

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
 Data File : VX025599.D
 Acq On : 08 Dec 2021 00:17
 Operator : JC/MD
 Sample : M4885-01ME
 Misc : 4.22g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9K8ME

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: VX025599.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	39	rVV	4914	10639	1.99%	0.242%
2	1.368	43	46	56	rVB	70840	77691	14.52%	1.766%
3	1.648	88	92	98	rBV	38513	47399	8.86%	1.077%
4	2.282	190	196	205	rBV	115228	189168	35.36%	4.300%
5	2.788	273	279	285	rVB3	1003	2436	0.46%	0.055%
6	2.837	285	287	288	rBV2	161	160	0.03%	0.004%
7	2.953	299	306	313	rBV2	3671	9095	1.70%	0.207%
8	3.319	364	366	369	rVV2	125	111	0.02%	0.003%
9	3.367	370	374	378	rVB2	170	232	0.04%	0.005%
10	3.526	398	400	402	rVB2	197	169	0.03%	0.004%
11	3.556	402	405	407	rBV2	175	245	0.05%	0.006%
12	3.825	447	449	451	rVB	170	123	0.02%	0.003%
13	4.294	524	526	529	rVB2	206	172	0.03%	0.004%
14	4.495	548	559	586	rBV2	21010	101260	18.93%	2.302%
15	4.806	607	610	611	rBV2	135	138	0.03%	0.003%
16	5.062	641	652	673	rVB	64118	204397	38.21%	4.646%
17	5.452	713	716	722	rBV3	345	743	0.14%	0.017%
18	5.538	728	730	733	rBV	113	144	0.03%	0.003%
19	5.611	740	742	747	rBB	144	136	0.03%	0.003%
20	5.879	784	786	788	rVB	167	163	0.03%	0.004%
21	5.971	788	801	816	rBV2	185901	534969	100.00%	12.160%
22	6.361	859	865	880	rVB2	2169	7265	1.36%	0.165%
23	6.763	921	931	948	rBV	125047	322828	60.35%	7.338%
24	6.989	966	968	973	rBV2	94	140	0.03%	0.003%
25	7.129	981	991	1003	rBV	132128	298025	55.71%	6.774%
26	7.312	1013	1021	1038	rVB	99966	237722	44.44%	5.403%
27	7.556	1059	1061	1063	rBV	216	192	0.04%	0.004%
28	7.629	1072	1073	1079	rBV2	110	204	0.04%	0.005%
29	7.769	1094	1096	1098	rBV	188	232	0.04%	0.005%
30	8.013	1135	1136	1139	rVB	207	116	0.02%	0.003%
31	8.263	1176	1177	1181	rBV2	148	158	0.03%	0.004%
32	8.330	1181	1188	1201	rBV	59332	108821	20.34%	2.474%
33	8.488	1211	1214	1215	rBV2	128	137	0.03%	0.003%
34	8.592	1229	1231	1234	rVV3	372	395	0.07%	0.009%
35	8.653	1234	1241	1249	rVV	264806	448299	83.80%	10.190%
36	8.720	1249	1252	1270	rVB2	3726	7462	1.39%	0.170%

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 Title : VOC Analysis

37	8.915	1282	1284	1285	rBV	141	115	0.02%	0.003%
38	8.958	1285	1291	1302	rVB	38260	66843	12.49%	1.519%
39	9.275	1338	1343	1351	rVV	39704	58789	10.99%	1.336%
40	9.397	1356	1363	1377	rBV	133206	225587	42.17%	5.128%
41	9.567	1388	1391	1395	rVB3	375	501	0.09%	0.011%
42	9.616	1395	1399	1403	rBV2	354	454	0.08%	0.010%
43	9.714	1412	1415	1419	rVB3	550	749	0.14%	0.017%
44	9.817	1430	1432	1434	rBV	203	109	0.02%	0.002%
45	10.061	1465	1472	1483	rBV	254508	377131	70.50%	8.572%
46	10.250	1501	1503	1506	rVB	145	113	0.02%	0.003%
47	10.305	1508	1512	1517	rVV3	1263	1882	0.35%	0.043%
48	10.360	1520	1521	1526	rVB	262	241	0.05%	0.005%
49	10.647	1564	1568	1571	rBV3	624	931	0.17%	0.021%
50	10.970	1619	1621	1624	rVB	217	185	0.03%	0.004%
51	11.122	1642	1646	1650	rBV2	2103	2990	0.56%	0.068%
52	11.195	1653	1658	1667	rBV	188865	242291	45.29%	5.507%
53	11.305	1675	1676	1682	rVB3	737	901	0.17%	0.020%
54	11.384	1686	1689	1698	rBV3	319	532	0.10%	0.012%
55	11.457	1698	1701	1702	rBV2	379	361	0.07%	0.008%
56	11.476	1702	1704	1707	rBV2	853	887	0.17%	0.020%
57	11.549	1713	1716	1718	rBV3	264	277	0.05%	0.006%
58	11.616	1725	1727	1728	rBV2	263	224	0.04%	0.005%
59	11.677	1735	1737	1739	rBV3	260	278	0.05%	0.006%
60	11.720	1741	1744	1745	rVV	425	530	0.10%	0.012%
61	11.756	1745	1750	1754	rVB2	2579	3811	0.71%	0.087%
62	11.841	1761	1764	1767	rBV3	485	542	0.10%	0.012%
63	11.939	1776	1780	1783	rVB4	1226	1638	0.31%	0.037%
64	12.024	1789	1794	1804	rBV	314286	382930	71.58%	8.704%
65	12.128	1807	1811	1812	rVV4	942	1199	0.22%	0.027%
66	12.146	1812	1814	1818	rVB2	1647	2128	0.40%	0.048%
67	12.232	1825	1828	1831	rBV3	204	256	0.05%	0.006%
68	12.262	1831	1833	1835	rBV	307	204	0.04%	0.005%
69	12.323	1835	1843	1851	rBV	321453	396273	74.07%	9.007%
70	12.427	1857	1860	1864	rVB3	1510	1583	0.30%	0.036%
71	12.482	1864	1869	1873	rVB3	417	800	0.15%	0.018%
72	12.664	1897	1899	1901	rBV2	538	407	0.08%	0.009%
73	12.847	1927	1929	1931	rBV2	123	118	0.02%	0.003%
74	12.975	1945	1950	1952	rBV	361	487	0.09%	0.011%
75	13.055	1960	1963	1967	rVB3	528	592	0.11%	0.013%
76	13.268	1993	1998	2002	rBV2	900	1160	0.22%	0.026%

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77	13.384	2015	2017	2018	rBV2	243	199	0.04%	0.005%
78	13.707	2064	2070	2074	rVV4	297	725	0.14%	0.016%
79	13.780	2077	2082	2090	rVB	1147	1536	0.29%	0.035%
80	13.841	2090	2092	2096	rBV2	448	575	0.11%	0.013%
81	13.951	2107	2110	2111	rBV	162	165	0.03%	0.004%
82	14.036	2121	2124	2128	rVB	766	837	0.16%	0.019%
83	14.146	2137	2142	2145	rBV3	355	645	0.12%	0.015%
84	14.207	2150	2152	2155	rVB2	246	220	0.04%	0.005%
85	14.231	2155	2156	2159	rBV2	137	123	0.02%	0.003%
86	14.524	2199	2204	2205	rBV3	318	442	0.08%	0.010%
87	14.756	2240	2242	2244	rBV2	648	670	0.13%	0.015%
88	14.780	2244	2246	2250	rVB3	660	693	0.13%	0.016%
89	14.932	2269	2271	2273	rVB2	243	136	0.03%	0.003%
90	14.975	2276	2278	2281	rBV3	228	247	0.05%	0.006%
91	15.152	2306	2307	2310	rBV	207	211	0.04%	0.005%
92	15.213	2312	2317	2324	rBV4	505	1090	0.20%	0.025%
93	15.371	2340	2343	2347	rBV2	374	568	0.11%	0.013%
94	15.487	2358	2362	2365	rVB3	555	667	0.12%	0.015%
95	15.694	2394	2396	2398	rBV	212	195	0.04%	0.004%
96	15.768	2407	2408	2411	rVB2	203	135	0.03%	0.003%
97	15.792	2411	2412	2413	rBV	266	150	0.03%	0.003%
98	16.042	2451	2453	2454	rVB	299	167	0.03%	0.004%
99	16.060	2454	2456	2457	rBV	221	179	0.03%	0.004%
100	16.322	2497	2499	2500	rBV	319	225	0.04%	0.005%

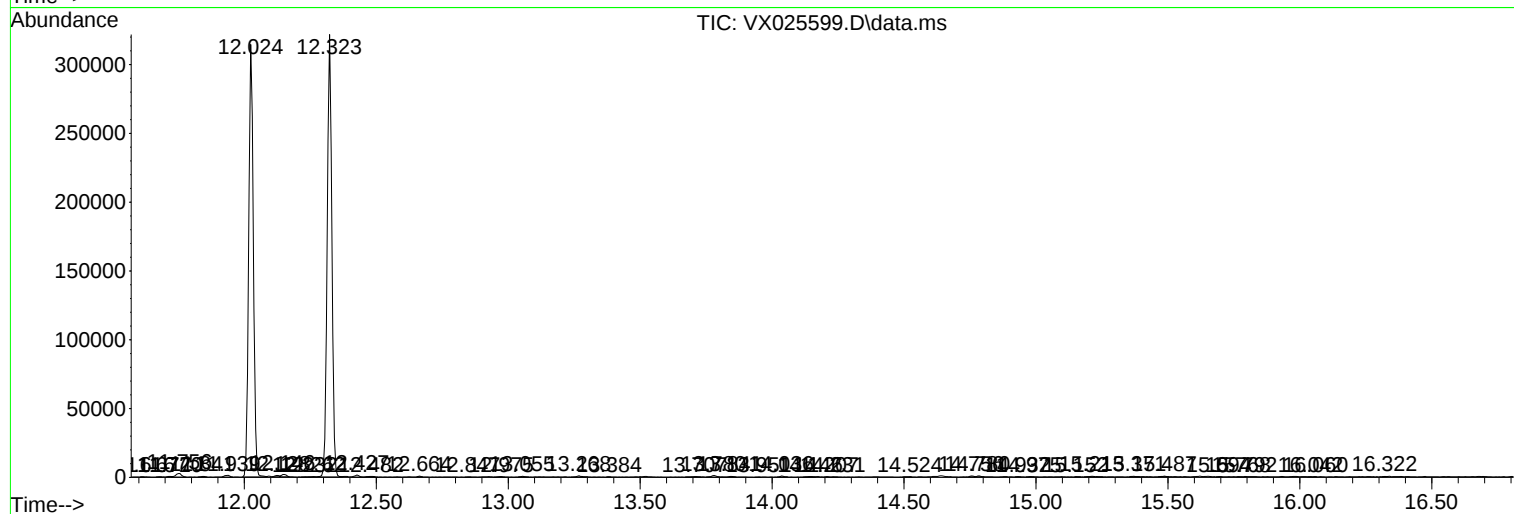
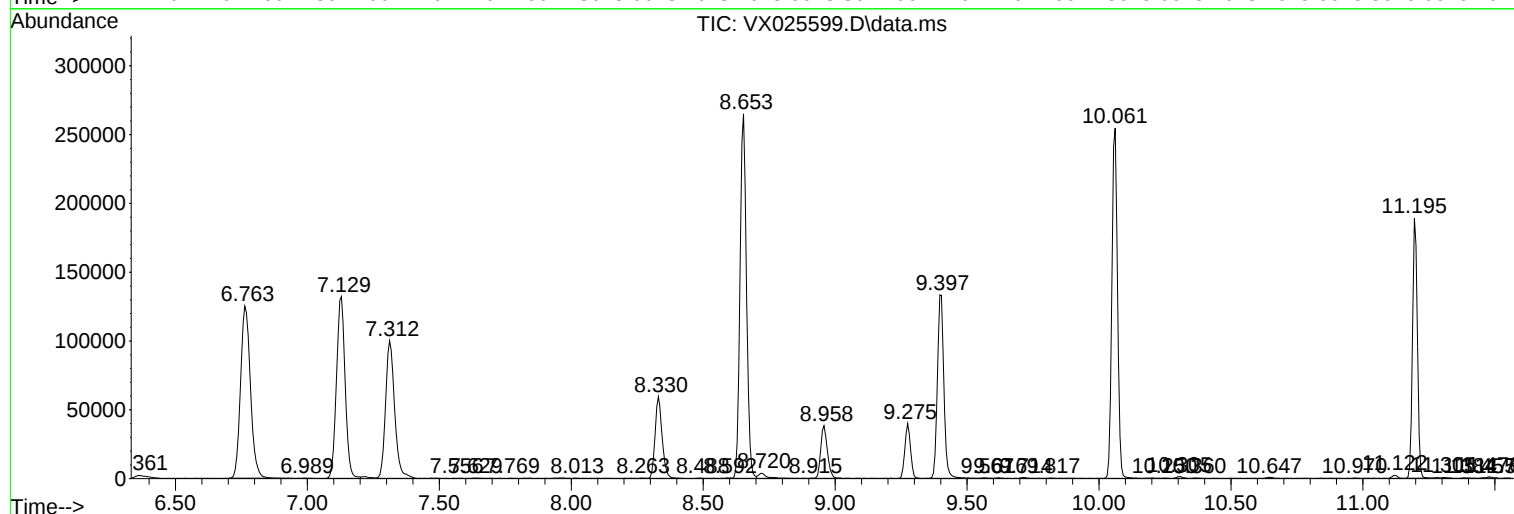
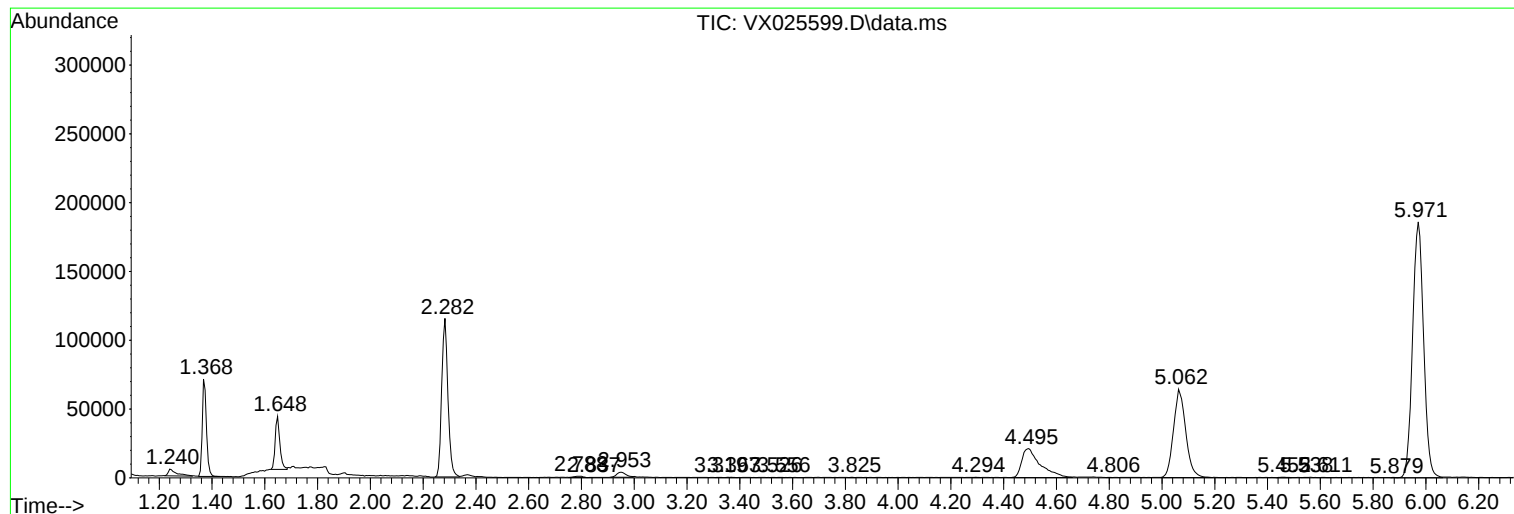
Sum of corrected areas: 4399415

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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



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
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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