

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039404.D
 Acq On : 20 Dec 2023 16:13
 Operator : JC/MD
 Sample : 05835-13DL 5X
 Misc : 2.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AR0DL

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: VX039404.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	23	25	33	rBV3	1854	3665	0.56%	0.070%
2	1.367	43	46	56	rVB	57355	64591	9.92%	1.242%
3	1.654	90	93	102	rVB	44808	64398	9.89%	1.238%
4	2.300	193	199	210	rBV	98854	156771	24.07%	3.015%
5	2.386	210	213	219	rVB3	2028	3074	0.47%	0.059%
6	2.508	231	233	235	rBV	295	270	0.04%	0.005%
7	2.703	259	265	274	rBV	2925	5540	0.85%	0.107%
8	2.788	274	279	286	rVV	2680	4769	0.73%	0.092%
9	2.940	296	304	319	rVB	18176	41946	6.44%	0.807%
10	3.190	343	345	348	rVB	212	161	0.02%	0.003%
11	3.227	348	351	354	rVV	156	177	0.03%	0.003%
12	3.306	363	364	365	rBV	258	153	0.02%	0.003%
13	3.379	374	376	378	rVB2	353	214	0.03%	0.004%
14	3.709	429	430	434	rBV	232	267	0.04%	0.005%
15	4.044	483	485	488	rVB2	244	264	0.04%	0.005%
16	4.068	488	489	491	rBV	285	216	0.03%	0.004%
17	4.160	502	504	506	rBV2	188	173	0.03%	0.003%
18	4.269	520	522	526	rVB	232	190	0.03%	0.004%
19	4.306	526	528	530	rBV2	173	225	0.03%	0.004%
20	4.452	542	552	567	rBV2	66242	198640	30.50%	3.820%
21	4.788	606	607	610	rVB	320	155	0.02%	0.003%
22	5.056	639	651	667	rBV	79996	259004	39.76%	4.981%
23	5.306	691	692	697	rVB2	204	147	0.02%	0.003%
24	5.452	715	716	718	rBV	223	146	0.02%	0.003%
25	5.964	789	800	819	rBV2	214596	651349	100.00%	12.526%
26	6.257	846	848	851	rVV2	213	239	0.04%	0.005%
27	6.281	851	852	856	rVV	213	180	0.03%	0.003%
28	6.312	856	857	860	rVB2	252	222	0.03%	0.004%
29	6.379	866	868	870	rVB	243	202	0.03%	0.004%
30	6.403	870	872	875	rVB2	342	301	0.05%	0.006%
31	6.757	921	930	952	rVV	173003	421900	64.77%	8.114%
32	7.037	974	976	978	rBV3	210	200	0.03%	0.004%
33	7.110	983	988	994	rVV5	1132	2636	0.40%	0.051%
34	7.305	1011	1020	1036	rBV	142662	310175	47.62%	5.965%
35	7.476	1044	1048	1051	rBV4	452	791	0.12%	0.015%
36	7.507	1051	1053	1055	rVB	392	256	0.04%	0.005%

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

37	7.580	1063	1065	1067	rBV	226	216	0.03%	0.004%
38	7.647	1074	1076	1079	rVB2	229	181	0.03%	0.003%
39	7.671	1079	1080	1081	rBV	320	145	0.02%	0.003%
40	7.744	1088	1092	1093	rBV2	160	215	0.03%	0.004%
41	7.970	1124	1129	1130	rBV2	827	1151	0.18%	0.022%
42	8.074	1143	1146	1147	rBV2	167	211	0.03%	0.004%
43	8.147	1155	1158	1160	rBV2	192	203	0.03%	0.004%
44	8.263	1175	1177	1179	rVV2	241	173	0.03%	0.003%
45	8.324	1181	1187	1202	rVV	83163	141835	21.78%	2.728%
46	8.488	1213	1214	1216	rVB	307	147	0.02%	0.003%
47	8.574	1226	1228	1229	rBV	262	186	0.03%	0.004%
48	8.647	1233	1240	1260	rBV	265746	429304	65.91%	8.256%
49	8.830	1268	1270	1273	rVB	247	191	0.03%	0.004%
50	8.951	1284	1290	1297	rBV	61766	93645	14.38%	1.801%
51	9.214	1331	1333	1335	rVB2	216	148	0.02%	0.003%
52	9.281	1341	1344	1348	rVB2	399	377	0.06%	0.007%
53	9.384	1356	1361	1381	rBV	326888	475217	72.96%	9.139%
54	9.701	1409	1413	1420	rBV2	1307	2318	0.36%	0.045%
55	9.793	1425	1428	1430	rBV2	213	248	0.04%	0.005%
56	10.055	1465	1471	1473	rBV	379253	572347	87.87%	11.007%
57	10.317	1510	1514	1515	rBV2	296	287	0.04%	0.006%
58	10.470	1537	1539	1541	rVV	238	212	0.03%	0.004%
59	10.695	1572	1576	1579	rBV2	140	250	0.04%	0.005%
60	10.750	1583	1585	1587	rBV	153	153	0.02%	0.003%
61	10.963	1617	1620	1626	rVB2	2413	2934	0.45%	0.056%
62	11.091	1638	1641	1644	rBV2	248	277	0.04%	0.005%
63	11.189	1652	1657	1668	rBV	274989	363503	55.81%	6.991%
64	11.317	1675	1678	1680	rBV	550	581	0.09%	0.011%
65	11.853	1764	1766	1768	rVB	256	149	0.02%	0.003%
66	11.884	1768	1771	1772	rBV	217	164	0.03%	0.003%
67	11.914	1774	1776	1779	rBV2	178	171	0.03%	0.003%
68	11.975	1779	1786	1788	rBV3	885	1057	0.16%	0.020%
69	12.024	1788	1794	1803	rVV	375531	503540	77.31%	9.684%
70	12.237	1826	1829	1832	rBV2	278	438	0.07%	0.008%
71	12.317	1837	1842	1853	rVV	307296	399007	61.26%	7.674%
72	12.762	1911	1915	1921	rVB2	2203	2915	0.45%	0.056%
73	13.024	1955	1958	1959	rBV	177	145	0.02%	0.003%
74	13.079	1964	1967	1970	rBV2	193	317	0.05%	0.006%
75	13.109	1970	1972	1973	rBV2	239	152	0.02%	0.003%
76	13.286	1999	2001	2003	rVB	202	155	0.02%	0.003%

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

Title : VOC Analysis

77	13.317	2003	2006	2008	rBV2	161	235	0.04%	0.005%
78	13.378	2015	2016	2020	rBV2	166	226	0.03%	0.004%
79	13.542	2041	2043	2046	rVB2	225	223	0.03%	0.004%
80	13.597	2049	2052	2056	rVB3	388	489	0.08%	0.009%
81	13.780	2080	2082	2088	rVV2	476	660	0.10%	0.013%
82	13.914	2102	2104	2106	rBV	170	157	0.02%	0.003%
83	13.932	2106	2107	2109	rBV	312	249	0.04%	0.005%
84	14.127	2135	2139	2143	rVB	3904	4920	0.76%	0.095%
85	14.207	2150	2152	2155	rBV2	214	177	0.03%	0.003%
86	14.249	2157	2159	2161	rBV	216	170	0.03%	0.003%
87	14.292	2164	2166	2169	rBV2	132	147	0.02%	0.003%
88	14.347	2173	2175	2177	rBV	157	156	0.02%	0.003%
89	14.444	2189	2191	2193	rBV	178	219	0.03%	0.004%
90	14.579	2211	2213	2216	rVV2	171	200	0.03%	0.004%
91	14.615	2217	2219	2222	rVV3	251	287	0.04%	0.006%
92	14.749	2240	2241	2243	rVB	261	172	0.03%	0.003%
93	14.780	2243	2246	2247	rBV	283	264	0.04%	0.005%
94	14.902	2264	2266	2268	rBV2	173	159	0.02%	0.003%
95	15.060	2290	2292	2293	rBV	298	224	0.03%	0.004%
96	15.365	2340	2342	2343	rBV2	271	222	0.03%	0.004%
97	15.377	2343	2344	2349	rVB2	499	648	0.10%	0.012%
98	15.487	2360	2362	2366	rBV2	285	387	0.06%	0.007%
99	15.584	2377	2378	2381	rBV	390	339	0.05%	0.007%
100	16.456	2519	2521	2524	rBV3	468	380	0.06%	0.007%

Sum of corrected areas: 5199782

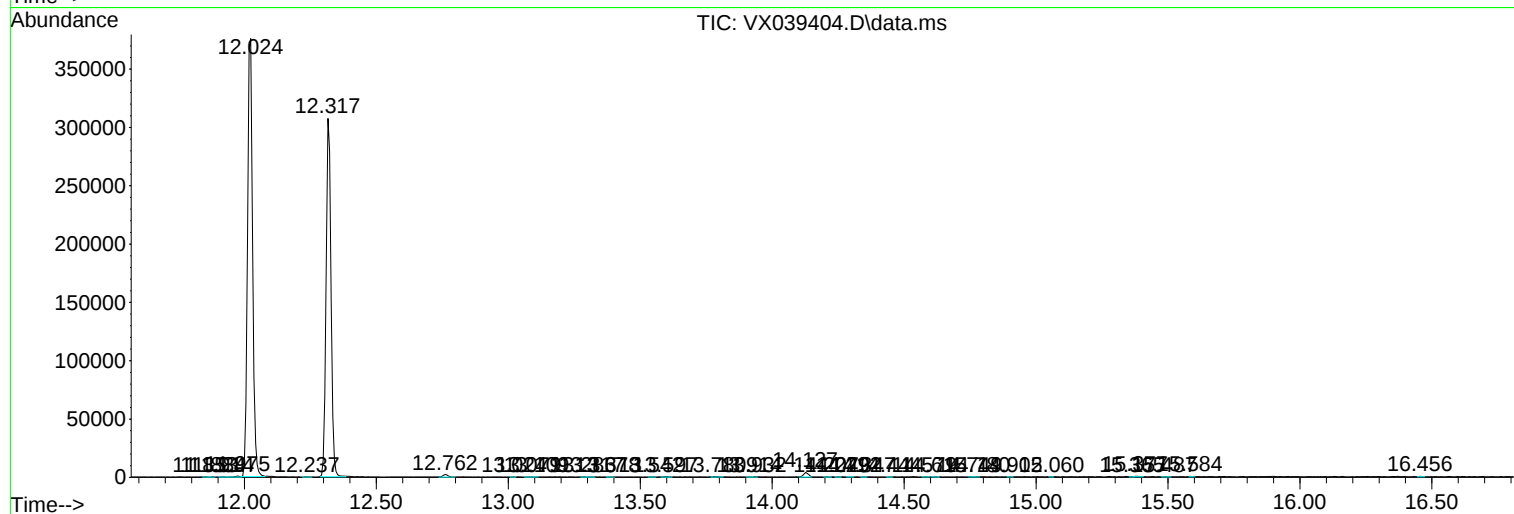
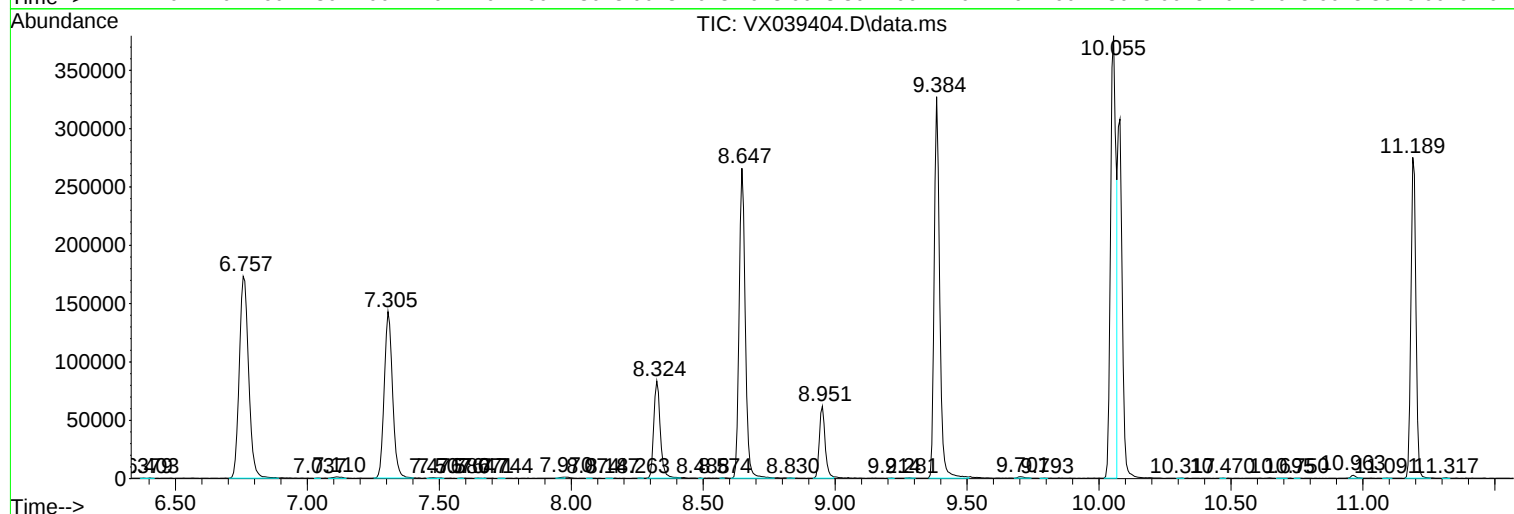
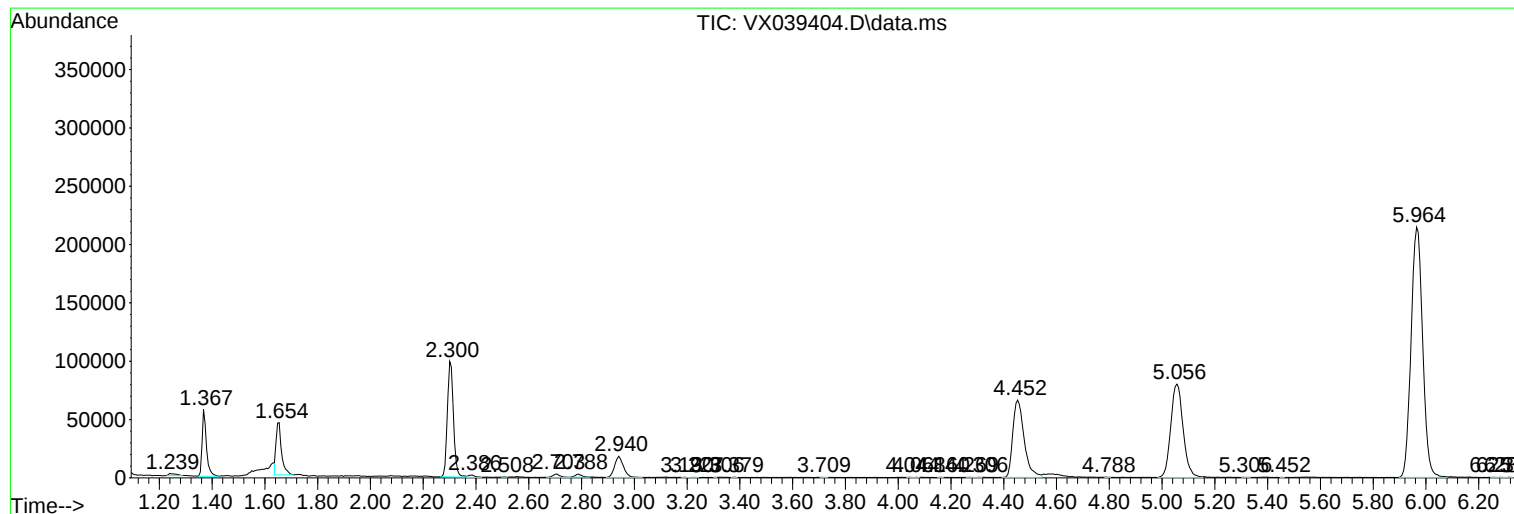
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
Quant Title : VOC Analysis

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