

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122321\
 Data File : VX025989.D
 Acq On : 23 Dec 2021 22:56
 Operator : JC/MD
 Sample : VX1223MBL01
 Misc : 5.0g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK657

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: VX025989.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	52	rVB	135446	130985	13.60%	1.840%
2	1.666	91	95	104	rVB	98938	124740	12.95%	1.753%
3	2.306	194	200	218	rVB	195216	331838	34.46%	4.662%
4	2.435	218	221	223	rBV3	649	759	0.08%	0.011%
5	2.514	230	234	239	rVB	1712	2790	0.29%	0.039%
6	2.794	276	280	288	rVB4	2738	4045	0.42%	0.057%
7	2.959	305	307	311	rVB2	292	271	0.03%	0.004%
8	3.099	323	330	336	rBV5	848	1733	0.18%	0.024%
9	3.361	371	373	376	rVB3	250	229	0.02%	0.003%
10	3.544	399	403	404	rVB2	208	224	0.02%	0.003%
11	4.093	492	493	496	rBV2	301	266	0.03%	0.004%
12	4.178	505	507	509	rVV	398	232	0.02%	0.003%
13	4.282	523	524	529	rBV2	235	391	0.04%	0.005%
14	4.459	544	553	567	rBV	78357	226609	23.53%	3.184%
15	4.782	603	606	608	rVV2	226	250	0.03%	0.004%
16	5.062	640	652	673	rVB2	119950	379417	39.40%	5.331%
17	5.379	702	704	705	rBV	314	223	0.02%	0.003%
18	5.489	718	722	724	rVB3	473	736	0.08%	0.010%
19	5.544	730	731	734	rBV	333	389	0.04%	0.005%
20	5.660	749	750	753	rBV	266	257	0.03%	0.004%
21	5.769	767	768	772	rVB2	222	275	0.03%	0.004%
22	5.977	789	802	817	rBV2	325460	963004	100.00%	13.531%
23	6.184	832	836	837	rVB2	300	294	0.03%	0.004%
24	6.214	839	841	842	rBV	305	225	0.02%	0.003%
25	6.452	878	880	884	rVB2	293	329	0.03%	0.005%
26	6.611	904	906	912	rVB2	223	232	0.02%	0.003%
27	6.763	922	931	945	rBV	208238	496715	51.58%	6.979%
28	6.915	954	956	959	rVV2	200	234	0.02%	0.003%
29	7.117	983	989	998	rVB7	2491	5709	0.59%	0.080%
30	7.312	1012	1021	1038	rBV	202719	440817	45.78%	6.194%
31	7.488	1045	1050	1055	rVB4	563	1126	0.12%	0.016%
32	7.653	1075	1077	1083	rBV2	183	254	0.03%	0.004%
33	7.757	1090	1094	1095	rBV	173	236	0.02%	0.003%
34	7.940	1119	1124	1125	rBV2	372	626	0.07%	0.009%
35	8.086	1144	1148	1151	rBV3	188	353	0.04%	0.005%
36	8.330	1180	1188	1197	rBV	125341	213123	22.13%	2.994%

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 Title : VOC Analysis

37	8.476	1209	1212	1214	rBV2	249	301	0.03%	0.004%
38	8.525	1218	1220	1225	rBV3	210	322	0.03%	0.005%
39	8.580	1225	1229	1231	rVB2	496	576	0.06%	0.008%
40	8.653	1234	1241	1248	rVV	479272	760917	79.01%	10.691%
41	8.720	1249	1252	1261	rVV	7418	11759	1.22%	0.165%
42	8.818	1263	1268	1269	rBV3	410	466	0.05%	0.007%
43	8.952	1284	1290	1301	rBV	89419	130322	13.53%	1.831%
44	9.104	1313	1315	1317	rBV3	332	334	0.03%	0.005%
45	9.281	1338	1344	1348	rBV	8386	14945	1.55%	0.210%
46	9.384	1356	1361	1375	rVB	363226	499749	51.89%	7.022%
47	9.641	1401	1403	1407	rVB2	346	396	0.04%	0.006%
48	9.702	1407	1413	1416	rBV4	1567	2177	0.23%	0.031%
49	9.933	1448	1451	1454	rBV	202	224	0.02%	0.003%
50	9.970	1454	1457	1458	rBV	320	254	0.03%	0.004%
51	10.055	1465	1471	1481	rBV	460338	610175	63.36%	8.573%
52	10.201	1491	1495	1500	rVB2	1380	1647	0.17%	0.023%
53	10.305	1508	1512	1517	rVB3	1673	2390	0.25%	0.034%
54	10.512	1544	1546	1551	rVB	310	376	0.04%	0.005%
55	10.653	1564	1569	1575	rBV5	1554	2735	0.28%	0.038%
56	10.750	1582	1585	1588	rBV2	242	300	0.03%	0.004%
57	10.963	1616	1620	1625	rBV3	889	1095	0.11%	0.015%
58	11.122	1642	1646	1650	rBV2	3441	4447	0.46%	0.062%
59	11.195	1652	1658	1668	rBV	365041	458493	47.61%	6.442%
60	11.317	1674	1678	1685	rVB	3354	5353	0.56%	0.075%
61	11.384	1685	1689	1691	rVB2	204	305	0.03%	0.004%
62	11.402	1691	1692	1696	rVB2	356	249	0.03%	0.003%
63	11.451	1696	1700	1702	rBV2	1030	1475	0.15%	0.021%
64	11.555	1714	1717	1719	rVB3	455	481	0.05%	0.007%
65	11.640	1729	1731	1734	rVB	285	277	0.03%	0.004%
66	11.689	1734	1739	1741	rBV4	555	831	0.09%	0.012%
67	11.750	1745	1749	1754	rVB3	3867	5106	0.53%	0.072%
68	11.835	1761	1763	1768	rVB2	592	828	0.09%	0.012%
69	11.933	1775	1779	1782	rBV3	1473	1838	0.19%	0.026%
70	11.969	1782	1785	1788	rVB3	1376	1738	0.18%	0.024%
71	12.024	1788	1794	1800	rBV	472513	592632	61.54%	8.327%
72	12.128	1808	1811	1812	rBV2	1160	1113	0.12%	0.016%
73	12.207	1821	1824	1826	rBV	234	272	0.03%	0.004%
74	12.323	1837	1843	1849	rVV	514179	647719	67.26%	9.101%
75	12.427	1857	1860	1864	rVB2	1058	1291	0.13%	0.018%
76	12.481	1865	1869	1877	rVB4	725	1514	0.16%	0.021%

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77	12.658	1896	1898	1901	rBV	878	524	0.05%	0.007%
78	12.768	1912	1916	1920	rBV3	1428	2028	0.21%	0.028%
79	12.981	1949	1951	1953	rBV	341	321	0.03%	0.005%
80	13.055	1960	1963	1965	rVB3	742	725	0.08%	0.010%
81	13.116	1970	1973	1977	rBV5	1377	1675	0.17%	0.024%
82	13.189	1983	1985	1989	rBV2	248	286	0.03%	0.004%
83	13.225	1989	1991	1993	rVB	283	226	0.02%	0.003%
84	13.506	2035	2037	2040	rVB2	202	259	0.03%	0.004%
85	13.591	2048	2051	2056	rVB3	1744	2098	0.22%	0.029%
86	13.713	2069	2071	2074	rVB	233	272	0.03%	0.004%
87	13.750	2074	2077	2078	rBV2	297	262	0.03%	0.004%
88	13.780	2078	2082	2087	rVB	1658	2118	0.22%	0.030%
89	13.963	2108	2112	2117	rVB3	1419	1852	0.19%	0.026%
90	14.012	2117	2120	2122	rBV	165	245	0.03%	0.003%
91	14.134	2134	2140	2145	rVV2	2400	3572	0.37%	0.050%
92	14.731	2235	2238	2241	rBV	366	427	0.04%	0.006%
93	15.329	2334	2336	2337	rBV	380	299	0.03%	0.004%
94	15.475	2359	2360	2365	rBV3	467	565	0.06%	0.008%
95	15.524	2365	2368	2369	rVV2	437	375	0.04%	0.005%
96	16.060	2454	2456	2460	rBV3	419	389	0.04%	0.005%
97	16.170	2470	2474	2478	rBV2	324	521	0.05%	0.007%
98	16.206	2478	2480	2483	rBV	400	362	0.04%	0.005%
99	16.353	2503	2504	2505	rBV	506	232	0.02%	0.003%
100	16.456	2519	2521	2523	rBV	394	267	0.03%	0.004%

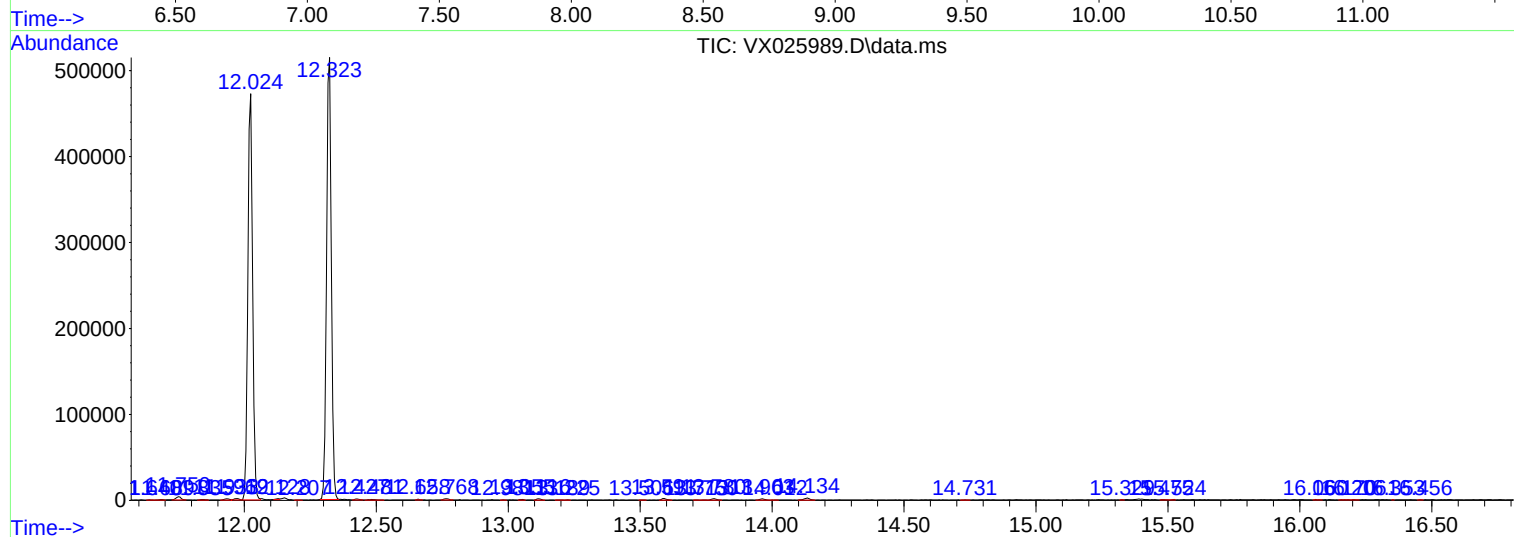
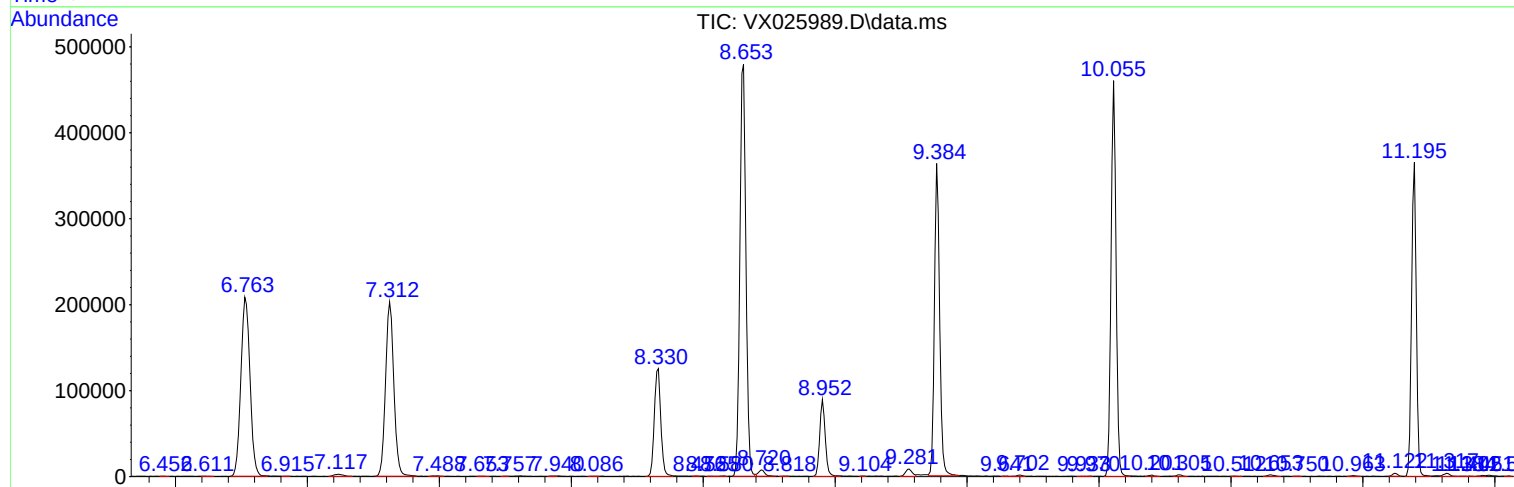
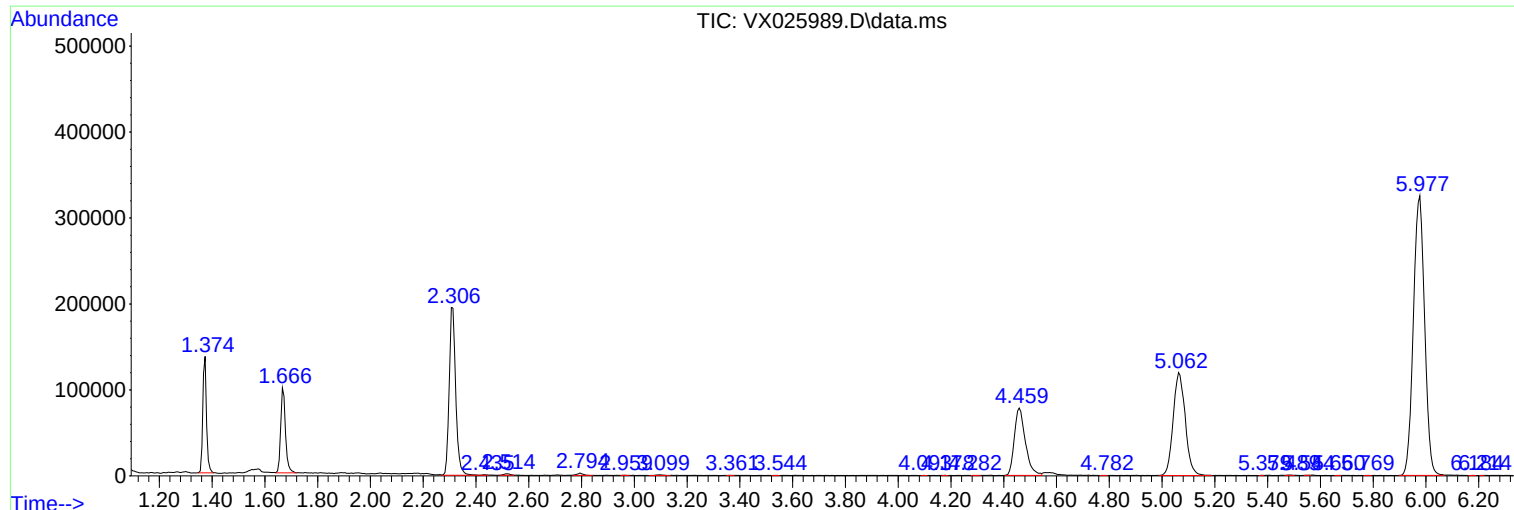
Sum of corrected areas: 7117258

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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