

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110921\
 Data File : VX025120.D
 Acq On : 09 Nov 2021 14:34
 Operator : JC/MD
 Sample : M4464-06ME 10X
 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GB7K4ME

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: VX025120.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	53	rBV	87701	89766	6.90%	1.291%
2	1.666	92	95	101	rVB	104960	117872	9.06%	1.695%
3	2.306	194	200	210	rBV	142229	252144	19.39%	3.626%
4	2.709	260	266	268	rBV3	1363	1835	0.14%	0.026%
5	3.056	319	323	327	rBV2	575	1163	0.09%	0.017%
6	3.221	346	350	356	rBB2	591	1347	0.10%	0.019%
7	3.324	365	367	370	rBV2	311	323	0.02%	0.005%
8	3.428	382	384	385	rBV	630	554	0.04%	0.008%
9	3.507	395	397	399	rVB	597	377	0.03%	0.005%
10	3.611	405	414	423	rVV2	13789	31942	2.46%	0.459%
11	3.959	470	471	473	rBV2	510	386	0.03%	0.006%
12	4.038	483	484	486	rVB	563	333	0.03%	0.005%
13	4.099	490	494	496	rVB2	441	444	0.03%	0.006%
14	4.129	496	499	501	rBV	433	334	0.03%	0.005%
15	4.154	501	503	507	rVB	484	416	0.03%	0.006%
16	4.215	507	513	515	rBV2	550	864	0.07%	0.012%
17	4.294	523	526	534	rVB4	1251	2429	0.19%	0.035%
18	4.385	540	541	544	rBV	681	644	0.05%	0.009%
19	4.489	547	558	570	rVV2	210040	639075	49.14%	9.190%
20	5.062	640	652	669	rVB2	95514	286753	22.05%	4.124%
21	5.391	695	706	716	rBV3	8280	26382	2.03%	0.379%
22	5.629	743	745	747	rBV	501	338	0.03%	0.005%
23	5.726	758	761	762	rBV	416	323	0.02%	0.005%
24	5.745	762	764	767	rBV2	275	290	0.02%	0.004%
25	5.818	773	776	778	rBV2	350	506	0.04%	0.007%
26	5.976	787	802	819	rBV2	226404	663449	51.02%	9.541%
27	6.172	831	834	837	rBV	372	407	0.03%	0.006%
28	6.202	837	839	840	rBV	499	487	0.04%	0.007%
29	6.348	860	863	865	rBV	309	358	0.03%	0.005%
30	6.415	872	874	877	rBV	452	452	0.03%	0.007%
31	6.495	882	887	889	rBV2	395	538	0.04%	0.008%
32	6.513	889	890	896	rVB2	364	277	0.02%	0.004%
33	6.562	896	898	899	rBV	569	394	0.03%	0.006%
34	6.763	922	931	947	rVB	165286	398709	30.66%	5.734%
35	7.129	985	991	1002	rVB6	10397	24859	1.91%	0.357%
36	7.220	1002	1006	1008	rBV6	701	842	0.06%	0.012%

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 Title : VOC Analysis

37	7.245	1008	1010	1013	rBV6	204	274	0.02%	0.004%
38	7.318	1013	1022	1033	rBV	138442	306352	23.56%	4.406%
39	7.476	1046	1048	1050	rBV2	826	645	0.05%	0.009%
40	7.811	1101	1103	1107	rVV2	473	548	0.04%	0.008%
41	7.872	1112	1113	1116	rVB	463	368	0.03%	0.005%
42	8.171	1161	1162	1164	rVB	444	275	0.02%	0.004%
43	8.330	1181	1188	1197	rVV	96623	158649	12.20%	2.281%
44	8.452	1205	1208	1211	rBV	763	832	0.06%	0.012%
45	8.476	1211	1212	1213	rBV	561	271	0.02%	0.004%
46	8.580	1226	1229	1234	rVB3	2021	2835	0.22%	0.041%
47	8.653	1234	1241	1247	rBV	321287	505989	38.91%	7.276%
48	8.720	1247	1252	1260	rVB	855905	1300431	100.00%	18.701%
49	8.952	1285	1290	1301	rVB	76769	109736	8.44%	1.578%
50	9.232	1334	1336	1339	rVB2	745	593	0.05%	0.009%
51	9.275	1339	1343	1348	rVB	2291	3528	0.27%	0.051%
52	9.336	1349	1353	1356	rBV	508	836	0.06%	0.012%
53	9.390	1356	1362	1377	rBV	230069	351649	27.04%	5.057%
54	10.055	1465	1471	1478	rBV	363403	482451	37.10%	6.938%
55	10.299	1507	1511	1517	rVB2	10822	15867	1.22%	0.228%
56	10.646	1565	1568	1572	rVB	3675	3840	0.30%	0.055%
57	10.854	1598	1602	1605	rBV2	1089	1529	0.12%	0.022%
58	11.195	1653	1658	1665	rBV	234183	307963	23.68%	4.429%
59	11.439	1695	1698	1699	rBV	830	741	0.06%	0.011%
60	11.536	1712	1714	1715	rBV	785	384	0.03%	0.006%
61	11.689	1735	1739	1741	rBV3	699	916	0.07%	0.013%
62	11.847	1764	1765	1768	rVB2	585	358	0.03%	0.005%
63	12.024	1789	1794	1803	rBV	334841	417695	32.12%	6.007%
64	12.085	1803	1804	1806	rBV	836	424	0.03%	0.006%
65	12.250	1826	1831	1834	rBV4	2649	3788	0.29%	0.054%
66	12.323	1837	1843	1850	rVB	323810	405524	31.18%	5.832%
67	12.427	1857	1860	1865	rVB4	2805	3756	0.29%	0.054%
68	12.859	1928	1931	1933	rBV3	678	668	0.05%	0.010%
69	12.890	1934	1936	1941	rBV2	448	702	0.05%	0.010%
70	12.969	1946	1949	1951	rBV	718	627	0.05%	0.009%
71	13.122	1972	1974	1976	rBV	443	417	0.03%	0.006%
72	13.182	1981	1984	1986	rBV	479	642	0.05%	0.009%
73	13.250	1991	1995	1996	rBV	345	348	0.03%	0.005%
74	13.262	1996	1997	2001	rBV3	746	857	0.07%	0.012%
75	13.341	2008	2010	2011	rBV	336	253	0.02%	0.004%
76	13.420	2021	2023	2028	rBV3	418	703	0.05%	0.010%

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

77	13.652	2057	2061	2063	rBV	533	627	0.05%	0.009%
78	13.688	2063	2067	2069	rBV2	403	479	0.04%	0.007%
79	13.756	2077	2078	2080	rBV2	310	284	0.02%	0.004%
80	13.853	2092	2094	2096	rBV	383	392	0.03%	0.006%
81	13.890	2098	2100	2105	rBV2	426	648	0.05%	0.009%
82	14.042	2124	2125	2127	rBV2	693	553	0.04%	0.008%
83	14.115	2135	2137	2138	rBV	483	327	0.03%	0.005%
84	14.243	2156	2158	2159	rBV	394	282	0.02%	0.004%
85	14.524	2202	2204	2205	rVB	417	273	0.02%	0.004%
86	14.682	2228	2230	2232	rBV	264	286	0.02%	0.004%
87	14.792	2247	2248	2251	rVB	466	269	0.02%	0.004%
88	14.822	2251	2253	2255	rBV	473	363	0.03%	0.005%
89	14.853	2255	2258	2262	rVV3	335	576	0.04%	0.008%
90	14.987	2277	2280	2283	rVB	327	412	0.03%	0.006%
91	15.030	2285	2287	2289	rBV	644	554	0.04%	0.008%
92	15.146	2305	2306	2309	rVB2	629	353	0.03%	0.005%
93	15.170	2309	2310	2313	rBV	482	440	0.03%	0.006%
94	15.206	2315	2316	2319	rBV2	511	539	0.04%	0.008%
95	15.316	2332	2334	2336	rBV2	550	431	0.03%	0.006%
96	15.365	2339	2342	2345	rBV2	677	847	0.07%	0.012%
97	15.591	2375	2379	2381	rBV2	605	913	0.07%	0.013%
98	15.713	2394	2399	2400	rBV2	471	892	0.07%	0.013%
99	16.036	2449	2452	2454	rBV3	636	830	0.06%	0.012%
100	16.566	2538	2539	2541	rBV	374	362	0.03%	0.005%

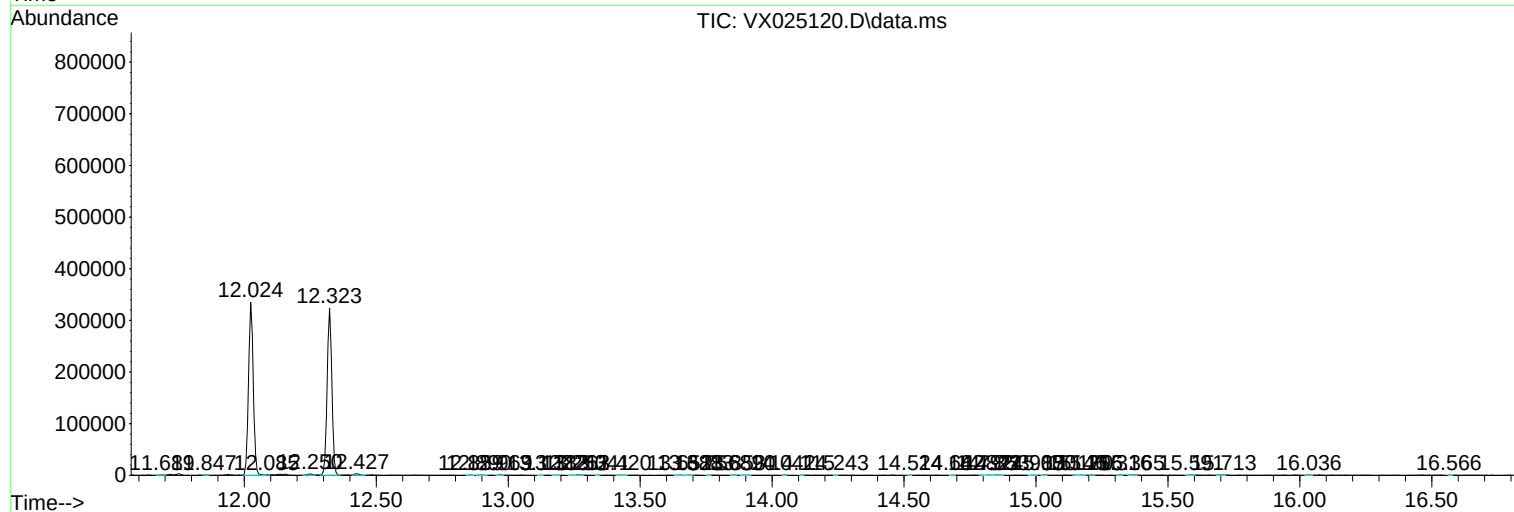
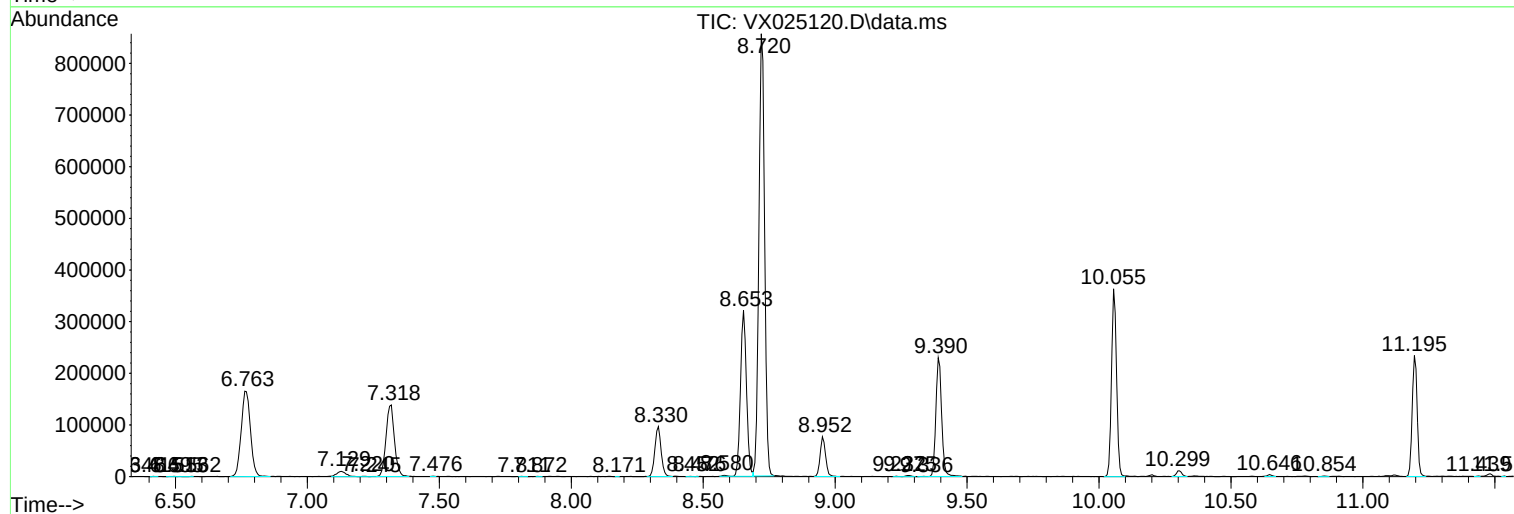
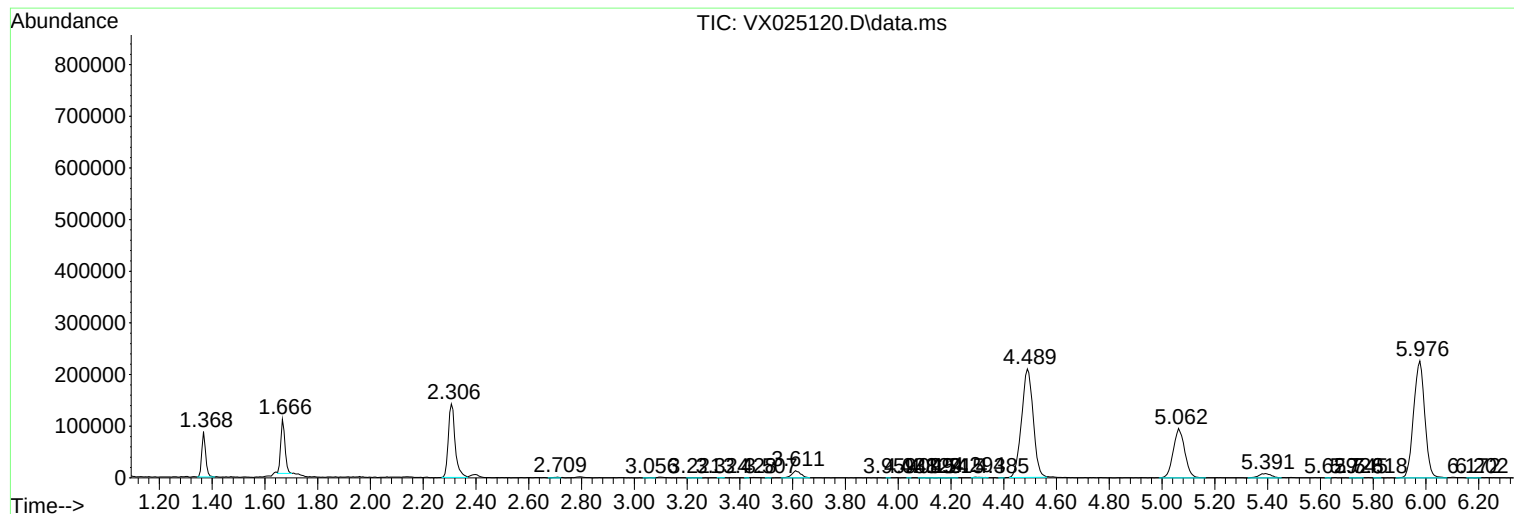
Sum of corrected areas: 6953808

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM110821WMA.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\SFAMXML110821WMA.M
Quant Title : VOC Analysis

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No Library Search Compounds Detected

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