

Supplementary Materials: Antimicrobial Activity of Xanthohumol and Its Selected Structural Analogues

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4-Hydroxy-4-methoxychalcone (8) (1.9 g, yield = 65%) m.p. = 180–183 °C (MeOH). IR (KBr) cm^{-1} : 3182, 1643, 1601, 1579, 1514, 1439, 1343, 1263, 1228, 1166, 1023, 978, 831. $^1\text{H-NMR}$ (600 MHz, acetone- d_6) δ (ppm): 8.91 (1H, s, –OH), 8.13 (2H, d, J = 8.8 Hz, H-2', H-6', AA'BB'), 8.00 (1H, d, J = 15.5 Hz, H- α), 7.72 (1H, d, J = 15.5 Hz, H- β), 7.70 (2H, d, J = 8.6 Hz, H-2, H-6, AA'BB'), 7.06 (2H, d, J = 8.8 Hz, H-3', H-5', AA'BB'), 6.92 (2H, d, J = 8.6 Hz, H-3, H-5, AA'BB'), 3.90 (3H, s, –OCH₃). UV (MeOH) λ_{max} : 347.4; 234.1 nm.

4-Chloro-4'-methoxychalcone (9) (2.5 g, yield = 78%) m.p. = 130–131 °C (MeOH). IR (KBr) cm^{-1} : 2962, 1656, 1605, 1510, 1492, 1330, 1254, 1223, 1177, 1092, 1024, 981, 818. $^1\text{H-NMR}$ (600 MHz, CDCl₃) δ (ppm): 8.03 (2H, d, J = 8.8 Hz, H-2', H-6', AA'BB'), 7.74 (1H, d, J = 15.6 Hz, H- α), 7.57 (2H, d, J = 8.5 Hz, H-2, H-6, AA'BB'), 7.51 (1H, d, J = 15.6 Hz, H- β), 7.38 (2H, d, J = 8.5 Hz, H-3, H-5, AA'BB'), 6.98 (2H, d, J = 8.8 Hz, H-3', H-5'), 3.89 (3H, s, –OCH₃). $^{13}\text{C-NMR}$ (150 MHz, CDCl₃) δ : 188.4 (C=O), 163.5, 142.4, 136.2, 133.6, 130.9, 130.8, 129.5, 129.2, 122.3, 113.9, 55.5 (–OCH₃). UV (MeOH) λ_{max} : 318.6; 229.3 nm.

4-Bromo-4'-methoxychalcone (10) (2.8 g, yield = 75%) m.p. = 150–151 °C (MeOH). IR (KBr) cm^{-1} : 3014, 1657, 1603, 1577, 1560, 1510, 1486, 1331, 1314, 1257, 1223, 1176, 1036, 1021, 979, 815. $^1\text{H-NMR}$ (600 MHz, CDCl₃) δ (ppm): 8.03 (2H, d, J = 7.7 Hz H-2', H-6'), 7.72 (1H, d, J = 15.6 Hz, H- α), 7.55–7.49 (5H, m, H-3, H-5, H-2, H-6, H- β), 6.98 (2H, d, J = 7.7 Hz, H-3', H-5'), 3.89 (3H, s, –OCH₃). $^{13}\text{C-NMR}$ (150 MHz, CDCl₃) δ : 188.4 (C=O), 163.5, 142.5, 134.0, 132.1, 130.9, 130.8, 129.7, 124.5, 122.4, 113.9, 55.5 (–OCH₃). UV (MeOH) λ_{max} : 320.5; 229.3 nm.

4'-Methoxy-4-nitrochalcone (11) (2.4 g, yield = 73%) m.p. = 170–172 °C (MeOH). IR (KBr) cm^{-1} : 2895, 1659, 1613, 1599, 1516, 1344, 1268, 1227, 1177, 1021, 826. $^1\text{H-NMR}$ (600 MHz, CDCl₃) δ (ppm): 8.27 (2H, d, J = 8.8 Hz H-2', H-6', AA'BB'), 8.05 (2H, d, J = 8.8 Hz, H-2, H-6, AA'BB'), 7.80 (1H, d, J = 15.7 Hz, H- α), 7.78 (2H, d, J = 8.8 Hz, H-3', H-5', AA'BB'), 7.65 (1H, d, J = 15.7 Hz, H- β), 7.00 (2H, d, J = 8.8 Hz, H-3, H-5, AA'BB'), 3.91 (3H, s, –OCH₃). $^{13}\text{C-NMR}$ (150 MHz, CDCl₃) δ : 187.7 (C=O), 163.9 (C-4'), 148.4 (C-1'), 141.3 (C-4), 140.7 (C- α), 131.0 (C-2, C-6), 130.5 (C-1), 128.8 (C-3', C-5'), 125.6 (C- β), 124.2 (C-2', C-6'), 114.0 (C-3, C-5), 55.6 (–OCH₃). UV (MeOH) λ_{max} : 323.4 nm.

4-Ethyl-4'-methoxychalcone (12) (2.7 g, yield = 85%) IR (KBr) cm^{-1} : 2967, 2933, 1655, 1603, 1569, 1510, 1421, 1333, 1315, 1260, 1223, 1175, 1113, 1032, 1015, 987, 826. $^1\text{H-NMR}$ (300 MHz, CDCl₃) δ (ppm): 8.07 (2H, d, J = 9.0 Hz, H-2', H-6', AA'BB'), 7.82 (1H, d, J = 15.6 Hz, H- α), 7.60 (2H, d, J = 8.1 Hz, H-2, H-6), 7.55 (1H, d, J = 15.6 Hz, H- β), 7.27 (2H, d, H-3, H-5), 7.01 (2H, d, J = 9.0 Hz, H-3', H-5', AA'BB'), 3.92 (3H, s, –OCH₃), 2.71 (2H, q, –CH₂), 1.28 (3H, t, J = 7.6 Hz, –CH₃). $^{13}\text{C-NMR}$ (75 MHz, CDCl₃) δ (ppm): 188.8 (C=O), 163.3, 147.1, 144.0, 132.5, 131.2, 130.7, 128.5, 120.9, 113.8, 55.5 (–OCH₃), 28.8 (–CH₂) 15.3 (–CH₃). UV (MeOH) λ_{max} : 325.3; 226.4 nm.

4-Ethoxy-4'-methoxychalcone (13) (2.8 g, yield = 84%) m.p. = 105–106 °C (EtOH). IR (KBr) cm^{-1} : 3055, 2936, 1655, 1602, 1572, 1509, 1492, 1445, 1422, 1336, 1309, 1286, 1259, 1225, 1187, 1035, 1016, 1187, 973, 992, 830, 763. $^1\text{H-NMR}$ (300 MHz, CDCl₃) δ (ppm): 8.03 (2H, d, J = 8.9 Hz, H-2', H-6', AA'BB'), 7.78 (1H, d, J = 15.6 Hz, H- α), 7.59 (2H, d, J = 8.8 Hz, H-2, H-6, AA'BB'), 7.43 (1H, d, J = 15.6 Hz, H- β), 6.98 (2H, d, J = 8.9 Hz, H-3', H-5', AA'BB'), 6.92 (2H, d, J = 8.8 Hz, H-3, H-5, AA'BB'), 4.07 (2H, q, –CH₂), 3.88 (3H, s, –OCH₃), 1.44 (3H, t, J = 7.0 Hz, –CH₃). $^{13}\text{C-NMR}$ (75 MHz, CDCl₃) δ (ppm): 188.7 (C=O), 163.2, 160.9, 143.9, 131.4, 130.7, 130.1, 127.6, 119.4, 114.8, 113.7, 63.6 (–CH₂–), 55.4 (–OCH₃), 14.7 (–CH₃). UV (MeOH) λ_{max} : 344.5; 234.1 nm.

4'-Methoxy-4-methylchalcone (14) (2.4 g, yield = 80%) m.p. = 125–127 °C (MeOH). IR (KBr) cm^{-1} : 3010, 2954, 1654, 1599, 1571, 1509, 1418, 1332, 1308, 1255, 1226, 1175, 1034, 1018, 985, 839, 811. $^1\text{H-NMR}$ (300 MHz, CDCl₃) δ (ppm): 8.04 (2H, d, J = 8.9 Hz, H-2', H-6', AA'BB'), 7.79 (1H, d, J = 15.6 Hz, H- α),

7.55 (2H, d, $J = 8.0$ Hz, H-2, H-6, AA'BB'), 7.51 (1H, d, $J = 15.6$ Hz, H- β), 7.22 (2H, d, $J = 8.0$ Hz, H-3, H-5, AA'BB'), 6.98 (2H, d, $J = 8.9$ Hz, H-3', H-5', AA'BB'), 3.89 (3H, s, -OCH₃), 2.39 (3H, s, -CH₃). ¹³C-NMR (75 MHz, CDCl₃) δ (ppm): 188.8 (C=O), 163.3, 144.0, 140.8, 132.3, 131.2, 130.7, 129.6, 128.4, 120.8, 113.8, 55.5 (-OCH₃) 21.5 (-CH₃). UV (MeOH) $\lambda_{\max}$: 326.2; 231.2 nm.

4'-Methoxychalcone (**15**) (2.4 g, yield = 85%) m.p. = 107–109 °C (MeOH). IR (KBr) cm⁻¹: 3056, 1655, 1603, 1573, 1446, 1337, 1260, 1036, 974, 830, 763. ¹H-NMR (600 MHz, CDCl₃) δ (ppm): 8.04 (2H, d, $J = 7.8$ Hz, H-2', H-6'), 7.80 (1H, d, $J = 15.6$ Hz, H- α), 7.64 (2H, d, $J = 7.04$ Hz, H-2, H-6), 7.55 (1H, d, $J = 15.6$ Hz, H- β), 7.41–7.39 (3H, m, H-3, H-4, H-5), 6.99 (2H, d, $J = 7.8$ Hz, H-3', H-5'), 3.89 (3H, s, -OCH₃). ¹³C-NMR (150 MHz, CDCl₃) δ (ppm): 188.7 (C=O), 163.4, 144.0, 135.1, 131.1, 130.8, 130.3, 128.9, 128.3, 121.9, 113.8, 55.5 (-OCH₃). UV (MeOH) $\lambda_{\max}$: 316.6; 227.4 nm.