

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039327.D
 Acq On : 18 Dec 2023 21:36
 Operator : JC/MD
 Sample : 05835-09 100X
 Misc : 3.02g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AQ1

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\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039327.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	56	rBV	89507	93197	7.45%	1.265%
2	1.666	91	95	105	rBV	61402	85890	6.87%	1.166%
3	2.307	194	200	212	rBV	163504	253965	20.30%	3.447%
4	2.703	263	265	269	rVB2	432	658	0.05%	0.009%
5	2.752	269	273	274	rBV2	298	271	0.02%	0.004%
6	2.788	275	279	286	rVB3	1721	3484	0.28%	0.047%
7	2.941	298	304	315	rVB2	3688	7728	0.62%	0.105%
8	3.489	393	394	397	rVV	248	188	0.02%	0.003%
9	3.611	412	414	418	rBV	259	334	0.03%	0.005%
10	3.983	472	475	477	rVB2	153	179	0.01%	0.002%
11	4.056	485	487	488	rBV	243	193	0.02%	0.003%
12	4.453	540	552	565	rBV	88690	251827	20.13%	3.418%
13	4.709	592	594	595	rBV	295	238	0.02%	0.003%
14	5.056	638	651	668	rBV	111772	332804	26.61%	4.517%
15	5.330	692	696	697	rBV2	186	196	0.02%	0.003%
16	5.343	697	698	701	rBV2	281	204	0.02%	0.003%
17	5.532	727	729	735	rBV3	258	339	0.03%	0.005%
18	5.696	754	756	759	rVB2	268	275	0.02%	0.004%
19	5.763	763	767	768	rVB	402	306	0.02%	0.004%
20	5.971	789	801	823	rBV2	272028	837358	66.94%	11.366%
21	6.324	856	859	862	rVV	298	326	0.03%	0.004%
22	6.519	888	891	893	rBV2	207	268	0.02%	0.004%
23	6.580	898	901	902	rBV2	228	232	0.02%	0.003%
24	6.605	902	905	907	rVV	239	205	0.02%	0.003%
25	6.763	922	931	944	rBV	217476	523736	41.87%	7.109%
26	7.031	973	975	977	rVB2	339	289	0.02%	0.004%
27	7.111	983	988	990	rBV2	1244	1844	0.15%	0.025%
28	7.306	1012	1020	1031	rBV	174257	380572	30.43%	5.166%
29	7.421	1037	1039	1041	rBV	265	194	0.02%	0.003%
30	7.562	1061	1062	1064	rBV2	348	258	0.02%	0.004%
31	7.757	1090	1094	1095	rBV2	159	187	0.01%	0.003%
32	7.891	1114	1116	1120	rBV2	154	233	0.02%	0.003%
33	7.958	1123	1127	1131	rVB2	252	355	0.03%	0.005%
34	8.062	1141	1144	1145	rBV2	217	230	0.02%	0.003%
35	8.190	1162	1165	1167	rBV	248	231	0.02%	0.003%
36	8.324	1179	1187	1200	rBV	114875	193668	15.48%	2.629%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
 Title : VOC Analysis

37	8.574	1226	1228	1234	rVB2	422	486	0.04%	0.007%
38	8.647	1234	1240	1263	rBV	394685	632558	50.57%	8.586%
39	8.952	1284	1290	1299	rBV	83407	126564	10.12%	1.718%
40	9.061	1306	1308	1314	rVB2	534	934	0.07%	0.013%
41	9.116	1314	1317	1320	rBV2	252	357	0.03%	0.005%
42	9.281	1340	1344	1348	rBV3	461	651	0.05%	0.009%
43	9.385	1355	1361	1379	rBV	397878	577253	46.15%	7.835%
44	9.695	1409	1412	1418	rVB5	729	1219	0.10%	0.017%
45	9.781	1424	1426	1428	rBV	261	213	0.02%	0.003%
46	10.055	1465	1471	1473	rBV	480758	686419	54.88%	9.317%
47	10.195	1491	1494	1497	rVB4	677	890	0.07%	0.012%
48	10.311	1510	1513	1516	rVB2	439	560	0.04%	0.008%
49	10.647	1562	1568	1577	rBV4	443	1430	0.11%	0.019%
50	10.817	1595	1596	1599	rVB2	220	178	0.01%	0.002%
51	10.860	1601	1603	1605	rBV2	214	234	0.02%	0.003%
52	10.964	1619	1620	1624	rVB2	409	484	0.04%	0.007%
53	11.092	1638	1641	1646	rVB2	597	755	0.06%	0.010%
54	11.189	1652	1657	1669	rBV	337024	433011	34.62%	5.878%
55	11.323	1675	1679	1680	rBV2	179	200	0.02%	0.003%
56	11.372	1683	1687	1690	rVV3	677	826	0.07%	0.011%
57	11.433	1694	1697	1699	rBV2	273	404	0.03%	0.005%
58	11.457	1699	1701	1709	rVB3	778	1339	0.11%	0.018%
59	11.518	1709	1711	1714	rBV2	150	193	0.02%	0.003%
60	11.683	1737	1738	1741	rBV2	270	243	0.02%	0.003%
61	11.750	1747	1749	1750	rVV	278	285	0.02%	0.004%
62	11.793	1753	1756	1757	rVB	257	218	0.02%	0.003%
63	11.969	1780	1785	1789	rBV	59476	73473	5.87%	0.997%
64	12.024	1789	1794	1806	rVB2	567232	1250824	100.00%	16.978%
65	12.317	1837	1842	1850	rBV	452785	582370	46.56%	7.905%
66	12.518	1870	1875	1876	rBV	217	305	0.02%	0.004%
67	12.597	1885	1888	1891	rBV	187	239	0.02%	0.003%
68	12.725	1906	1909	1910	rBV2	215	199	0.02%	0.003%
69	12.756	1912	1914	1919	rVV2	556	899	0.07%	0.012%
70	12.799	1919	1921	1924	rVB2	197	197	0.02%	0.003%
71	13.067	1959	1965	1970	rVB6	2712	5085	0.41%	0.069%
72	13.116	1970	1973	1977	rBV4	1527	2101	0.17%	0.029%
73	13.329	2005	2008	2009	rBV2	190	180	0.01%	0.002%
74	13.597	2048	2052	2057	rVB2	674	895	0.07%	0.012%
75	13.786	2078	2083	2088	rBV3	634	1048	0.08%	0.014%
76	13.841	2091	2092	2094	rBV	265	214	0.02%	0.003%

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 Title : VOC Analysis

77	13.969	2110	2113	2116	rVB3	394	526	0.04%	0.007%
78	14.128	2135	2139	2145	rBV2	1379	2016	0.16%	0.027%
79	14.176	2145	2147	2149	rBV	171	177	0.01%	0.002%
80	14.250	2157	2159	2164	rBV2	155	202	0.02%	0.003%
81	14.335	2171	2173	2178	rVB2	243	327	0.03%	0.004%
82	14.414	2182	2186	2190	rBV2	263	498	0.04%	0.007%
83	14.469	2193	2195	2197	rBV	225	181	0.01%	0.002%
84	14.597	2215	2216	2219	rBV2	240	236	0.02%	0.003%
85	14.646	2222	2224	2225	rBV	332	210	0.02%	0.003%
86	14.664	2225	2227	2231	rVB2	208	307	0.02%	0.004%
87	14.701	2231	2233	2235	rBV2	196	219	0.02%	0.003%
88	14.896	2263	2265	2267	rBV	260	212	0.02%	0.003%
89	14.987	2278	2280	2282	rBV2	288	232	0.02%	0.003%
90	15.030	2285	2287	2291	rVB2	287	258	0.02%	0.004%
91	15.341	2336	2338	2340	rVB2	305	183	0.01%	0.002%
92	15.390	2344	2346	2352	rVB3	722	1115	0.09%	0.015%
93	15.469	2357	2359	2360	rBV	276	220	0.02%	0.003%
94	15.512	2364	2366	2367	rBV	261	188	0.02%	0.003%
95	15.646	2386	2388	2390	rBV	235	184	0.01%	0.002%
96	15.792	2408	2412	2414	rBV2	190	201	0.02%	0.003%
97	15.938	2434	2436	2439	rBV2	328	251	0.02%	0.003%
98	16.176	2473	2475	2478	rBV	255	195	0.02%	0.003%
99	16.377	2504	2508	2511	rBV	320	466	0.04%	0.006%
100	16.658	2552	2554	2555	rBV2	317	235	0.02%	0.003%

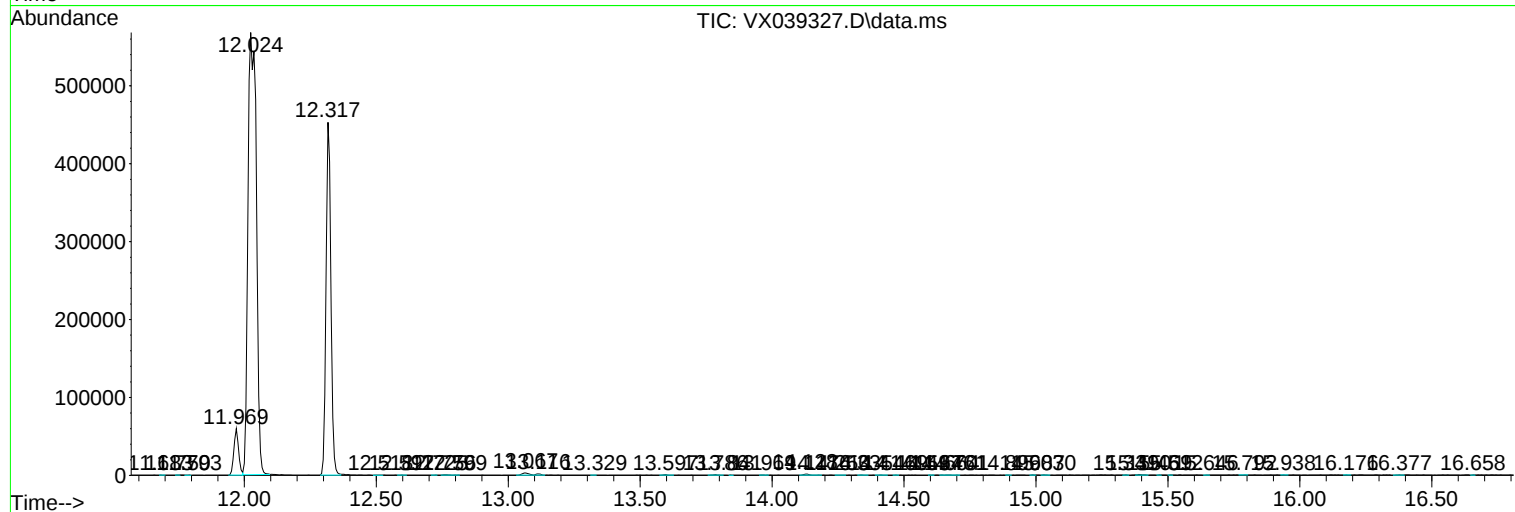
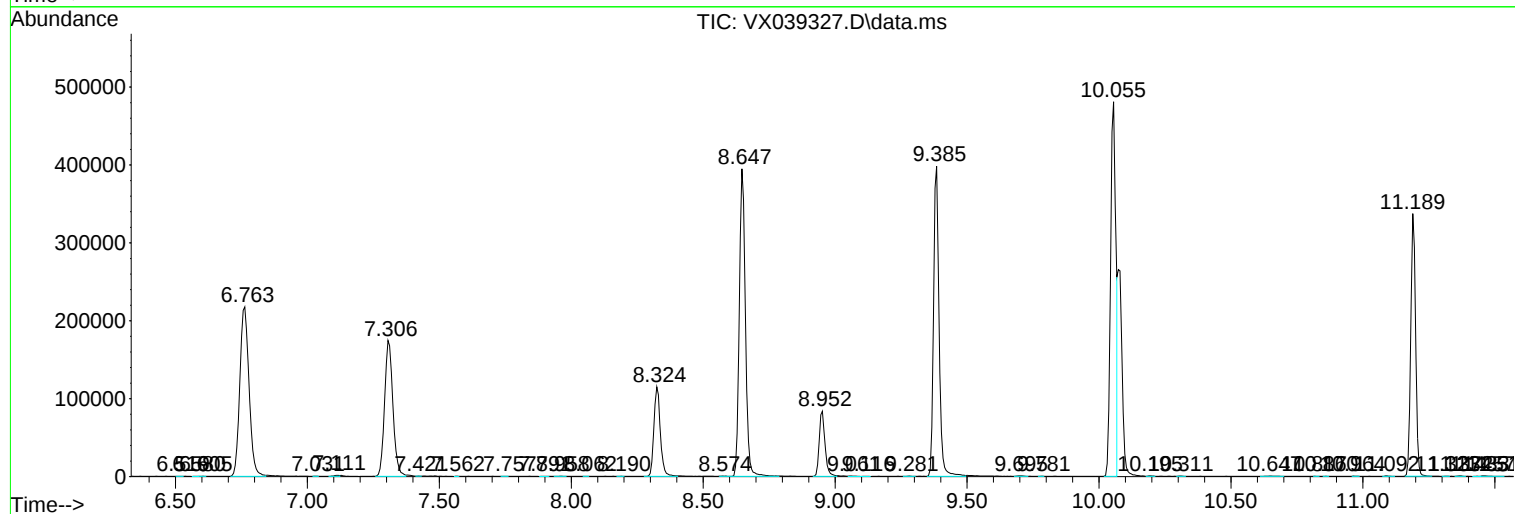
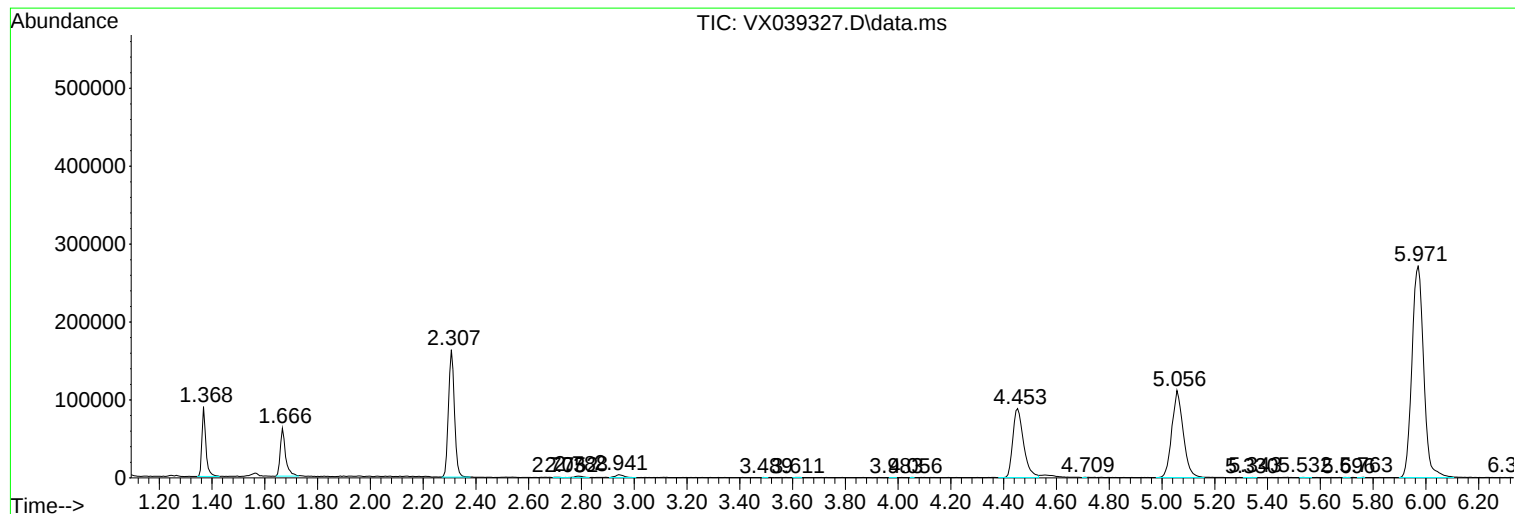
Sum of corrected areas: 7367234

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.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\SFAMXML120523WMA.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