

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
 Data File : VX025674.D
 Acq On : 09 Dec 2021 21:03
 Operator : JC/MD
 Sample : M5004-01 20X
 Misc : 5.27g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGKW0

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: VX025674.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	43	46	53	rVB	64772	62150	15.04%	1.917%
2	1.660	90	94	103	rVB	45913	61031	14.77%	1.883%
3	2.306	194	200	210	rBV	95034	153853	37.23%	4.746%
4	2.453	223	224	227	rBV	287	242	0.06%	0.007%
5	2.501	231	232	236	rBV	424	444	0.11%	0.014%
6	2.794	274	280	288	rBV3	1366	2656	0.64%	0.082%
7	2.855	288	290	293	rBV	243	232	0.06%	0.007%
8	2.946	298	305	315	rVB	4860	11373	2.75%	0.351%
9	3.014	315	316	318	rBV	295	192	0.05%	0.006%
10	3.178	341	343	346	rBV2	271	306	0.07%	0.009%
11	3.288	359	361	363	rVB	314	187	0.05%	0.006%
12	3.459	387	389	390	rVV	250	181	0.04%	0.006%
13	3.544	401	403	404	rBV	245	205	0.05%	0.006%
14	3.824	448	449	451	rBV	250	193	0.05%	0.006%
15	3.922	461	465	466	rBV2	269	224	0.05%	0.007%
16	4.391	538	542	543	rBV2	284	298	0.07%	0.009%
17	4.458	543	553	567	rBV	29552	83895	20.30%	2.588%
18	4.672	586	588	590	rBV2	249	243	0.06%	0.007%
19	4.739	597	599	602	rVB2	280	232	0.06%	0.007%
20	4.818	610	612	615	rBV2	239	212	0.05%	0.007%
21	4.910	624	627	628	rBV2	362	388	0.09%	0.012%
22	4.928	628	630	633	rVV	298	291	0.07%	0.009%
23	5.062	640	652	667	rBV	51416	166068	40.19%	5.122%
24	5.275	686	687	690	rBV	257	264	0.06%	0.008%
25	5.416	708	710	713	rVB	229	195	0.05%	0.006%
26	5.495	721	723	724	rBV	307	287	0.07%	0.009%
27	5.544	728	731	732	rBV2	245	329	0.08%	0.010%
28	5.739	761	763	765	rVB	306	193	0.05%	0.006%
29	5.970	790	801	817	rBV2	137908	413248	100.00%	12.747%
30	6.495	884	887	892	rBV2	214	411	0.10%	0.013%
31	6.763	922	931	945	rVV	112382	269051	65.11%	8.299%
32	6.860	945	947	949	rVB2	328	238	0.06%	0.007%
33	6.988	966	968	971	rBV	355	316	0.08%	0.010%
34	7.116	982	989	996	rBV6	3078	6842	1.66%	0.211%
35	7.312	1012	1021	1034	rVV	82602	181561	43.94%	5.600%
36	7.421	1037	1039	1041	rVB	275	192	0.05%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
 Data File : VX025674.D
 Acq On : 09 Dec 2021 21:03
 Operator : JC/MD
 Sample : M5004-01 20X
 Misc : 5.27g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGKW0

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

37	7.452	1041	1044	1048	rBV2	337	449	0.11%	0.014%
38	7.763	1093	1095	1098	rVB2	281	301	0.07%	0.009%
39	7.818	1101	1104	1108	rVV2	331	433	0.10%	0.013%
40	7.878	1112	1114	1116	rVB	257	188	0.05%	0.006%
41	7.964	1125	1128	1129	rBV2	315	300	0.07%	0.009%
42	8.031	1136	1139	1143	rBV	251	285	0.07%	0.009%
43	8.122	1153	1154	1157	rBV	327	296	0.07%	0.009%
44	8.324	1180	1187	1198	rBV	58902	96336	23.31%	2.971%
45	8.445	1205	1207	1209	rBV	227	192	0.05%	0.006%
46	8.653	1232	1241	1249	rBV	218214	346655	83.89%	10.693%
47	8.720	1249	1252	1259	rVB	2962	4374	1.06%	0.135%
48	8.830	1268	1270	1272	rVB2	250	184	0.04%	0.006%
49	8.854	1272	1274	1276	rBV	242	242	0.06%	0.007%
50	8.951	1285	1290	1298	rBV	42385	59065	14.29%	1.822%
51	9.128	1317	1319	1321	rBV2	239	195	0.05%	0.006%
52	9.275	1339	1343	1348	rVB3	3399	4751	1.15%	0.147%
53	9.384	1356	1361	1375	rBV	127366	184988	44.76%	5.706%
54	9.665	1406	1407	1410	rBV	324	282	0.07%	0.009%
55	9.860	1438	1439	1442	rVV2	204	211	0.05%	0.007%
56	9.909	1445	1447	1449	rVB2	351	291	0.07%	0.009%
57	9.939	1449	1452	1453	rBV2	228	278	0.07%	0.009%
58	10.055	1465	1471	1484	rVB	241949	323657	78.32%	9.983%
59	10.299	1509	1511	1512	rBV2	431	382	0.09%	0.012%
60	10.476	1538	1540	1541	rVB	325	210	0.05%	0.006%
61	11.122	1642	1646	1649	rBV2	1580	1769	0.43%	0.055%
62	11.195	1652	1658	1667	rVB	154192	192560	46.60%	5.940%
63	11.750	1746	1749	1755	rVB3	1092	1566	0.38%	0.048%
64	11.841	1761	1764	1766	rBV3	363	410	0.10%	0.013%
65	11.933	1775	1779	1782	rBV3	949	1251	0.30%	0.039%
66	12.024	1789	1794	1802	rBV	247188	304141	73.60%	9.381%
67	12.122	1808	1810	1812	rBV3	454	523	0.13%	0.016%
68	12.323	1835	1843	1850	rBV	226359	286799	69.40%	8.846%
69	12.420	1857	1859	1864	rVB2	428	607	0.15%	0.019%
70	12.469	1864	1867	1869	rBV2	232	267	0.06%	0.008%
71	12.494	1869	1871	1872	rBV	198	191	0.05%	0.006%
72	12.524	1874	1876	1878	rBV	311	259	0.06%	0.008%
73	12.768	1913	1916	1917	rVB	415	312	0.08%	0.010%
74	12.969	1947	1949	1952	rVB	299	269	0.07%	0.008%
75	13.182	1982	1984	1987	rVB	241	253	0.06%	0.008%
76	13.292	2000	2002	2003	rBV	239	192	0.05%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
 Data File : VX025674.D
 Acq On : 09 Dec 2021 21:03
 Operator : JC/MD
 Sample : M5004-01 20X
 Misc : 5.27g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGKW0

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\SFAMXLM112221WMA.M
 Title : VOC Analysis

77	13.323	2005	2007	2010	rVB	345	338	0.08%	0.010%
78	13.353	2010	2012	2013	rBV	258	182	0.04%	0.006%
79	13.780	2079	2082	2085	rBV3	298	517	0.13%	0.016%
80	13.835	2088	2091	2094	rVB2	219	269	0.07%	0.008%
81	13.957	2109	2111	2116	rVB2	170	204	0.05%	0.006%
82	14.060	2122	2128	2130	rBV	324	537	0.13%	0.017%
83	14.133	2137	2140	2144	rVB3	462	580	0.14%	0.018%
84	14.225	2153	2155	2158	rBV	224	294	0.07%	0.009%
85	14.329	2170	2172	2173	rVB	314	195	0.05%	0.006%
86	14.426	2186	2188	2189	rBV	332	228	0.06%	0.007%
87	14.737	2237	2239	2244	rVV	188	217	0.05%	0.007%
88	14.810	2250	2251	2254	rBV3	329	368	0.09%	0.011%
89	14.883	2260	2263	2265	rBV2	384	622	0.15%	0.019%
90	15.011	2282	2284	2285	rVB2	311	184	0.04%	0.006%
91	15.036	2285	2288	2290	rBV2	200	311	0.08%	0.010%
92	15.097	2296	2298	2302	rVB3	294	427	0.10%	0.013%
93	15.584	2376	2378	2380	rBV2	259	205	0.05%	0.006%
94	15.956	2437	2439	2443	rVB3	311	371	0.09%	0.011%
95	16.048	2452	2454	2455	rBV	393	248	0.06%	0.008%
96	16.145	2469	2470	2472	rBV	304	246	0.06%	0.008%
97	16.401	2510	2512	2515	rBV	230	297	0.07%	0.009%
98	16.596	2542	2544	2545	rBV2	332	248	0.06%	0.008%
99	16.706	2559	2562	2565	rBV2	274	425	0.10%	0.013%
100	16.731	2565	2566	2570	rBV	328	361	0.09%	0.011%

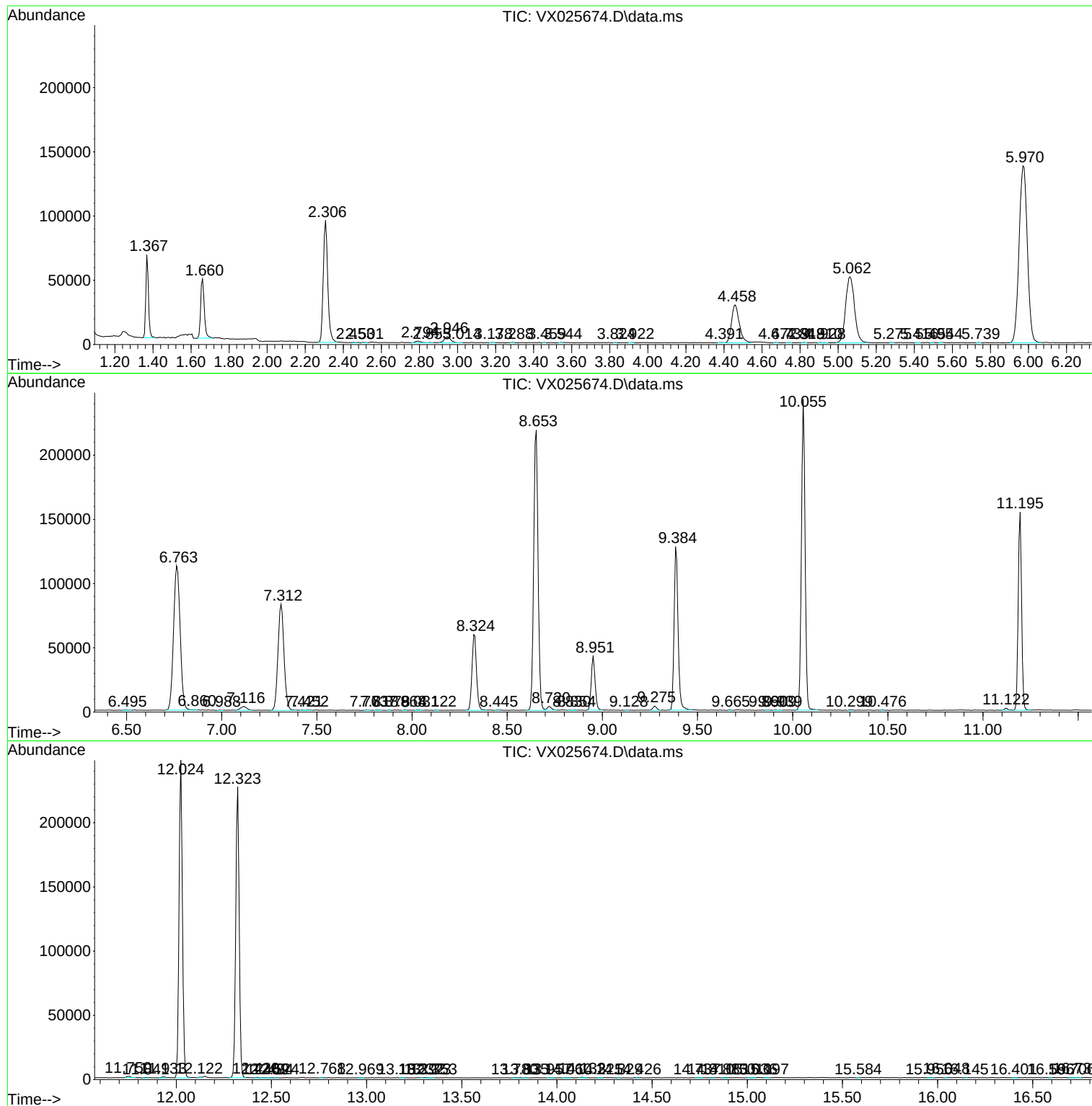
Sum of corrected areas: 3242011

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025674.D
Acq On : 09 Dec 2021 21:03
Operator : JC/MD
Sample : M5004-01 20X
Misc : 5.27g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKW0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025674.D
Acq On : 09 Dec 2021 21:03
Operator : JC/MD
Sample : M5004-01 20X
Misc : 5.27g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKW0

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

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025674.D
Acq On : 09 Dec 2021 21:03
Operator : JC/MD
Sample : M5004-01 20X
Misc : 5.27g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKW0

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

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