

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020823\
 Data File : VX034056.D
 Acq On : 07 Feb 2023 13:01
 Operator : JC/MD
 Sample : 01394-01ME
 Misc : 2.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C1149ME

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\SFAMXML020223WMA.M
 Title : VOC Analysis

Signal : TIC: VX034056.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	26	28	31	rVB2	815	747	0.10%	0.013%
2	1.374	43	47	61	rBV	47440	90954	11.88%	1.558%
3	1.526	70	72	73	rBV2	391	262	0.03%	0.004%
4	1.544	73	75	76	rBV	704	574	0.07%	0.010%
5	1.569	76	79	80	rBV2	1053	1052	0.14%	0.018%
6	1.648	89	92	109	rBV	18841	48487	6.33%	0.830%
7	2.081	158	163	164	rBV	152	248	0.03%	0.004%
8	2.288	191	197	212	rBV	156549	242631	31.69%	4.155%
9	2.630	252	253	258	rBV2	148	213	0.03%	0.004%
10	2.776	272	277	285	rBV3	1847	4071	0.53%	0.070%
11	2.947	298	305	310	rBV	2078	4617	0.60%	0.079%
12	3.038	318	320	323	rBV	153	224	0.03%	0.004%
13	3.123	333	334	336	rBV	171	158	0.02%	0.003%
14	3.392	376	378	381	rBV2	153	168	0.02%	0.003%
15	3.416	381	382	383	rBV	253	181	0.02%	0.003%
16	3.489	389	394	395	rBV	140	209	0.03%	0.004%
17	3.520	398	399	407	rVB	109	234	0.03%	0.004%
18	3.599	407	412	414	rBB2	135	227	0.03%	0.004%
19	3.623	414	416	417	rBV2	158	146	0.02%	0.003%
20	3.642	417	419	421	rVB	167	148	0.02%	0.003%
21	3.770	437	440	442	rBV	194	198	0.03%	0.003%
22	3.794	442	444	448	rVB	138	167	0.02%	0.003%
23	3.825	448	449	453	rBB	141	144	0.02%	0.002%
24	3.855	453	454	456	rBV	168	161	0.02%	0.003%
25	3.934	465	467	470	rBV	141	144	0.02%	0.002%
26	4.062	486	488	490	rBV	120	145	0.02%	0.002%
27	4.459	545	553	575	rBV2	43994	143547	18.75%	2.458%
28	4.891	622	624	627	rBV2	132	166	0.02%	0.003%
29	5.056	634	651	668	rBV	97674	311055	40.63%	5.327%
30	5.373	700	703	704	rBV	302	285	0.04%	0.005%
31	5.550	725	732	740	rVB2	807	2120	0.28%	0.036%
32	5.836	775	779	783	rBV	124	240	0.03%	0.004%
33	5.958	787	799	816	rBV2	267450	765626	100.00%	13.112%
34	6.227	841	843	845	rBV	159	156	0.02%	0.003%
35	6.355	858	864	865	rBV2	379	499	0.07%	0.009%
36	6.458	878	881	886	rVB2	184	348	0.05%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020823\
 Data File : VX034056.D
 Acq On : 07 Feb 2023 13:01
 Operator : JC/MD
 Sample : 01394-01ME
 Misc : 2.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C1149ME

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\SFAMXML020223WMA.M
 Title : VOC Analysis

37	6.501	886	888	889	rBV	169	140	0.02%	0.002%
38	6.562	897	898	901	rBB	201	136	0.02%	0.002%
39	6.598	901	904	906	rBV	159	212	0.03%	0.004%
40	6.757	920	930	944	rBV	202263	479274	62.60%	8.208%
41	7.111	982	988	997	rVB5	1548	3930	0.51%	0.067%
42	7.208	997	1004	1011	rBV4	919	2333	0.30%	0.040%
43	7.300	1011	1019	1036	rVV	158693	352120	45.99%	6.030%
44	7.482	1045	1049	1053	rVB3	306	472	0.06%	0.008%
45	7.787	1097	1099	1102	rBV	123	128	0.02%	0.002%
46	7.903	1114	1118	1120	rBV2	103	168	0.02%	0.003%
47	8.068	1141	1145	1146	rBV	177	231	0.03%	0.004%
48	8.171	1159	1162	1166	rBV	149	160	0.02%	0.003%
49	8.324	1179	1187	1197	rBV	99855	165248	21.58%	2.830%
50	8.476	1210	1212	1216	rVB	185	179	0.02%	0.003%
51	8.513	1216	1218	1220	rBV2	161	177	0.02%	0.003%
52	8.549	1222	1224	1227	rBV2	107	152	0.02%	0.003%
53	8.647	1233	1240	1255	rBV	398184	636446	83.13%	10.899%
54	8.811	1265	1267	1268	rVB	260	166	0.02%	0.003%
55	8.866	1274	1276	1278	rVB	230	191	0.02%	0.003%
56	8.891	1278	1280	1284	rBV2	234	355	0.05%	0.006%
57	8.946	1284	1289	1301	rBV	68803	105887	13.83%	1.813%
58	9.116	1314	1317	1321	rBV3	168	333	0.04%	0.006%
59	9.275	1340	1343	1345	rBV2	371	362	0.05%	0.006%
60	9.397	1356	1363	1382	rVV	145171	313288	40.92%	5.365%
61	9.708	1411	1414	1417	rBV2	359	397	0.05%	0.007%
62	9.799	1428	1429	1432	rBV2	164	184	0.02%	0.003%
63	10.055	1465	1471	1488	rVV	366724	532054	69.49%	9.112%
64	10.201	1491	1495	1499	rBV3	368	531	0.07%	0.009%
65	10.305	1507	1512	1517	rBV3	567	1042	0.14%	0.018%
66	10.610	1560	1562	1565	rBV	144	159	0.02%	0.003%
67	10.646	1565	1568	1569	rBV2	291	248	0.03%	0.004%
68	10.945	1613	1617	1618	rBV	119	134	0.02%	0.002%
69	10.964	1618	1620	1625	rVB2	321	484	0.06%	0.008%
70	11.012	1625	1628	1629	rBV	236	252	0.03%	0.004%
71	11.085	1636	1640	1641	rBV	121	158	0.02%	0.003%
72	11.134	1646	1648	1650	rVV	112	142	0.02%	0.002%
73	11.195	1652	1658	1672	rVB	288308	382485	49.96%	6.550%
74	11.311	1672	1677	1682	rBV	1219	1768	0.23%	0.030%
75	11.451	1698	1700	1702	rVV	317	270	0.04%	0.005%
76	11.524	1709	1712	1715	rBV	198	360	0.05%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020823\
 Data File : VX034056.D
 Acq On : 07 Feb 2023 13:01
 Operator : JC/MD
 Sample : 01394-01ME
 Misc : 2.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C1149ME

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\SFAMXML020223WMA.M
 Title : VOC Analysis

77	11.713	1742	1743	1746	rVB2	244	169	0.02%	0.003%
78	11.762	1748	1751	1753	rBV2	343	363	0.05%	0.006%
79	11.908	1773	1775	1779	rBV2	99	128	0.02%	0.002%
80	11.969	1783	1785	1788	rBV	214	185	0.02%	0.003%
81	12.024	1789	1794	1805	rVV	468525	577254	75.40%	9.886%
82	12.323	1837	1843	1856	rBV	504345	646921	84.50%	11.079%
83	12.634	1891	1894	1895	rBV	151	174	0.02%	0.003%
84	12.762	1910	1915	1922	rVB3	1865	2541	0.33%	0.044%
85	12.841	1926	1928	1930	rBV	138	133	0.02%	0.002%
86	12.860	1930	1931	1934	rBV2	163	150	0.02%	0.003%
87	12.969	1946	1949	1954	rBV2	136	300	0.04%	0.005%
88	13.097	1968	1970	1972	rBV	108	129	0.02%	0.002%
89	13.122	1972	1974	1977	rVV	191	200	0.03%	0.003%
90	13.500	2033	2036	2037	rBV	136	154	0.02%	0.003%
91	13.597	2050	2052	2056	rVB2	325	296	0.04%	0.005%
92	13.713	2067	2071	2076	rVB	194	309	0.04%	0.005%
93	13.963	2110	2112	2118	rVB2	357	539	0.07%	0.009%
94	14.024	2118	2122	2123	rBV	172	209	0.03%	0.004%
95	14.134	2134	2140	2147	rVV2	1796	2757	0.36%	0.047%
96	14.237	2153	2157	2159	rBV	223	285	0.04%	0.005%
97	14.676	2227	2229	2230	rBV	243	238	0.03%	0.004%
98	15.243	2320	2322	2327	rBV3	279	462	0.06%	0.008%
99	15.390	2344	2346	2353	rVB3	1521	1824	0.24%	0.031%
100	16.597	2542	2544	2545	rBV	296	216	0.03%	0.004%

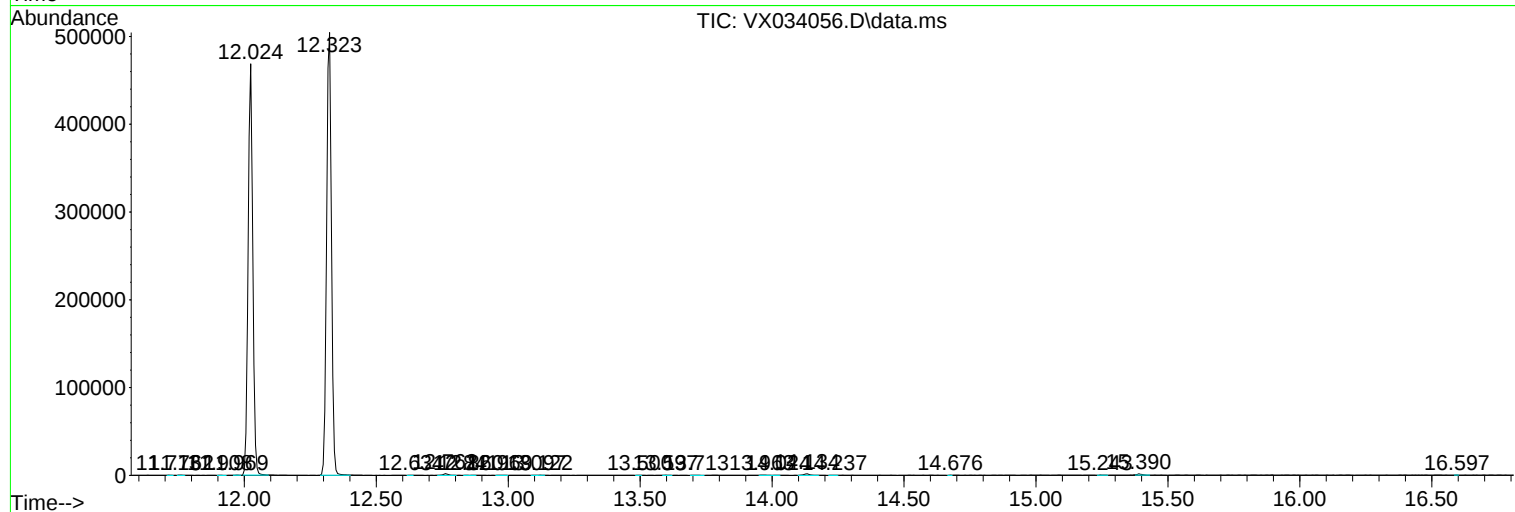
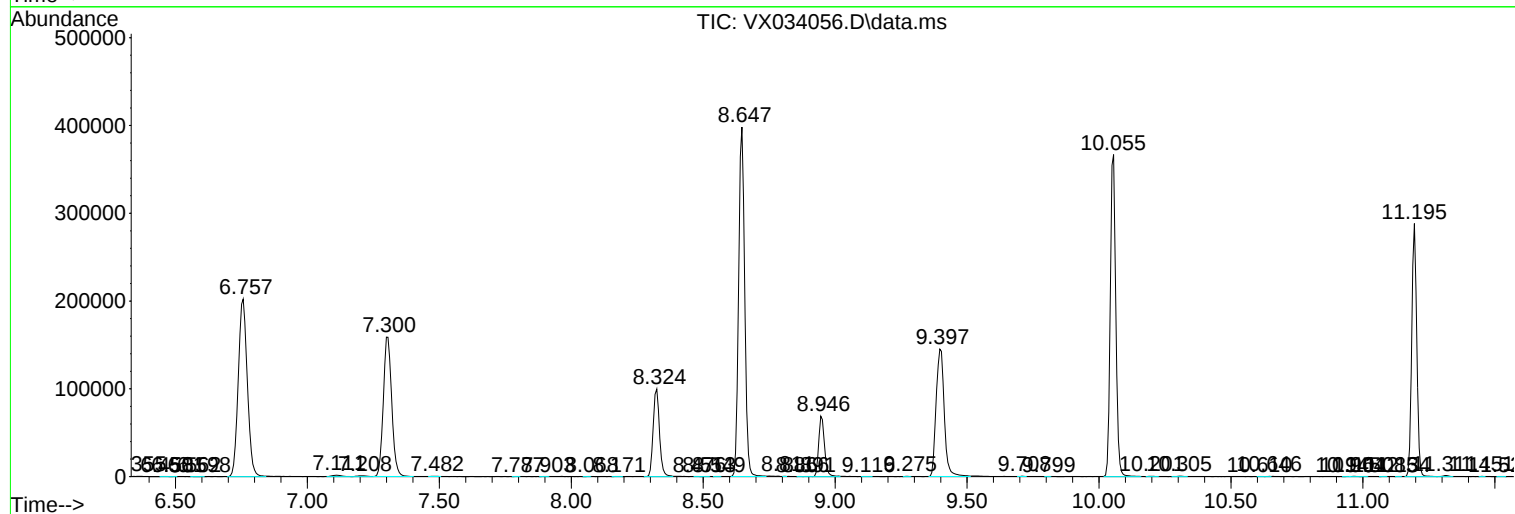
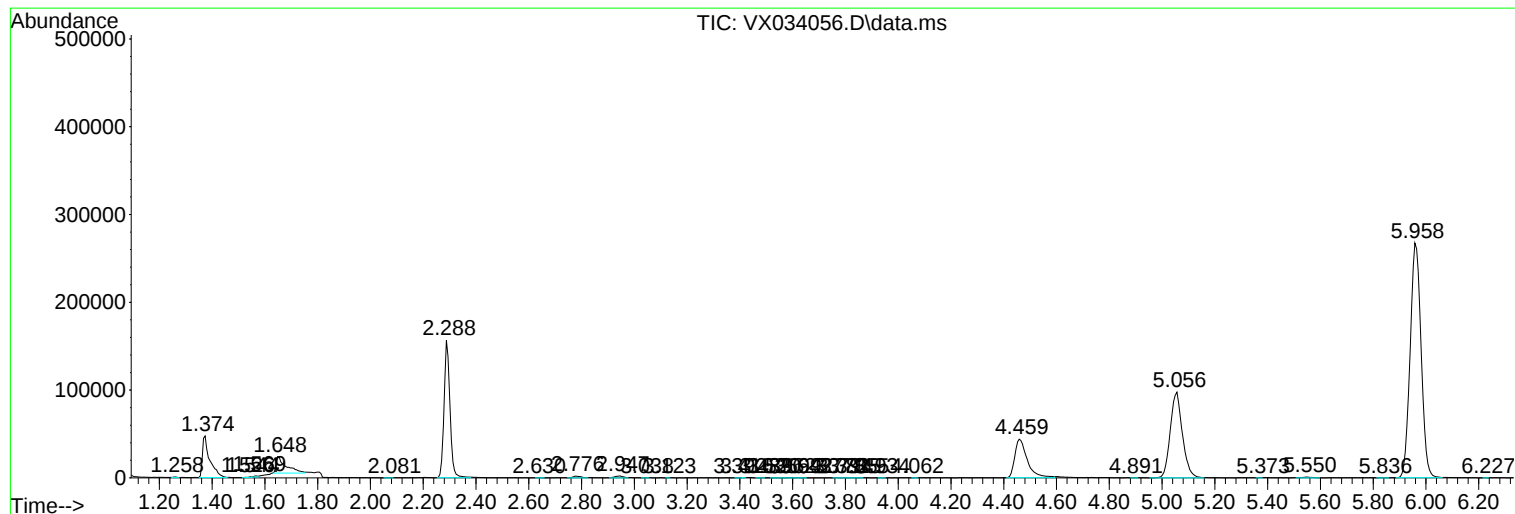
Sum of corrected areas: 5839244

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020823\
Data File : VX034056.D
Acq On : 07 Feb 2023 13:01
Operator : JC/MD
Sample : 01394-01ME
Misc : 2.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C1149ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML020223WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020823\
Data File : VX034056.D
Acq On : 07 Feb 2023 13:01
Operator : JC/MD
Sample : 01394-01ME
Misc : 2.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C1149ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML020223WMA.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\VX020823\
Data File : VX034056.D
Acq On : 07 Feb 2023 13:01
Operator : JC/MD
Sample : 01394-01ME
Misc : 2.82g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C1149ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML020223WMA.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