973	rVB2	330	269	0.02%	0.003%
28	7.111	982	988	994	rVV5	2067	4318	0.40%	0.052%
29	7.306	1011	1020	1035	rBV	230511	497779	45.98%	5.992%
30	7.476	1046	1048	1051	rVB2	554	501	0.05%	0.006%
31	7.708	1083	1086	1088	rBV2	157	239	0.02%	0.003%
32	7.757	1092	1094	1097	rBV2	215	230	0.02%	0.003%
33	7.799	1097	1101	1111	rVB3	463	1139	0.11%	0.014%
34	7.934	1118	1123	1126	rBV3	560	1056	0.10%	0.013%
35	8.031	1137	1139	1142	rBV3	215	230	0.02%	0.003%
36	8.202	1166	1167	1171	rVB	223	230	0.02%	0.003%

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 Title : VOC Analysis

37	8.324	1180	1187	1200	rBV	154211	245618	22.69%	2.956%
38	8.482	1207	1213	1214	rBV	248	441	0.04%	0.005%
39	8.574	1225	1228	1233	rVB3	555	797	0.07%	0.010%
40	8.647	1233	1240	1248	rBV	598484	912539	84.29%	10.984%
41	8.714	1248	1251	1260	rVB	8421	13957	1.29%	0.168%
42	8.952	1283	1290	1299	rBV	102556	153837	14.21%	1.852%
43	9.104	1312	1315	1317	rBV2	379	450	0.04%	0.005%
44	9.275	1339	1343	1345	rBV2	2180	2978	0.28%	0.036%
45	9.385	1355	1361	1379	rVB	394596	553916	51.17%	6.667%
46	9.506	1379	1381	1384	rVV3	598	479	0.04%	0.006%
47	9.555	1387	1389	1392	rBV3	280	283	0.03%	0.003%
48	9.695	1410	1412	1417	rVB2	1048	1336	0.12%	0.016%
49	9.842	1433	1436	1439	rBV	204	290	0.03%	0.003%
50	10.055	1465	1471	1481	rBV	574934	766685	70.82%	9.228%
51	10.195	1491	1494	1498	rVB2	1013	1109	0.10%	0.013%
52	10.256	1498	1504	1506	rBV	221	381	0.04%	0.005%
53	10.299	1508	1511	1517	rVB4	1722	2160	0.20%	0.026%
54	10.384	1522	1525	1528	rVB2	251	248	0.02%	0.003%
55	10.616	1561	1563	1565	rBV2	354	303	0.03%	0.004%
56	10.647	1565	1568	1573	rVV4	951	1392	0.13%	0.017%
57	10.866	1602	1604	1607	rBV2	361	426	0.04%	0.005%
58	10.890	1607	1608	1613	rBV2	315	342	0.03%	0.004%
59	10.964	1617	1620	1624	rVB4	428	598	0.06%	0.007%
60	11.043	1631	1633	1636	rVB2	227	248	0.02%	0.003%
61	11.085	1636	1640	1642	rBV2	223	359	0.03%	0.004%
62	11.122	1642	1646	1650	rVB	4294	5822	0.54%	0.070%
63	11.195	1652	1658	1665	rBV	410973	515858	47.65%	6.209%
64	11.323	1674	1679	1686	rVB3	2345	4258	0.39%	0.051%
65	11.384	1686	1689	1690	rBV2	348	402	0.04%	0.005%
66	11.451	1698	1700	1701	rBV2	592	552	0.05%	0.007%
67	11.543	1713	1715	1719	rVB2	604	567	0.05%	0.007%
68	11.616	1725	1727	1728	rBV	421	280	0.03%	0.003%
69	11.713	1741	1743	1744	rBV2	579	494	0.05%	0.006%
70	11.750	1744	1749	1753	rVB3	3997	5865	0.54%	0.071%
71	11.841	1760	1764	1769	rVB3	1067	1423	0.13%	0.017%
72	11.890	1769	1772	1774	rVB2	247	316	0.03%	0.004%
73	11.933	1774	1779	1783	rBV4	2279	3458	0.32%	0.042%
74	11.969	1783	1785	1788	rVB3	1008	968	0.09%	0.012%
75	12.024	1788	1794	1800	rBV	612936	763928	70.56%	9.195%
76	12.128	1806	1811	1812	rBV4	1764	2349	0.22%	0.028%

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77	12.152	1812	1815	1820	rVV	3215	3751	0.35%	0.045%
78	12.323	1835	1843	1850	rBV	603992	795871	73.52%	9.580%
79	12.421	1856	1859	1864	rVB3	1425	1897	0.18%	0.023%
80	12.634	1891	1894	1896	rBV	530	556	0.05%	0.007%
81	12.768	1912	1916	1922	rVB3	1292	1898	0.18%	0.023%
82	12.817	1922	1924	1927	rBV2	473	545	0.05%	0.007%
83	12.969	1947	1949	1952	rVB2	460	343	0.03%	0.004%
84	13.055	1960	1963	1969	rVV5	893	1169	0.11%	0.014%
85	13.116	1971	1973	1975	rVV	711	583	0.05%	0.007%
86	13.396	2016	2019	2020	rBV2	246	279	0.03%	0.003%
87	13.469	2030	2031	2034	rBV3	338	379	0.04%	0.005%
88	13.591	2048	2051	2056	rBV3	484	703	0.06%	0.008%
89	13.695	2066	2068	2069	rBV	280	259	0.02%	0.003%
90	13.780	2076	2082	2086	rBV3	1566	2167	0.20%	0.026%
91	13.926	2104	2106	2109	rVB3	263	237	0.02%	0.003%
92	13.963	2109	2112	2115	rBV3	560	678	0.06%	0.008%
93	14.134	2135	2140	2144	rBV	3582	4859	0.45%	0.058%
94	14.402	2182	2184	2188	rBV3	344	381	0.04%	0.005%
95	14.719	2234	2236	2238	rBV	372	240	0.02%	0.003%
96	15.530	2367	2369	2372	rBV3	447	454	0.04%	0.005%
97	15.835	2417	2419	2423	rVB3	785	985	0.09%	0.012%
98	16.024	2448	2450	2451	rBV2	596	381	0.04%	0.005%
99	16.292	2492	2494	2499	rVB3	597	736	0.07%	0.009%
100	16.328	2499	2500	2501	rBV	551	276	0.03%	0.003%

Sum of corrected areas: 8308057

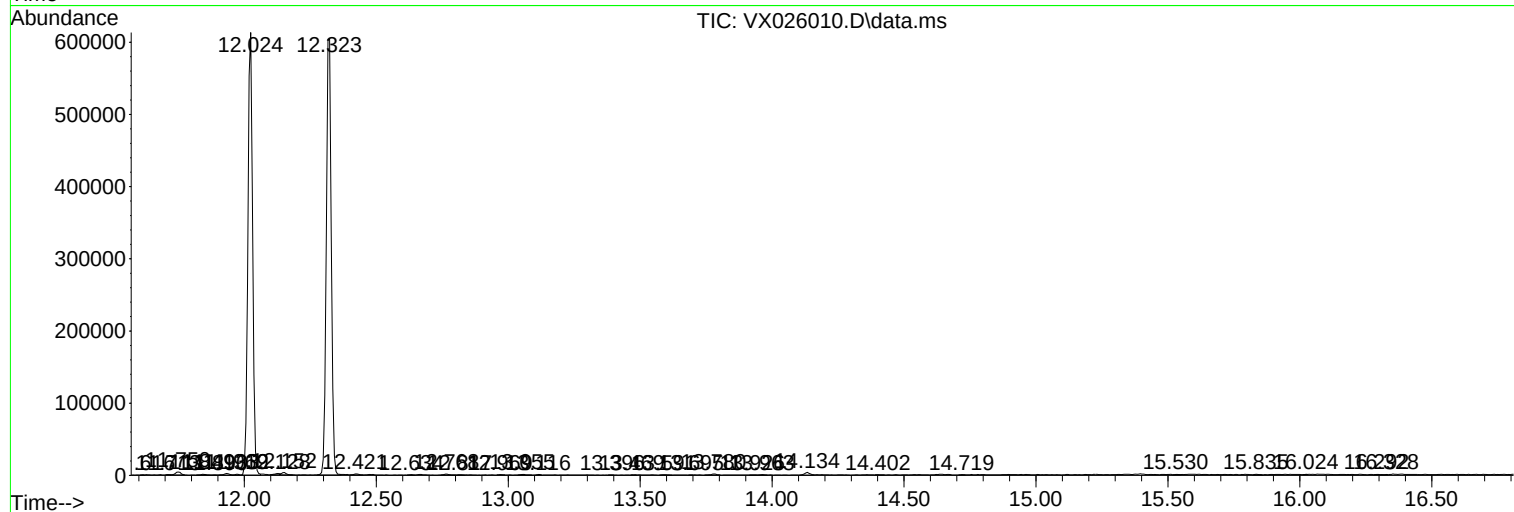
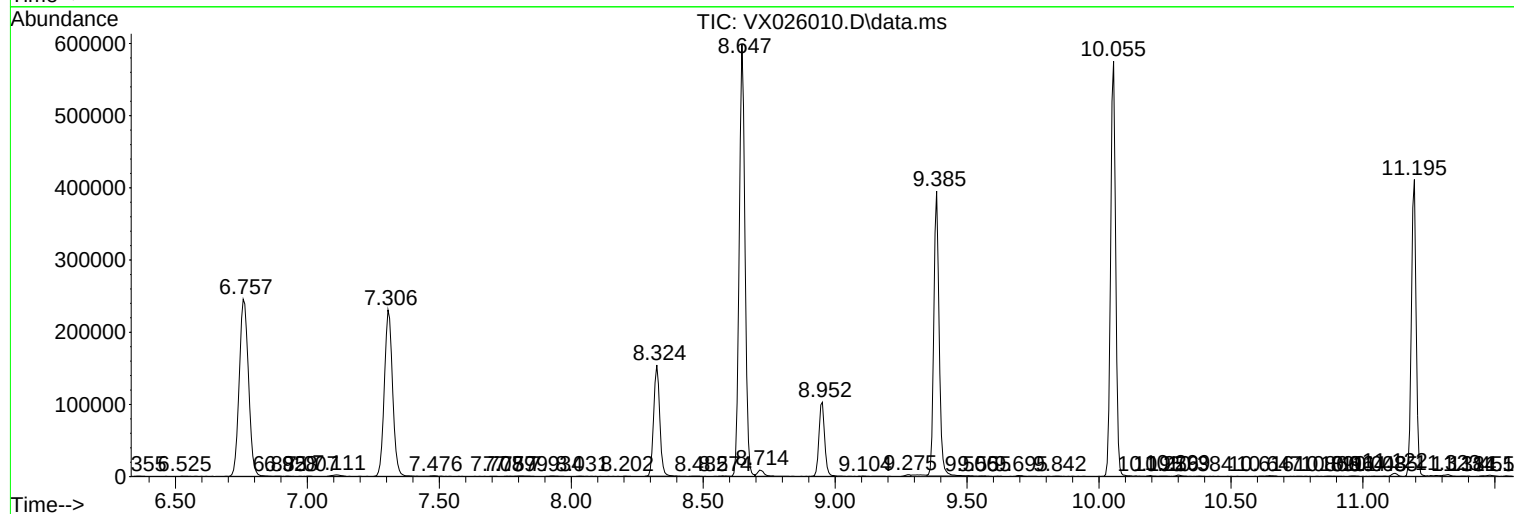
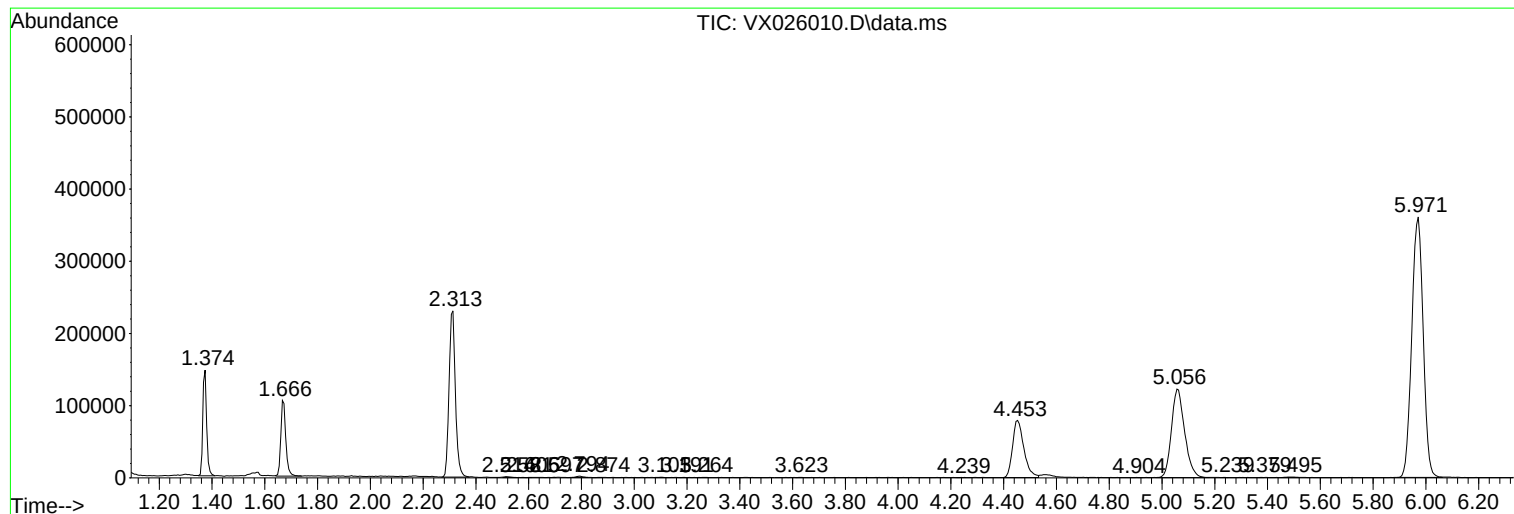
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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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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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