

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
 Data File : VX039151.D
 Acq On : 11 Dec 2023 18:03
 Operator : JC/MD
 Sample : 05752-05 100X
 Misc : 4.14g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AW6

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: VX039151.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	23	26	34	rVB2	3167	5936	0.18%	0.042%
2	1.367	42	46	54	rBV	123740	129707	3.85%	0.927%
3	1.666	91	95	110	rVB	82823	117916	3.50%	0.843%
4	2.306	194	200	211	rBV	217910	339541	10.09%	2.427%
5	2.581	243	245	248	rBV	219	205	0.01%	0.001%
6	2.690	260	263	268	rVB	486	594	0.02%	0.004%
7	2.788	275	279	286	rVB4	1390	2445	0.07%	0.017%
8	2.867	290	292	295	rVB2	280	275	0.01%	0.002%
9	2.946	297	305	311	rBV2	3652	7721	0.23%	0.055%
10	3.428	382	384	387	rVV2	209	208	0.01%	0.001%
11	3.526	398	400	402	rVV	227	184	0.01%	0.001%
12	4.300	525	527	529	rBV2	168	195	0.01%	0.001%
13	4.452	543	552	565	rBV	94138	266972	7.93%	1.908%
14	5.056	637	651	667	rBV	127695	411818	12.23%	2.943%
15	5.397	703	707	712	rVB3	493	653	0.02%	0.005%
16	5.489	720	722	726	rBV2	233	328	0.01%	0.002%
17	5.800	771	773	776	rVB2	367	318	0.01%	0.002%
18	5.836	776	779	783	rBV2	211	460	0.01%	0.003%
19	5.964	788	800	820	rBV2	343818	1052615	31.27%	7.523%
20	6.519	889	891	894	rBV2	204	252	0.01%	0.002%
21	6.568	898	899	903	rVB2	310	200	0.01%	0.001%
22	6.757	920	930	948	rBV	266558	656232	19.49%	4.690%
23	7.062	979	980	983	rBV2	254	307	0.01%	0.002%
24	7.116	983	989	997	rVB4	1785	3606	0.11%	0.026%
25	7.202	1001	1003	1004	rBV2	328	229	0.01%	0.002%
26	7.305	1012	1020	1041	rBV	216193	477833	14.19%	3.415%
27	7.482	1046	1049	1052	rBV4	899	1150	0.03%	0.008%
28	7.665	1077	1079	1081	rVB	300	220	0.01%	0.002%
29	7.702	1083	1085	1089	rVV2	236	346	0.01%	0.002%
30	7.738	1089	1091	1093	rVB2	271	220	0.01%	0.002%
31	7.763	1093	1095	1098	rBV	345	310	0.01%	0.002%
32	8.104	1149	1151	1153	rVB2	274	194	0.01%	0.001%
33	8.263	1173	1177	1178	rBV2	165	203	0.01%	0.001%
34	8.324	1181	1187	1203	rBV	153491	260983	7.75%	1.865%
35	8.574	1227	1228	1231	rBV2	277	306	0.01%	0.002%
36	8.647	1233	1240	1257	rVV	529282	820611	24.38%	5.865%

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 Title : VOC Analysis

37	8.848	1272	1273	1277	rBV3	319	304	0.01%	0.002%
38	8.951	1284	1290	1304	rBV	113671	175887	5.22%	1.257%
39	9.195	1328	1330	1332	rBV	296	239	0.01%	0.002%
40	9.275	1341	1343	1346	rVB2	324	231	0.01%	0.002%
41	9.311	1348	1349	1352	rBV2	176	177	0.01%	0.001%
42	9.384	1355	1361	1379	rBV	429164	628866	18.68%	4.494%
43	9.549	1386	1388	1390	rVB3	516	393	0.01%	0.003%
44	9.701	1409	1413	1419	rVB2	1586	2257	0.07%	0.016%
45	9.939	1449	1452	1453	rVV	239	264	0.01%	0.002%
46	10.055	1465	1471	1490	rBV2	564716	986931	29.32%	7.053%
47	10.281	1505	1508	1510	rVB2	289	301	0.01%	0.002%
48	10.311	1510	1513	1514	rBV	244	180	0.01%	0.001%
49	10.415	1528	1530	1532	rVB	245	217	0.01%	0.002%
50	10.561	1551	1554	1557	rVB	214	213	0.01%	0.002%
51	10.598	1557	1560	1564	rBV2	162	237	0.01%	0.002%
52	10.793	1590	1592	1595	rBV2	163	179	0.01%	0.001%
53	11.091	1637	1641	1644	rVB3	772	959	0.03%	0.007%
54	11.189	1652	1657	1666	rBV	410881	515629	15.32%	3.685%
55	11.305	1674	1676	1683	rVB3	532	685	0.02%	0.005%
56	11.366	1683	1686	1689	rBV2	203	266	0.01%	0.002%
57	11.469	1701	1703	1706	rBV2	238	239	0.01%	0.002%
58	11.701	1738	1741	1743	rBV	351	375	0.01%	0.003%
59	11.878	1767	1770	1773	rBV2	170	234	0.01%	0.002%
60	11.969	1780	1785	1789	rBV	57303	73306	2.18%	0.524%
61	12.036	1789	1796	1806	rVB2	2109477	3366481	100.00%	24.059%
62	12.323	1837	1843	1854	rBV2	660486	1179563	35.04%	8.430%
63	12.487	1867	1870	1871	rBV2	302	278	0.01%	0.002%
64	12.603	1886	1889	1890	rBV2	291	242	0.01%	0.002%
65	12.713	1904	1907	1908	rBV2	312	326	0.01%	0.002%
66	12.756	1911	1914	1920	rBV2	385	627	0.02%	0.004%
67	12.841	1924	1928	1930	rVB2	176	233	0.01%	0.002%
68	12.920	1937	1941	1948	rVB2	10816	14317	0.43%	0.102%
69	13.054	1959	1963	1970	rVV2	11534	22292	0.66%	0.159%
70	13.109	1970	1972	1979	rVB4	2076	2662	0.08%	0.019%
71	13.195	1982	1986	1992	rVV2	9828	12947	0.38%	0.093%
72	13.347	2009	2011	2013	rVV2	194	198	0.01%	0.001%
73	13.384	2013	2017	2023	rVB4	1747	2337	0.07%	0.017%
74	13.432	2023	2025	2030	rBV2	418	472	0.01%	0.003%
75	13.469	2030	2031	2033	rBV	270	179	0.01%	0.001%
76	13.548	2043	2044	2045	rBV	257	183	0.01%	0.001%

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 Title : VOC Analysis

77	13.585	2045	2050	2063	rVV	1518245	1869149	55.52%	13.358%
78	13.719	2070	2072	2075	rVB2	656	658	0.02%	0.005%
79	13.749	2075	2077	2080	rBV2	343	440	0.01%	0.003%
80	13.823	2086	2089	2095	rVB2	188	361	0.01%	0.003%
81	13.957	2106	2111	2121	rBV	394852	493237	14.65%	3.525%
82	14.127	2135	2139	2143	rBV3	665	978	0.03%	0.007%
83	14.347	2173	2175	2180	rBV3	259	347	0.01%	0.002%
84	14.451	2191	2192	2194	rBV	222	238	0.01%	0.002%
85	14.542	2205	2207	2210	rVV	288	312	0.01%	0.002%
86	14.621	2217	2220	2223	rBV2	344	441	0.01%	0.003%
87	14.652	2223	2225	2228	rBV3	162	194	0.01%	0.001%
88	14.725	2234	2237	2238	rBV2	260	289	0.01%	0.002%
89	14.780	2241	2246	2252	rVB3	11029	15365	0.46%	0.110%
90	14.914	2267	2268	2271	rVB	430	262	0.01%	0.002%
91	14.999	2279	2282	2285	rVB2	306	379	0.01%	0.003%
92	15.243	2317	2322	2331	rBV	36238	53932	1.60%	0.385%
93	15.383	2344	2345	2348	rVB2	518	489	0.01%	0.003%
94	15.438	2352	2354	2358	rVB2	410	477	0.01%	0.003%
95	15.499	2362	2364	2366	rVB2	273	195	0.01%	0.001%
96	15.688	2394	2395	2397	rBV	297	216	0.01%	0.002%
97	15.743	2402	2404	2407	rVB2	276	259	0.01%	0.002%
98	15.773	2407	2409	2411	rBV	245	182	0.01%	0.001%
99	15.883	2424	2427	2429	rBV2	413	561	0.02%	0.004%
100	16.475	2522	2524	2526	rBV2	256	186	0.01%	0.001%

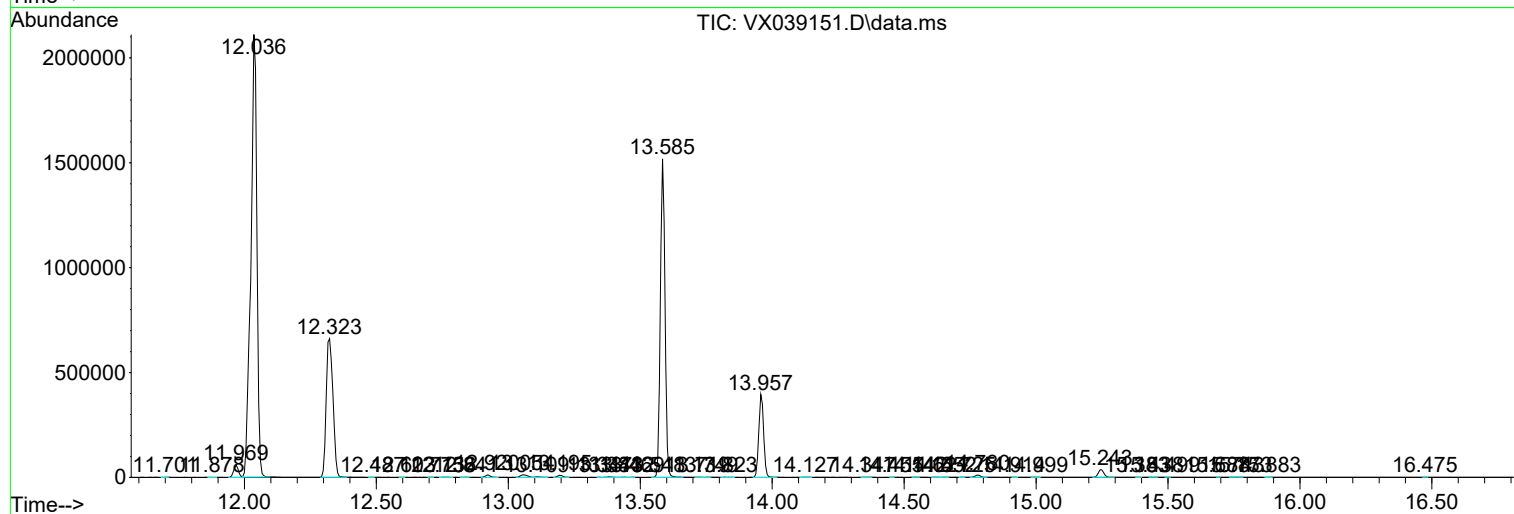
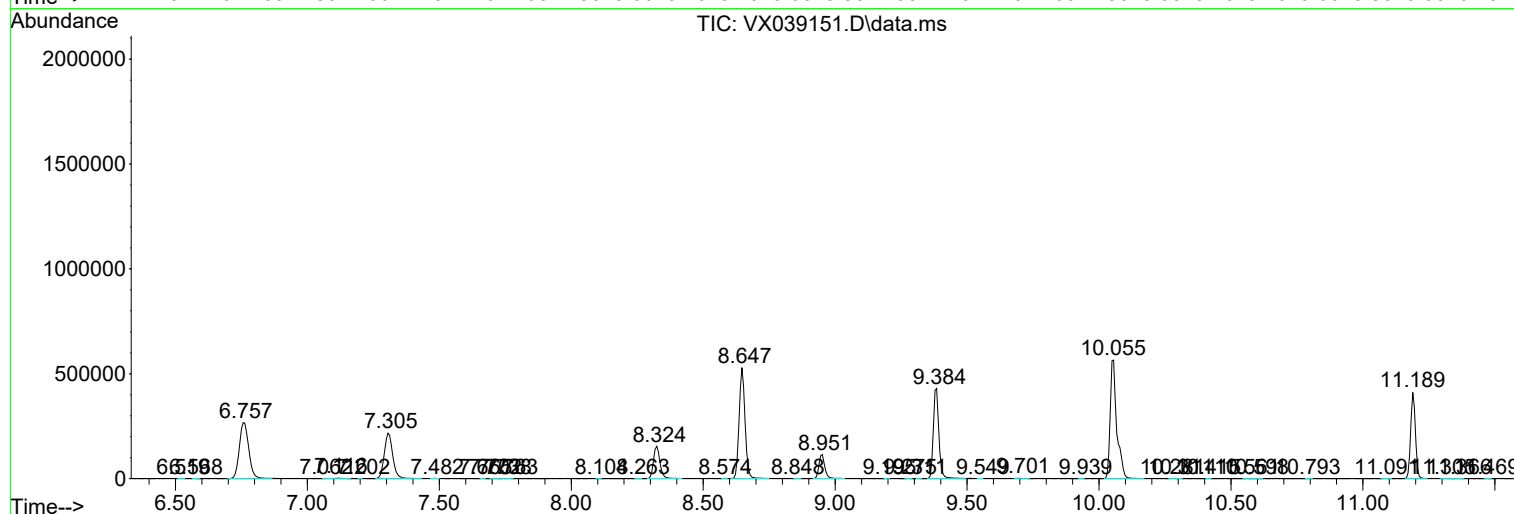
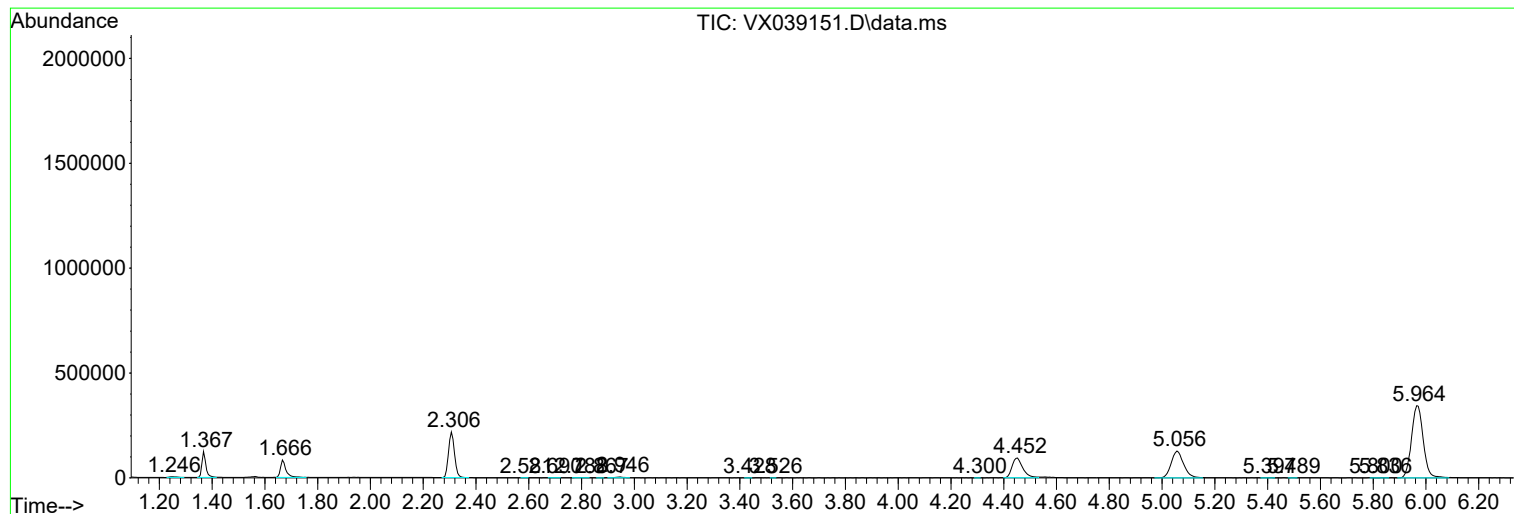
Sum of corrected areas: 13992346

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.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
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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