

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122521\
 Data File : VX026032.D
 Acq On : 25 Dec 2021 13:42
 Operator : JC/MD
 Sample : VX1225MBL01
 Misc : 5.0G/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 1 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: VX026032.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	56	rVB	155447	162816	15.97%	2.148%
2	1.666	91	95	105	rBV	113789	143674	14.09%	1.896%
3	2.313	194	201	220	rBV	226607	381003	37.36%	5.027%
4	2.532	230	237	245	rVB4	1000	2729	0.27%	0.036%
5	2.685	258	262	263	rBV3	272	319	0.03%	0.004%
6	2.715	263	267	271	rVB3	457	775	0.08%	0.010%
7	2.794	276	280	284	rVV3	1725	2674	0.26%	0.035%
8	3.380	375	376	378	rBV	341	253	0.02%	0.003%
9	4.196	504	510	512	rBV2	354	573	0.06%	0.008%
10	4.459	544	553	567	rBV2	74342	233394	22.89%	3.079%
11	5.062	640	652	676	rVV3	106780	395519	38.79%	5.218%
12	5.233	678	680	682	rVB	399	236	0.02%	0.003%
13	5.483	719	721	723	rVV2	519	413	0.04%	0.005%
14	5.696	755	756	759	rVB	381	290	0.03%	0.004%
15	5.971	789	801	820	rVV2	342797	1019725	100.00%	13.453%
16	6.227	841	843	848	rBV2	412	507	0.05%	0.007%
17	6.336	859	861	862	rBV	363	250	0.02%	0.003%
18	6.544	891	895	902	rBV3	369	851	0.08%	0.011%
19	6.702	917	921	922	rBV2	188	236	0.02%	0.003%
20	6.763	922	931	948	rBV	221773	516860	50.69%	6.819%
21	7.068	978	981	983	rVV2	279	321	0.03%	0.004%
22	7.117	983	989	998	rVB6	2888	7254	0.71%	0.096%
23	7.232	1004	1008	1010	rBV2	215	263	0.03%	0.003%
24	7.312	1010	1021	1035	rBV	213691	460644	45.17%	6.077%
25	7.489	1044	1050	1053	rBV3	603	1171	0.11%	0.015%
26	7.671	1076	1080	1082	rVV2	151	256	0.03%	0.003%
27	7.799	1095	1101	1104	rBV2	413	736	0.07%	0.010%
28	7.897	1113	1117	1118	rVB	237	272	0.03%	0.004%
29	7.927	1120	1122	1123	rBV	337	273	0.03%	0.004%
30	8.049	1139	1142	1147	rBV3	291	374	0.04%	0.005%
31	8.123	1152	1154	1159	rBV	212	290	0.03%	0.004%
32	8.177	1159	1163	1164	rBV2	220	253	0.02%	0.003%
33	8.324	1181	1187	1199	rBV	142244	229180	22.47%	3.024%
34	8.470	1209	1211	1214	rVB3	404	430	0.04%	0.006%
35	8.574	1225	1228	1230	rBV2	319	436	0.04%	0.006%
36	8.647	1233	1240	1248	rBV	520604	828108	81.21%	10.925%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122521\
 Data File : VX026032.D
 Acq On : 25 Dec 2021 13:42
 Operator : JC/MD
 Sample : VX1225MBL01
 Misc : 5.0G/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 1 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

37	8.720	1248	1252	1259	rVB2	7755	12679	1.24%	0.167%
38	8.952	1284	1290	1300	rBV	96248	140665	13.79%	1.856%
39	9.135	1319	1320	1324	rVB	346	355	0.03%	0.005%
40	9.183	1326	1328	1331	rVB2	347	245	0.02%	0.003%
41	9.232	1335	1336	1338	rBV	292	235	0.02%	0.003%
42	9.281	1338	1344	1349	rBV	7961	15703	1.54%	0.207%
43	9.385	1356	1361	1375	rVB	376732	516504	50.65%	6.814%
44	9.702	1406	1413	1417	rBV4	1258	1928	0.19%	0.025%
45	9.836	1433	1435	1437	rBV2	297	304	0.03%	0.004%
46	9.866	1437	1440	1441	rBV	243	294	0.03%	0.004%
47	10.055	1465	1471	1487	rBV	478867	634293	62.20%	8.368%
48	10.195	1491	1494	1500	rVV3	680	1019	0.10%	0.013%
49	10.299	1508	1511	1516	rVV3	1675	2167	0.21%	0.029%
50	10.403	1527	1528	1533	rVB	281	366	0.04%	0.005%
51	10.640	1564	1567	1569	rBV	843	1052	0.10%	0.014%
52	10.817	1591	1596	1597	rBV2	349	420	0.04%	0.006%
53	10.970	1620	1621	1623	rVB	551	254	0.02%	0.003%
54	11.122	1641	1646	1650	rVB2	4642	5866	0.58%	0.077%
55	11.195	1652	1658	1665	rBV	366004	473108	46.40%	6.242%
56	11.317	1674	1678	1685	rVB4	4891	8272	0.81%	0.109%
57	11.384	1687	1689	1690	rBV	318	293	0.03%	0.004%
58	11.451	1698	1700	1701	rBV2	539	310	0.03%	0.004%
59	11.476	1701	1704	1713	rVB4	1711	3425	0.34%	0.045%
60	11.555	1713	1717	1719	rBV3	670	727	0.07%	0.010%
61	11.677	1732	1737	1740	rBV3	665	975	0.10%	0.013%
62	11.750	1745	1749	1753	rVB2	4411	5755	0.56%	0.076%
63	11.841	1761	1764	1774	rVB4	1093	1472	0.14%	0.019%
64	11.933	1774	1779	1783	rBV3	2457	3215	0.32%	0.042%
65	11.969	1783	1785	1788	rBV2	950	988	0.10%	0.013%
66	12.024	1788	1794	1801	rBV	507328	622882	61.08%	8.218%
67	12.128	1808	1811	1813	rBV4	1739	2528	0.25%	0.033%
68	12.152	1813	1815	1820	rVB2	3401	3711	0.36%	0.049%
69	12.238	1826	1829	1830	rBV	364	260	0.03%	0.003%
70	12.323	1835	1843	1850	rVV	533458	697438	68.39%	9.201%
71	12.378	1850	1852	1856	rVV4	1158	1191	0.12%	0.016%
72	12.427	1858	1860	1864	rVB	1177	1346	0.13%	0.018%
73	12.530	1875	1877	1880	rVB	432	236	0.02%	0.003%
74	12.628	1890	1893	1894	rBV2	669	490	0.05%	0.006%
75	12.664	1896	1899	1903	rVB3	1012	1111	0.11%	0.015%
76	12.762	1911	1915	1920	rBV2	2738	3855	0.38%	0.051%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122521\
 Data File : VX026032.D
 Acq On : 25 Dec 2021 13:42
 Operator : JC/MD
 Sample : VX1225MBL01
 Misc : 5.0G/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 1 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\SFAMXML122321WMA.M
 Title : VOC Analysis

77	12.860	1928	1931	1932	rBV	239	242	0.02%	0.003%
78	12.945	1941	1945	1947	rVV2	281	464	0.05%	0.006%
79	12.975	1947	1950	1951	rVV3	355	373	0.04%	0.005%
80	13.000	1953	1954	1958	rVV2	274	252	0.02%	0.003%
81	13.061	1959	1964	1969	rVV4	603	1119	0.11%	0.015%
82	13.122	1971	1974	1977	rVV2	549	593	0.06%	0.008%
83	13.164	1977	1981	1984	rVV2	254	330	0.03%	0.004%
84	13.597	2048	2052	2054	rVB3	417	622	0.06%	0.008%
85	13.780	2079	2082	2085	rBV2	763	952	0.09%	0.013%
86	13.963	2109	2112	2116	rVB2	638	776	0.08%	0.010%
87	14.134	2134	2140	2145	rVV	4085	5443	0.53%	0.072%
88	14.286	2162	2165	2168	rBV2	312	351	0.03%	0.005%
89	14.426	2186	2188	2189	rVB2	426	285	0.03%	0.004%
90	14.445	2189	2191	2194	rBV	314	324	0.03%	0.004%
91	14.591	2211	2215	2217	rBV2	220	272	0.03%	0.004%
92	14.743	2235	2240	2244	rBV3	312	514	0.05%	0.007%
93	14.786	2245	2247	2250	rVB	336	275	0.03%	0.004%
94	14.908	2264	2267	2268	rBV2	407	424	0.04%	0.006%
95	15.091	2295	2297	2299	rBV3	271	331	0.03%	0.004%
96	15.402	2343	2348	2354	rVB4	1860	2967	0.29%	0.039%
97	15.944	2435	2437	2440	rBV3	314	352	0.03%	0.005%
98	16.243	2485	2486	2489	rBV3	412	345	0.03%	0.005%
99	16.298	2493	2495	2498	rVV2	563	477	0.05%	0.006%
100	16.713	2561	2563	2564	rBV	355	251	0.02%	0.003%

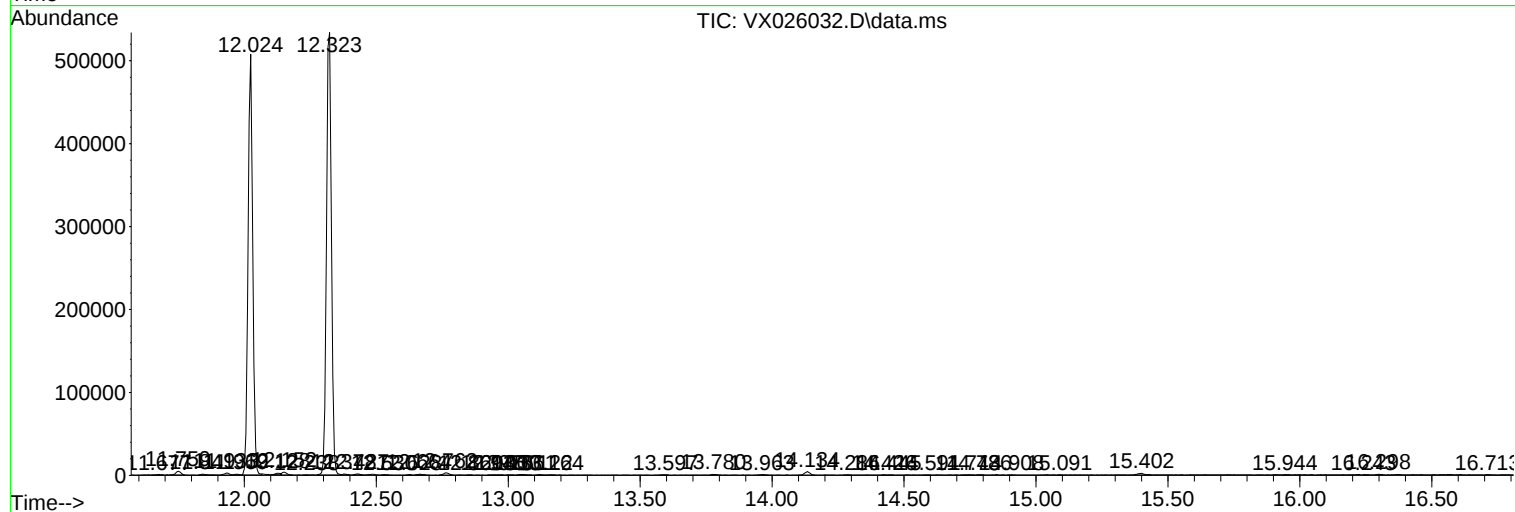
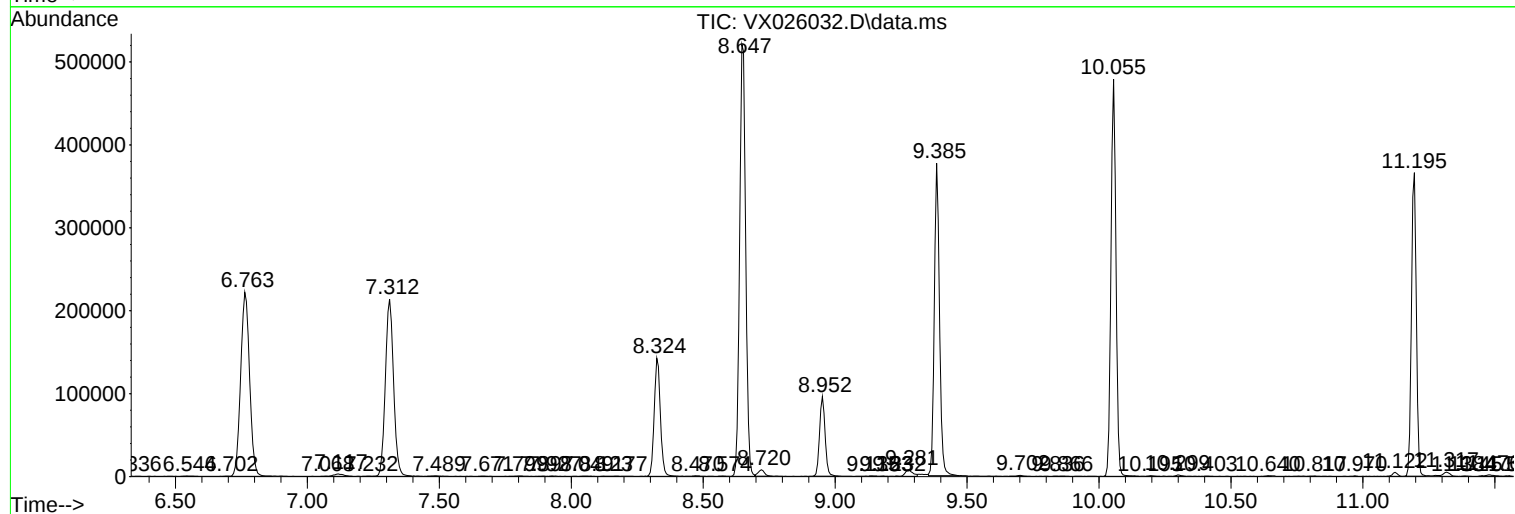
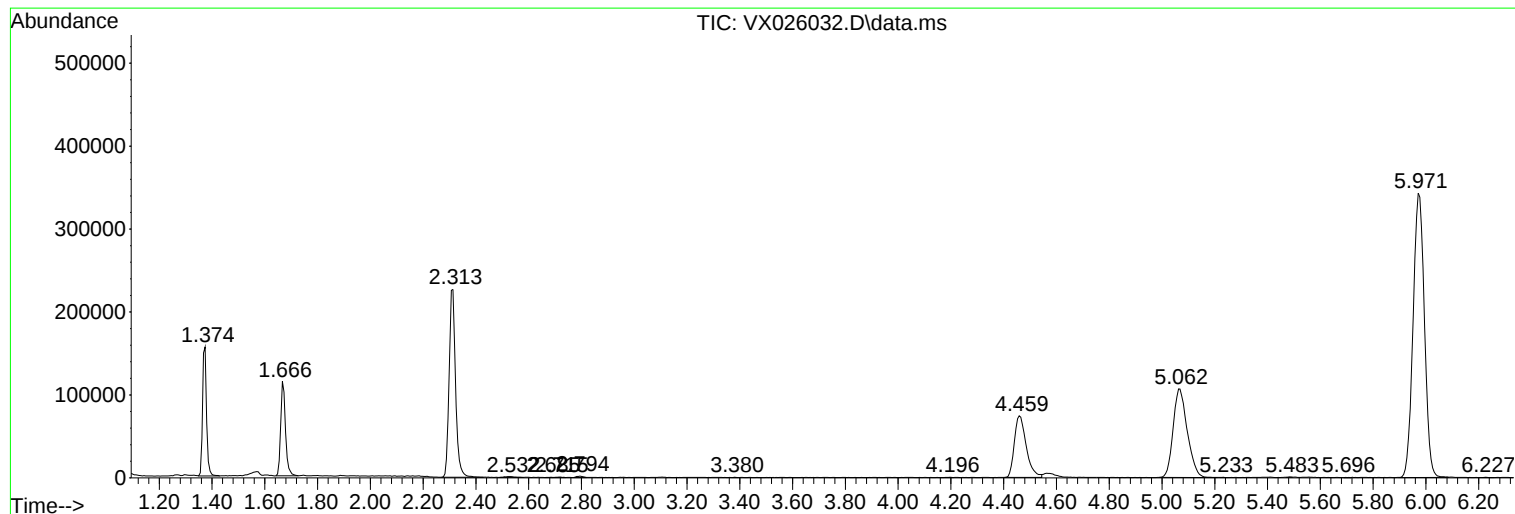
Sum of corrected areas: 7579629

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122521\
Data File : VX026032.D
Acq On : 25 Dec 2021 13:42
Operator : JC/MD
Sample : VX1225MBL01
Misc : 5.0G/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK659

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122521\
Data File : VX026032.D
Acq On : 25 Dec 2021 13:42
Operator : JC/MD
Sample : VX1225MBL01
Misc : 5.0G/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK659

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

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122521\
Data File : VX026032.D
Acq On : 25 Dec 2021 13:42
Operator : JC/MD
Sample : VX1225MBL01
Misc : 5.0G/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK659

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.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