

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110821\
 Data File : VX025101.D
 Acq On : 08 Nov 2021 17:31
 Operator : JC/MD
 Sample : M4464-04ME 10X
 Misc : 7.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GB7K2ME

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\SFAMXLM110821WMA.M

Title : VOC Analysis

Signal : TIC: VX025101.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	42	46	55	rVB	122730	128621	9.26%	1.297%
2	1.660	91	94	100	rVB	59684	75883	5.46%	0.765%
3	2.306	194	200	209	rBV	227243	362000	26.05%	3.651%
4	2.392	210	214	223	rVB	27875	47847	3.44%	0.483%
5	2.508	230	233	238	rVB	2166	3368	0.24%	0.034%
6	2.916	297	300	301	rBV2	449	543	0.04%	0.005%
7	3.099	324	330	334	rBV3	2176	4030	0.29%	0.041%
8	3.245	352	354	357	rVB	771	450	0.03%	0.005%
9	3.477	391	392	396	rVB	373	291	0.02%	0.003%
10	3.520	396	399	401	rBV	544	497	0.04%	0.005%
11	3.562	404	406	407	rVV	326	240	0.02%	0.002%
12	3.617	407	415	425	rVV2	23062	54788	3.94%	0.553%
13	4.154	502	503	505	rBV	302	254	0.02%	0.003%
14	4.373	537	539	540	rBV	478	300	0.02%	0.003%
15	4.495	545	559	573	rBV3	210991	692591	49.84%	6.985%
16	4.769	602	604	607	rVB3	295	293	0.02%	0.003%
17	4.812	607	611	613	rBV3	347	469	0.03%	0.005%
18	5.062	641	652	666	rVB2	126933	390686	28.12%	3.940%
19	5.294	688	690	694	rBV	347	380	0.03%	0.004%
20	5.367	700	702	703	rBV	930	934	0.07%	0.009%
21	5.464	716	718	719	rBV	513	511	0.04%	0.005%
22	5.556	727	733	741	rBV3	1278	3339	0.24%	0.034%
23	5.629	741	745	748	rBV2	657	720	0.05%	0.007%
24	5.763	764	767	768	rBV	392	321	0.02%	0.003%
25	5.830	775	778	779	rBV	470	473	0.03%	0.005%
26	5.977	790	802	817	rVV2	315137	933900	67.21%	9.419%
27	6.208	838	840	842	rBV2	546	524	0.04%	0.005%
28	6.263	848	849	851	rBV2	401	327	0.02%	0.003%
29	6.403	870	872	874	rVB2	376	257	0.02%	0.003%
30	6.446	876	879	881	rBV	484	571	0.04%	0.006%
31	6.672	914	916	920	rVB3	699	747	0.05%	0.008%
32	6.763	923	931	946	rVB	189039	452647	32.58%	4.565%
33	7.043	975	977	980	rBV	419	445	0.03%	0.004%
34	7.129	980	991	1010	rVV	636017	1389511	100.00%	14.014%
35	7.312	1013	1021	1034	rVV	148320	323380	23.27%	3.262%
36	7.568	1060	1063	1065	rBV2	670	628	0.05%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110821\
 Data File : VX025101.D
 Acq On : 08 Nov 2021 17:31
 Operator : JC/MD
 Sample : M4464-04ME 10X
 Misc : 7.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GB7K2ME

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\SFAMXLM110821WMA.M
 Title : VOC Analysis

37	7.793	1093	1100	1102	rBV3	456	954	0.07%	0.010%
38	7.994	1132	1133	1135	rBV	382	361	0.03%	0.004%
39	8.086	1146	1148	1151	rBV	391	343	0.02%	0.003%
40	8.196	1162	1166	1167	rBV	466	626	0.05%	0.006%
41	8.330	1181	1188	1195	rBV	111834	184725	13.29%	1.863%
42	8.427	1203	1204	1205	rBV	520	258	0.02%	0.003%
43	8.580	1224	1229	1234	rBV3	7655	13272	0.96%	0.134%
44	8.653	1234	1241	1247	rVV	414369	653703	47.05%	6.593%
45	8.720	1247	1252	1264	rVB	800065	1200905	86.43%	12.112%
46	8.952	1285	1290	1297	rBV	91475	138750	9.99%	1.399%
47	9.086	1309	1312	1313	rBV	496	358	0.03%	0.004%
48	9.275	1341	1343	1348	rVB2	2473	2629	0.19%	0.027%
49	9.317	1348	1350	1355	rBV3	427	648	0.05%	0.007%
50	9.391	1355	1362	1373	rBV	305167	437909	31.52%	4.417%
51	10.055	1466	1471	1482	rVB	525992	720652	51.86%	7.268%
52	10.159	1487	1488	1490	rBB	434	252	0.02%	0.003%
53	10.305	1508	1512	1517	rVB2	3454	4750	0.34%	0.048%
54	10.738	1582	1583	1586	rVB	544	351	0.03%	0.004%
55	10.774	1586	1589	1592	rBV2	503	700	0.05%	0.007%
56	10.963	1617	1620	1625	rVB3	2019	2437	0.18%	0.025%
57	11.067	1635	1637	1639	rVB	395	320	0.02%	0.003%
58	11.091	1639	1641	1642	rBV	636	396	0.03%	0.004%
59	11.122	1642	1646	1650	rVV	3697	5088	0.37%	0.051%
60	11.195	1653	1658	1667	rBV	335194	417152	30.02%	4.207%
61	11.280	1670	1672	1673	rBV	632	637	0.05%	0.006%
62	11.451	1697	1700	1703	rBV	2354	2806	0.20%	0.028%
63	11.543	1714	1715	1719	rBV	596	533	0.04%	0.005%
64	11.573	1719	1720	1722	rBV	540	366	0.03%	0.004%
65	11.658	1733	1734	1736	rBV	327	275	0.02%	0.003%
66	11.750	1746	1749	1756	rVB3	5217	7297	0.53%	0.074%
67	11.817	1758	1760	1762	rBV	594	464	0.03%	0.005%
68	11.854	1762	1766	1770	rVB2	482	703	0.05%	0.007%
69	11.908	1774	1775	1776	rBV	411	254	0.02%	0.003%
70	11.975	1782	1786	1789	rVB3	2864	3873	0.28%	0.039%
71	12.024	1789	1794	1804	rBV	523136	637250	45.86%	6.427%
72	12.323	1838	1843	1851	rVB	470792	584536	42.07%	5.896%
73	12.561	1880	1882	1883	rBV	438	362	0.03%	0.004%
74	12.664	1897	1899	1901	rBV	892	674	0.05%	0.007%
75	12.939	1940	1944	1945	rBV	559	681	0.05%	0.007%
76	13.170	1979	1982	1983	rBV	456	462	0.03%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110821\
 Data File : VX025101.D
 Acq On : 08 Nov 2021 17:31
 Operator : JC/MD
 Sample : M4464-04ME 10X
 Misc : 7.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GB7K2ME

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\SFAMXML110821WMA.M
 Title : VOC Analysis

77	13.286	2000	2001	2003	rBV	510	355	0.03%	0.004%
78	13.536	2039	2042	2044	rBV	384	496	0.04%	0.005%
79	13.554	2044	2045	2048	rVV2	502	524	0.04%	0.005%
80	13.591	2048	2051	2054	rVV2	2437	2507	0.18%	0.025%
81	13.652	2057	2061	2062	rBV2	401	488	0.04%	0.005%
82	13.695	2067	2068	2070	rVB	500	330	0.02%	0.003%
83	13.853	2092	2094	2098	rVB	391	466	0.03%	0.005%
84	13.902	2098	2102	2103	rBV	261	289	0.02%	0.003%
85	13.914	2103	2104	2107	rBV	551	614	0.04%	0.006%
86	14.201	2149	2151	2152	rBV	474	440	0.03%	0.004%
87	14.969	2273	2277	2280	rBV2	317	650	0.05%	0.007%
88	15.079	2293	2295	2296	rBV	439	252	0.02%	0.003%
89	15.158	2304	2308	2313	rBV3	693	1263	0.09%	0.013%
90	15.237	2319	2321	2322	rBV	509	276	0.02%	0.003%
91	15.268	2322	2326	2327	rVB2	572	517	0.04%	0.005%
92	15.286	2327	2329	2331	rBV2	760	396	0.03%	0.004%
93	15.688	2393	2395	2402	rBV2	539	831	0.06%	0.008%
94	15.969	2439	2441	2442	rBV2	589	438	0.03%	0.004%
95	16.164	2471	2473	2474	rBV	472	341	0.02%	0.003%
96	16.286	2491	2493	2495	rBV	554	594	0.04%	0.006%
97	16.334	2499	2501	2502	rBV	565	341	0.02%	0.003%
98	16.395	2510	2511	2512	rBV	632	310	0.02%	0.003%
99	16.450	2518	2520	2521	rVB	692	314	0.02%	0.003%
100	16.475	2521	2524	2526	rBV2	481	421	0.03%	0.004%

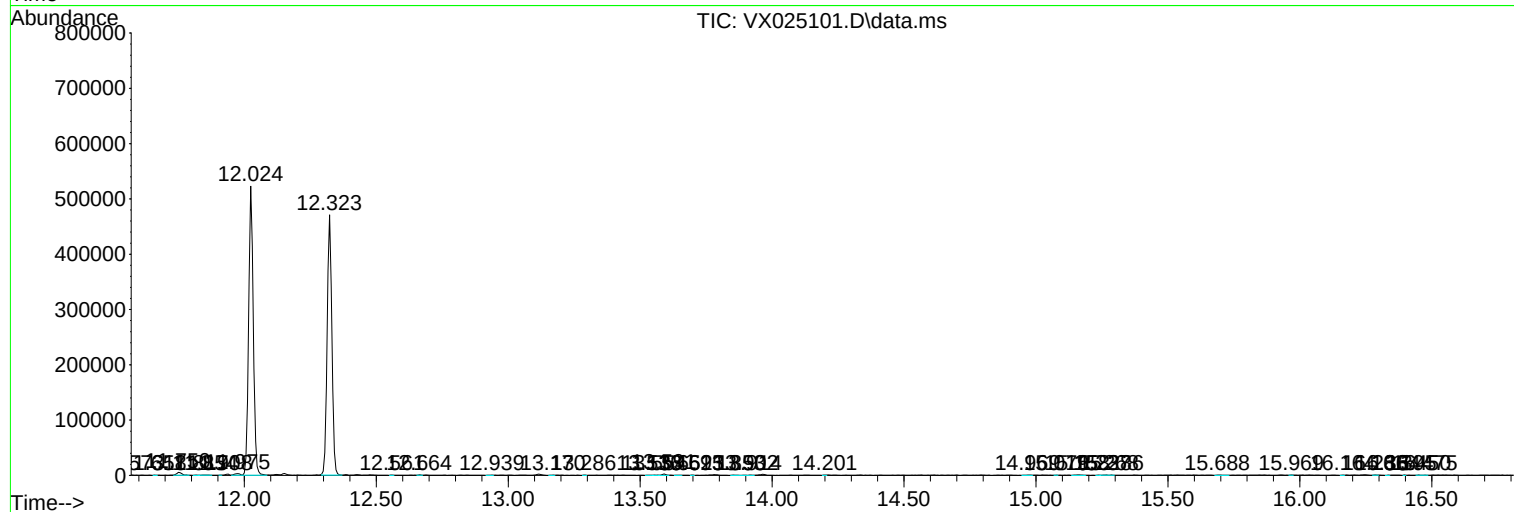
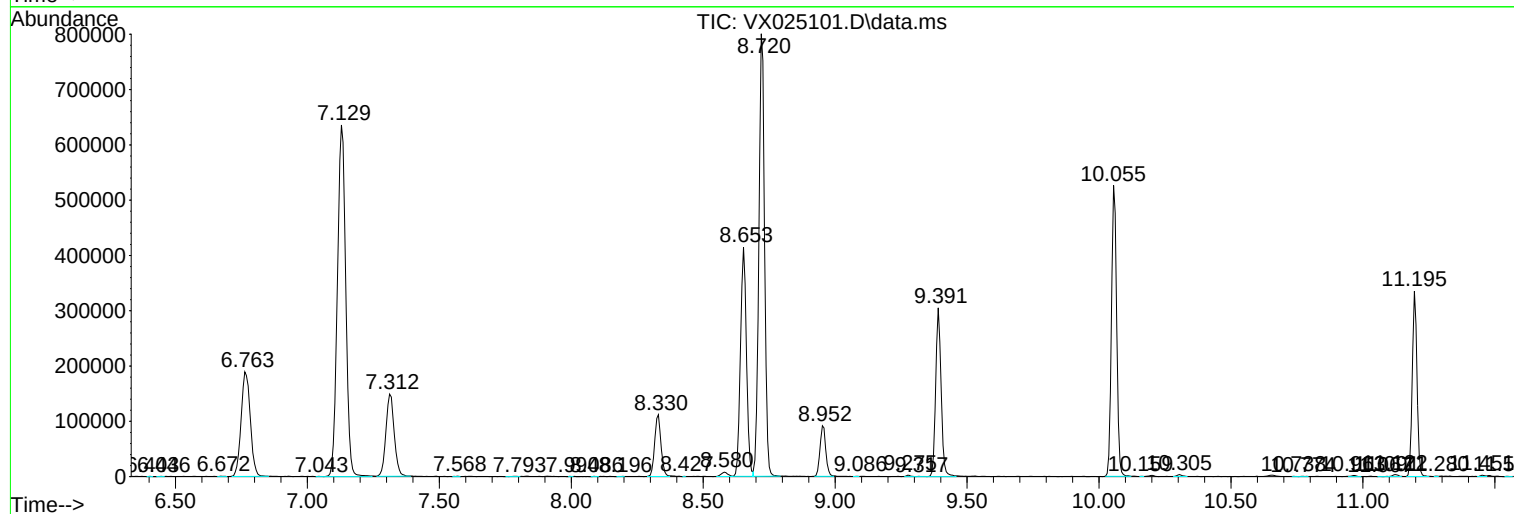
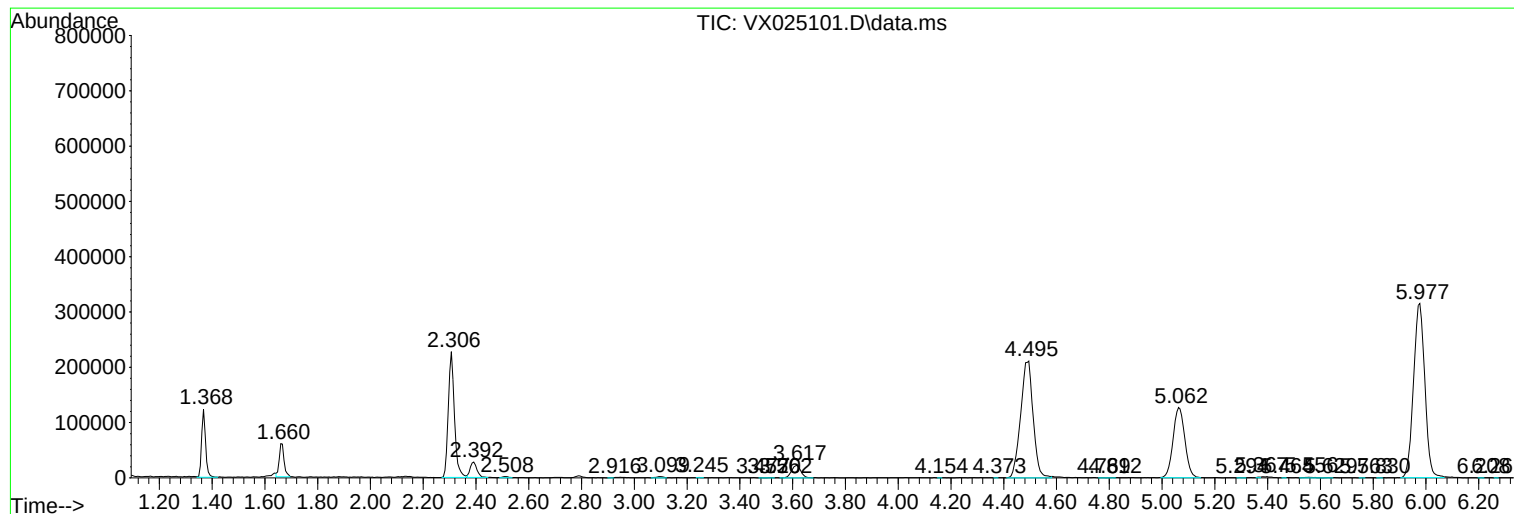
Sum of corrected areas: 9914931

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110821\
Data File : VX025101.D
Acq On : 08 Nov 2021 17:31
Operator : JC/MD
Sample : M4464-04ME 10X
Misc : 7.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GB7K2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML110821WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110821\
Data File : VX025101.D
Acq On : 08 Nov 2021 17:31
Operator : JC/MD
Sample : M4464-04ME 10X
Misc : 7.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GB7K2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML110821WMA.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\VX110821\
Data File : VX025101.D
Acq On : 08 Nov 2021 17:31
Operator : JC/MD
Sample : M4464-04ME 10X
Misc : 7.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GB7K2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML110821WMA.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