

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122123\
 Data File : VX039416.D
 Acq On : 21 Dec 2023 09:53
 Operator : JC/MD
 Sample : VX1221MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK656

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: VX039416.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	58	rVB	101004	110840	13.26%	1.704%
2	1.672	91	96	108	rBV	67940	100889	12.07%	1.551%
3	2.306	194	200	211	rBV	182909	282562	33.80%	4.345%
4	2.508	229	233	234	rBV2	875	1088	0.13%	0.017%
5	2.788	274	279	288	rVB4	3321	6656	0.80%	0.102%
6	2.934	298	303	311	rVB4	1649	3928	0.47%	0.060%
7	3.087	326	328	335	rVB4	474	1012	0.12%	0.016%
8	3.361	371	373	376	rVB2	244	231	0.03%	0.004%
9	3.447	385	387	390	rBV2	166	222	0.03%	0.003%
10	3.581	408	409	412	rVB2	314	225	0.03%	0.003%
11	3.605	412	413	416	rBV2	283	305	0.04%	0.005%
12	3.709	425	430	432	rBV2	239	399	0.05%	0.006%
13	3.959	467	471	473	rBV	188	255	0.03%	0.004%
14	4.032	479	483	484	rBV2	186	251	0.03%	0.004%
15	4.074	487	490	493	rVB2	307	275	0.03%	0.004%
16	4.117	493	497	499	rBV2	172	251	0.03%	0.004%
17	4.343	528	534	537	rBV2	247	441	0.05%	0.007%
18	4.440	542	550	567	rBV	74716	216616	25.91%	3.331%
19	4.867	618	620	622	rBV	403	392	0.05%	0.006%
20	5.050	638	650	667	rBV2	104529	338448	40.48%	5.205%
21	5.385	703	705	707	rVB2	417	288	0.03%	0.004%
22	5.544	728	731	733	rVV2	460	573	0.07%	0.009%
23	5.568	733	735	739	rVB3	392	365	0.04%	0.006%
24	5.678	751	753	756	rBV2	258	265	0.03%	0.004%
25	5.812	772	775	778	rBV2	179	254	0.03%	0.004%
26	5.964	787	800	817	rBV2	273266	835993	100.00%	12.856%
27	6.184	834	836	840	rBV3	241	277	0.03%	0.004%
28	6.269	848	850	854	rBV2	387	509	0.06%	0.008%
29	6.757	921	930	947	rBV	199248	477590	57.13%	7.344%
30	7.111	984	988	995	rVB4	1583	3190	0.38%	0.049%
31	7.306	1011	1020	1039	rBV	172239	387741	46.38%	5.963%
32	7.464	1044	1046	1047	rVV	375	321	0.04%	0.005%
33	7.482	1047	1049	1056	rVV	736	974	0.12%	0.015%
34	7.818	1102	1104	1106	rBV	243	232	0.03%	0.004%
35	7.915	1117	1120	1122	rBV2	173	216	0.03%	0.003%
36	7.946	1122	1125	1126	rBV2	234	236	0.03%	0.004%

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

37	8.220	1168	1170	1173	rVB2	252	268	0.03%	0.004%
38	8.251	1173	1175	1176	rBV	270	212	0.03%	0.003%
39	8.318	1180	1186	1201	rBV	115081	198788	23.78%	3.057%
40	8.500	1213	1216	1217	rBV2	361	330	0.04%	0.005%
41	8.574	1225	1228	1233	rVB3	755	1031	0.12%	0.016%
42	8.647	1233	1240	1251	rBV	400437	650296	77.79%	10.000%
43	8.946	1284	1289	1300	rBV	86185	129304	15.47%	1.988%
44	9.128	1316	1319	1321	rBV	184	211	0.03%	0.003%
45	9.226	1332	1335	1337	rBV	196	260	0.03%	0.004%
46	9.275	1340	1343	1347	rVB2	647	691	0.08%	0.011%
47	9.378	1355	1360	1379	rBV	348153	501989	60.05%	7.719%
48	9.781	1424	1426	1427	rBV	281	216	0.03%	0.003%
49	9.817	1430	1432	1435	rBV2	224	276	0.03%	0.004%
50	9.921	1447	1449	1452	rVB	278	224	0.03%	0.003%
51	9.958	1452	1455	1457	rBV2	205	224	0.03%	0.003%
52	10.049	1465	1470	1484	rBV	419817	586522	70.16%	9.019%
53	10.201	1491	1495	1499	rVB2	665	1148	0.14%	0.018%
54	10.244	1500	1502	1505	rVB3	331	296	0.04%	0.005%
55	10.281	1505	1508	1510	rBV	247	337	0.04%	0.005%
56	10.305	1510	1512	1513	rBV2	431	384	0.05%	0.006%
57	10.409	1527	1529	1530	rVB	385	201	0.02%	0.003%
58	10.720	1579	1580	1583	rBV2	245	216	0.03%	0.003%
59	10.963	1616	1620	1624	rVB4	997	1270	0.15%	0.020%
60	11.091	1639	1641	1644	rVB2	482	371	0.04%	0.006%
61	11.189	1652	1657	1668	rVB	332929	422534	50.54%	6.498%
62	11.311	1673	1677	1682	rVB2	944	1236	0.15%	0.019%
63	11.451	1697	1700	1705	rBV2	945	1357	0.16%	0.021%
64	11.500	1705	1708	1711	rVB	224	248	0.03%	0.004%
65	11.671	1734	1736	1738	rVV2	395	286	0.03%	0.004%
66	11.756	1746	1750	1756	rVB3	819	1236	0.15%	0.019%
67	11.969	1781	1785	1788	rBV2	1166	1408	0.17%	0.022%
68	12.018	1788	1793	1804	rBV	474164	606207	72.51%	9.322%
69	12.171	1816	1818	1822	rVB2	385	413	0.05%	0.006%
70	12.250	1829	1831	1833	rBV	241	203	0.02%	0.003%
71	12.317	1837	1842	1852	rBV	461848	587845	70.32%	9.040%
72	12.512	1872	1874	1877	rVV2	412	361	0.04%	0.006%
73	12.640	1892	1895	1896	rVV	247	227	0.03%	0.003%
74	12.677	1898	1901	1902	rVV2	212	199	0.02%	0.003%
75	12.707	1902	1906	1909	rVV2	203	333	0.04%	0.005%
76	12.762	1909	1915	1919	rVV2	4241	5899	0.71%	0.091%

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77	12.859	1928	1931	1932	rVB2	258	234	0.03%	0.004%
78	12.878	1932	1934	1937	rBV2	200	230	0.03%	0.004%
79	12.933	1942	1943	1946	rBV	257	253	0.03%	0.004%
80	13.116	1967	1973	1977	rBV3	1466	2009	0.24%	0.031%
81	13.201	1985	1987	1990	rVV	249	219	0.03%	0.003%
82	13.439	2023	2026	2030	rVB2	240	307	0.04%	0.005%
83	13.469	2030	2031	2034	rBV	252	213	0.03%	0.003%
84	13.512	2036	2038	2041	rVB2	261	222	0.03%	0.003%
85	13.554	2044	2045	2048	rBV2	188	204	0.02%	0.003%
86	13.591	2048	2051	2055	rVV3	1698	2115	0.25%	0.033%
87	13.701	2067	2069	2073	rBV2	313	326	0.04%	0.005%
88	13.774	2076	2081	2085	rBV	2769	3549	0.42%	0.055%
89	13.963	2108	2112	2116	rBV2	2013	2165	0.26%	0.033%
90	14.128	2135	2139	2145	rVB	5756	7817	0.94%	0.120%
91	14.268	2159	2162	2165	rVB2	205	281	0.03%	0.004%
92	14.408	2182	2185	2188	rBV	165	221	0.03%	0.003%
93	14.506	2199	2201	2203	rVB2	275	205	0.02%	0.003%
94	14.603	2215	2217	2220	rBV	295	400	0.05%	0.006%
95	14.823	2251	2253	2256	rBV	331	338	0.04%	0.005%
96	15.158	2306	2308	2310	rBV	225	267	0.03%	0.004%
97	15.322	2333	2335	2338	rVV2	415	325	0.04%	0.005%
98	15.359	2338	2341	2343	rVV2	416	468	0.06%	0.007%
99	15.383	2343	2345	2349	rVB3	642	858	0.10%	0.013%
100	16.408	2510	2513	2516	rVB2	330	362	0.04%	0.006%

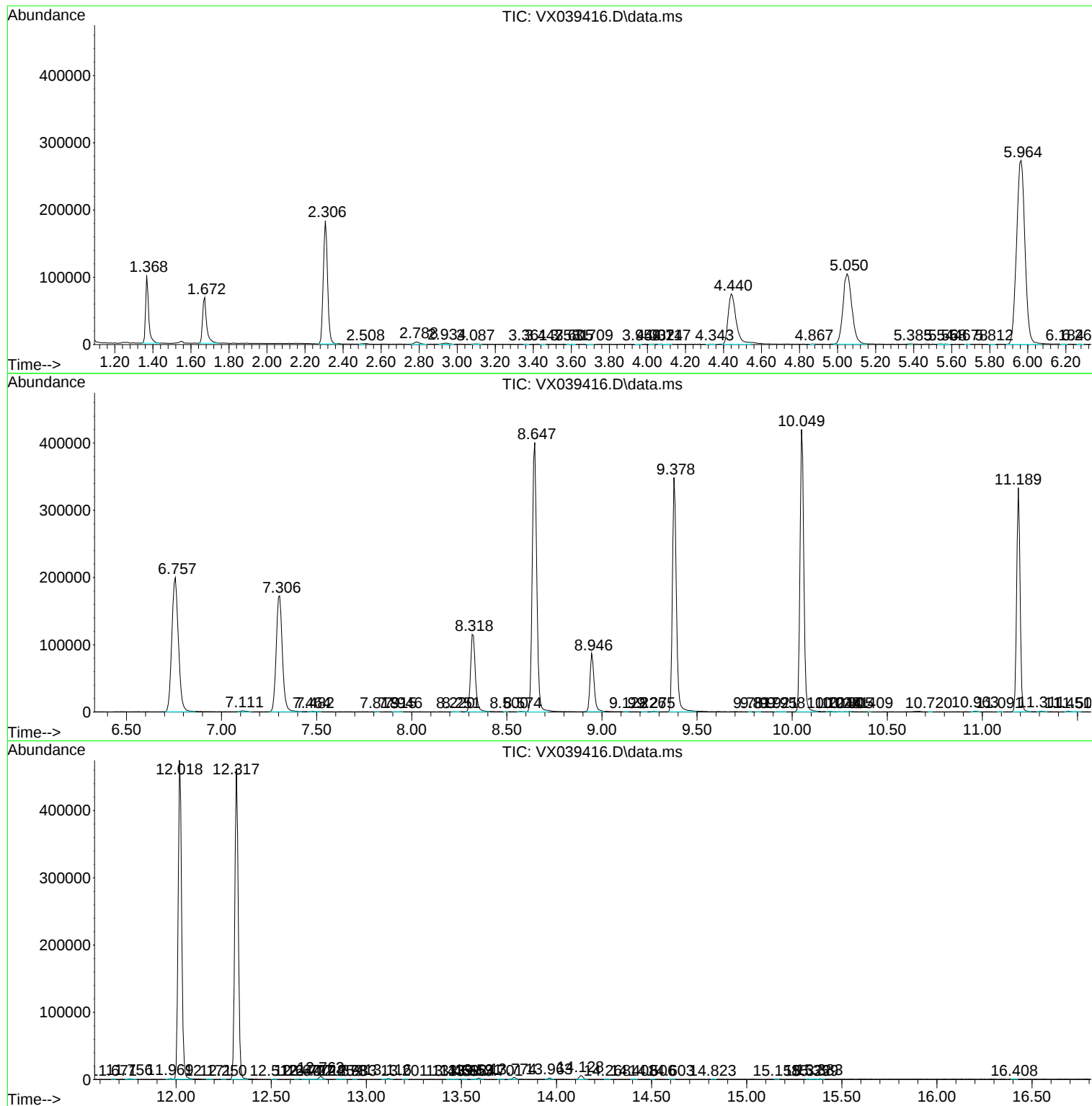
Sum of corrected areas: 6502955

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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 Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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