

Supplementary Data

Microwave assisted synthesis, antibacterial activity against *Bordetella bronchiseptica* of a library of 3'-hydroxy-aryl and heteroaryl chalcones and molecular descriptors-based SAR

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Structural data of Set 1

1-(3'-Hydroxyphenyl)-3-(phenyl)-2-propen-1-one (1) R_f 0.71^a. Yield 74%. m.p. 127-130 °C. IR (KBr) cm⁻¹: 3248, 1644, 1593. ¹H- NMR (CDCl₃, 300 MHz,) δ: 10.0 (1H, s), 7.83 (1H, d, J=15.9 Hz), 7.60 (1H, d, J=15.9 Hz), 6.46-7.42 (9H, m). MS (m/z): 224.0 (M⁺).

1-(3'-Hydroxyphenyl)-3-(2-hydroxyphenyl)-2-propen-1-one (2) R_f 0.23^b. Yield 55%. m.p. 152 °C. IR (KBr) cm⁻¹: 3364, 1652, 1606. ¹H-NMR (CDCl₃, 300 MHz) δ: 9.90 (1H, bs), 7.83 (1H, d, J= 15.9 Hz), 7.50 (1H, d, J=15.9 Hz), 6.63-7.48 (8H,m). MS (m/z): 240.0 (M⁺).

1-(3'-Hydroxyphenyl)-3-(3-hydroxyphenyl)-2-propen-1-one (3) R_f 0.18^b. Yield 54%. m.p. 182 °C. IR (KBr) cm⁻¹: 3409, 1644, 1585. ¹H- NMR (CDCl₃, 300 MHz) δ: 9.85 (1H, s), 9.68 (1H, s), 7.71 (1H, d, J= 15.6 Hz), 7.59 (1H, d, J= 15.6 Hz), 6.86-7.59 (8H, m). MS (m/z): 240.0 (M⁺).

1-(3'-Hydroxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one (4) R_f 0.16^b. Yield 51%. m.p. 194-195 °C. IR (KBr) cm⁻¹: 3339, 1653, 1561. ¹H- NMR (CDCl₃, 300 MHz) δ: 10.06 (1H, s), 9.73 (1H, s), 7.88 (1H, d, J=8.7 Hz), 7.56 (1H, d, J= 9.0 Hz), 7.16-7.50 (8H, m). MS (m/z): 240.0 (M⁺).

1-(3'-Hydroxyphenyl)-3-(2-methoxyphenyl)-2-propen-1-one (5) R_f 0.68^a. Yield 57%. m.p. 128 °C. IR (KBr) cm⁻¹: 3347, 1651, 1555. ¹H-NMR (300 MHz, CDCl₃) δ: 9.00 (1H, bs), 8.16 (1H, d, J=15.6 Hz), 7.42 (1H, d, J=15.3 Hz), 6.66-7.56 (8H, m), 3.84 (3H, s). MS (m/z): 254.0 (M⁺).

1-(3'-Hydroxyphenyl)-3-(3-methoxyphenyl)-2-propen-1-one (6) R_f 0.62^a. Yield 55%. m.p. 143 °C. IR (KBr) cm⁻¹: 3361, 1660, 1576. ¹H- NMR (CDCl₃, 300 MHz) δ: 9.87 (1H, bs), 7.83 (1H, d, J=15.6 Hz), 7.67 (1H, d, J=15.8 Hz), 6.76-7.58 (8H, m), 4.59 (3H, s). MS (m/z): 254.0 (M⁺).

1-(3'-Hydroxyphenyl)-3-(4-methoxyphenyl)-2-propen-1-one (7) R_f 0.65^a. Yield 61%. IR (KBr) cm^{-1} : 3350, 1651, 1546. $^1\text{H-NMR}$ (DMSO-d_6 , 300 MHz) δ : 8.96 (1H, bs), 7.85 (1H, d, $J=15.6$ Hz), 7.58 (1H, d, $J=15.6$ Hz), 3.41 (3H, s). MS (m/z): 254.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(3,4-dimethoxyphenyl)-2-propen-1-one (8) R_f 0.46^a. Yield 63%. m.p. 135 °C. IR (KBr) cm^{-1} : 3447, 1648, 1567. $^1\text{H-NMR}$ (CDCl_3 , 300 MHz) δ : 8.42 (1H, bs), 8.00 (1H, d, $J=15.6$ Hz), 7.55 (1H, d, $J=15.6$ Hz), 6.63-7.59 (7H, m), 3.47 (6H, s). MS (m/z): 284.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(4-hydroxy, 3-methoxyphenyl)-2-propen-1-one (9) R_f 0.57^c. Yield 59%. m.p. 210 °C. IR (KBr) cm^{-1} : 3462, 1627, 1535. $^1\text{H-NMR}$ (CDCl_3 , 300 MHz) δ : 8.32 (2H, bs), 8.01 (1H, d, $J=14.9$ Hz), 7.25 (1H, d, $J=14.9$ Hz), 6.46-7.56 (7H, m), 3.73 (3H, s). MS (m/z): 270.0 (M^+).

1-(3'-Hydroxyphenyl)-2-(2-fluorophenyl)-2-propene-1-one (10) R_f 0.62^c. Yield 83%. m.p. 96 °C. IR (KBr) cm^{-1} : 3362, 1629, 1532. $^1\text{H-NMR}$ (DMSO-d_6 , 300 MHz) δ : 9.9 (1H, s), 8.13 (1H, d, $J=15.3$ Hz), 7.81-7.89 (8H, m), 7.68 (1H, d, $J=15.3$ Hz). MS (m/z): 242.0 (M^+).

1-(3'-Hydroxyphenyl)-2-(3-fluorophenyl)-2-propene-1-one (11) R_f 0.64^c. Yield 87%. m.p. 81-2 °C. IR (KBr) cm^{-1} : 3435, 1657, 1553. $^1\text{H-NMR}$ (DMSO-d_6 , 300 MHz) δ : 10.0 (1H, s), 8.21 (1H, d, $J=15.5$ Hz), 7.84-8.13 (8H, m), 7.71 (1H, d, $J=15.5$ Hz). MS (m/z): 242.0 (M^+).

1-(3'-Hydroxyphenyl)-2-(4-fluorophenyl)-2-propen-1-one (12) R_f 0.63^c. Yield 91%. m.p. 136 °C. IR (KBr) cm^{-1} : 3297, 1647, 1568. $^1\text{H-NMR}$ (DMSO-d_6 , 300 MHz) δ : 9.90 (1H, s), 8.34 (1H, d, $J=15.9$ Hz), 7.85 (1H, d, $J=15.9$ Hz), 7.77-8.21 (8H, m). MS (m/z): 242.1 (M^+).

1-(3'-Hydroxyphenyl)-3-(2-chlorophenyl)-2-propen-1-one (13) R_f 0.64^a. Yield 84%. m.p. 150 °C. IR (KBr) cm^{-1} : 3327, 1652, 1585. $^1\text{H-NMR}$ (CDCl_3 , 300 MHz) δ : 10.10 (1H, bs), 7.83 (1H, d, $J=15.9$ Hz), 7.64 (1H, d, $J=15.9$ Hz), 7.61-7.53 (3H, m). MS (m/z): 258.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(3-chlorophenyl)-2-propen-1-one (14) R_f 0.66^a. Yield 80%. m.p. 127-128 °C. IR (KBr) cm^{-1} : 3404, 1661, 1582. $^1\text{H-NMR}$ (CDCl_3 , 300 MHz) δ : 8.76 (1H, bs), 8.10 (1H, d, $J=15.6$ Hz), 7.62 (1H, d, $J=15.9$ Hz), 7.04-7.93 (8H, m). MS (m/z): 258.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(4-chlorophenyl)-2-propen-1-one (15) R_f 0.57^a. Yield 88%. IR (KBr) cm^{-1} : 3317, 1646, 1546. $^1\text{H-NMR}$ (CDCl_3 , 300 MHz) δ : 10.03 (1H, bs), 8.10 (1H, d, $J=15.6$ Hz), 7.63 (1H, d, $J=15.4$ Hz), 7.06-8.05 (8H, m). MS (m/z): 258.0 (M^+).

1-(3'-Hydroxyphenyl)-2-(3-bromophenyl)-2-propen-1-one (16) R_f 0.67^a. Yield 76%. m.p. 182 °C. IR (KBr) cm^{-1} : 3409, 1661, 1584; $^1\text{H-NMR}$ (CDCl_3 , 300 MHz) δ : 8.79 (1H, bs), 8.13 (1H, d, $J=15.6$ Hz), 7.51 (1H, d, $J=15.6$ Hz), 7.01-7.63 (8H, m). MS (m/z): 303.0 (M^+), 305.0 ($\text{M}^+ + 2$).

1-(3'-Hydroxyphenyl)-2-(4-bromophenyl)-2-propen-1-one (17) R_f 0.68^a. Yield 88%. m.p. 109-11 °C. IR (KBr) cm^{-1} : 3398, 1660, 1527. $^1\text{H-NMR}$ (DMSO-d_6 , 300 MHz) δ : 8.01 (1H, bs), 7.74 (1H, d, $J=15.6$ Hz), 7.51 (1H, d, $J=15.6$ Hz), 7.13-7.65 (8H, m). MS (m/z): 303.0 (M^+), 305.0 ($\text{M}^+ + 2$).

1-(3'-Hydroxyphenyl)-3-(2-nitrophenyl)-2-propen-1-one (18) R_f 0.72^a. Yield 84%. m.p. 187-189 °C. IR (KBr) cm^{-1} : 3259, 1632, 1524. $^1\text{H-NMR}$ (DMSO-d_6 , 300 MHz) δ : 10.23 (1H, bs), 8.26 (1H, d, $J=15.6$ Hz), 7.83 (1H, d, $J=15.6$ Hz), 7.47-8.19 (8H, m). MS (m/z): 269.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(3-nitrophenyl)-2-propen-1-one (19) R_f 0.64^a. Yield 87%. m.p. 207-209 °C. IR (KBr) cm^{-1} : 3411, 1664, 1553. $^1\text{H-NMR}$ (DMSO- d_6 , 300 MHz) δ : 10.10 (1H, bs), 8.19 (1H, d, $J=15.6$ Hz), 7.82 (1H, d, $J=15.6$ Hz), 7.47-8.27 (8H, m). MS (m/z): 268.9 (M^+).

1-(3'-Hydroxyphenyl)-3-(4-nitrophenyl)-2-propen-1-one (20) R_f 0.70^a. Yield 93%. m.p. 160 °C. IR (KBr) cm^{-1} : 3400, 1658, 1574. $^1\text{H-NMR}$ (DMSO- d_6 , 300 MHz) δ : 10.01 (1H, bs), 8.14 (1H, d, $J=15.6$ Hz), 7.82 (1H, d, $J=15.6$ Hz), 7.28-8.06 (8H, m). MS (m/z): 269.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(4-N,N-dimethylphenyl)-2-propen-1-one (21) R_f 0.62^c. Yield 67%. m.p. 169-171 °C. IR (KBr) cm^{-1} : 3447, 1567. $^1\text{H-NMR}$ (DMSO- d_6 , 300 MHz) δ : 8.76 (1H, bs), 8.00 (1H, d, $J=15.5$ Hz), 7.55 (1H, d, $J=15.3$ Hz), 6.38-7.41 (8H, m), 3.0 (6H, s). MS (m/z): 267.1 (M^+).

1-(3'-Hydroxyphenyl)-3-(4-methylphenyl)-2-propen-1-one (22) R_f 0.75^a. Yield 55%. m.p. 119-120 °C. IR (KBr) cm^{-1} : 3412, 1653, 1566. $^1\text{H-NMR}$ (DMSO- d_6 , 300 MHz) δ : 8.89 (1H, bs), 7.86 (1H, d, $J=16.5$ Hz), 7.61 (1H, d, $J=15.6$ Hz), 7.01-7.57 (8H, m), 2.33 (3H, s). MS (m/z): 239.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(2-methyl-3,5-dimethoxyphenyl)-2-propen-1-one (23) R_f 0.60^c. Yield 63%. m.p. 142-143 °C. IR (KBr) cm^{-1} : 3438, 1647, 1566. $^1\text{H-NMR}$ (DMSO- d_6 , 300 MHz) δ : 8.87 (1H, bs), 8.00 (1H, d, $J=16.0$ Hz), 7.43 (1H, d, $J=15.9$ Hz), 3.87 (6H, s), 2.44 (3H, s). MS (m/z): 298.0 (M^+).

Structural data of Set 2

1-(3'-Hydroxyphenyl)-3-(pyridin-2-yl)-2-propen-1-one (24) R_f 0.71^a. Yield 60%. m.p. 146 °C. IR (KBr) cm^{-1} : 3400, 1628, 1571. $^1\text{H-NMR}$ (CDCl_3 , 300 MHz) δ : 8.96 (1H, bs), 8.20 (1H, d, $J=15.31$ Hz), 8.05 (1H, d, $J=15.0$ Hz), 7.36-8.49 (4H, m), 6.62-7.24 (4H, m). MS (m/z): 225.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(pyridin-3-yl)-2-propen-1-one (25) R_f 0.65^a. Yield 59%. m.p. 187-190 °C. IR (KBr) cm^{-1} : 3412, 1643, 1555. $^1\text{H-NMR}$ (CDCl_3 , 300 MHz) δ : 9.10 (1H, bs), 8.29-8.50 (4H, m), 7.90 (1H, d, $J=15.7$ Hz), 7.49 (1H, d, $J=15.5$ Hz), 6.65-7.46 (4H, m). MS (m/z): 225.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(pyridin-4-yl)-2-propen-1-one (26) R_f 0.69^a. Yield 54%. m.p. 175-177 °C. IR (KBr) cm^{-1} : 3404, 1659, 1541. $^1\text{H-NMR}$ (DMSO- d_6 , 300 MHz) δ : 8.79 (1H, bs), 8.13 (1H, d, $J=16.0$ Hz), 8.06 (1H, d, $J=15.6$ Hz), 7.53-8.62 (4H, m), 7.03-7.51 (4H, m). MS (m/z): 225.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(pyrrol-2-yl)-2-propen-1-one (27) R_f 0.64^c. Yield 62%. m.p. 197 °C. IR (KBr) cm^{-1} : 3412, 1661, 1571. $^1\text{H-NMR}$ (Acetone- d_6) δ : 10.84 (1H, bs), 7.59 (1H, d, $J=15.3$ Hz), 7.37 (1H, d, $J=15.3$ Hz), 7.40-7.58 (3H, m), 6.13-6.58 (4H, m), 6.11 (1H, s). MS (m/z): 213.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(furan-2-yl)-2-propen-1-one (28) R_f 0.45^c. Yield 51%. m.p. 152 °C. IR (KBr) cm^{-1} : 3423, 1656, 1544. $^1\text{H-NMR}$ (DMSO- d_6 , 300 MHz) δ : 9.84 (1H, bs), 7.91 (1H, d, $J=15.6$ Hz), 7.44 (1H, d, $J=15.6$ Hz), 7.13-7.78 (4H, m), 6.65-7.80 (3H, m). MS (m/z): 214.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(indol-3-yl)-2-propen-1-one (29) R_f 0.51^c. Yield 50%. m.p. 196-199 °C. IR (KBr) cm^{-1} : 3400, 1627, 1537. $^1\text{H-NMR}$ (CDCl_3 , 300 MHz,) δ : 9.82 (1H, bs), 8.29 (1H, bs), 7.66-8.12 (4H, m), 7.53 (1H, d, $J=9.0$ Hz), 7.21 (1H, d, $J=7.2$ Hz), 7.24 (1H, s), 7.24-7.47 (1H, m). MS (m/z): 263.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(thien-2-yl)-2-propen-1-one (30) R_f 0.67^c. Yield 76%. m.p. 123 °C. IR (KBr) cm^{-1} : 3466, 1642, 1535. $^1\text{H-NMR}$ (DMSO-d_6 , 300 MHz) δ : 9.90 (1H, bs), 7.91 (1H, d, $J=15.0$ Hz), 7.55 (d, $J=15.0$ Hz), 7.31-7.86 (3H, m), 7.03-7.49 (4H, m). MS (m/z): 230.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(5-methylthien-2-yl)-2-propen-1-one (31) R_f 0.66^a. Yield 69%. m.p. 114-115 °C. IR (KBr) cm^{-1} : 3402, 1624, 1537. $^1\text{H-NMR}$ (DMSO-d_6 , 300 MHz) δ : 9.83 (1H, bs), 7.79 (1H, d, $J=15.3$ Hz), 7.53 (1H, d, $J=15.3$ Hz), 7.00 (1H, d, $J=3.3$ Hz), 6.88 (1H, d, $J=3.6$ Hz), 6.91-7.21 (4H, m), 2.50 (3H, s). MS (m/z): 244.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(5-bromothien-2-yl)-2-propen-1-one (32) R_f 0.58^a. Yield 66%. m.p. 133-136 °C. IR (KBr) cm^{-1} : 3458, 1665, 1557. $^1\text{H-NMR}$ (DMSO-d_6 , 300 MHz) δ : 9.87 (1H, bs), 7.80 (1H, d, $J=15.3$ Hz), 7.29 (1H, d, $J=15.3$ Hz), 7.05 (1H, d, $J=3.0$ Hz), 7.03 (1H, d, $J=3.7$ Hz), 6.91-7.21 (4H, m). MS (m/z): 309.0 (M^+).

1-(3'-Hydroxyphenyl)-3-(5-nitrothien-2-yl)-2-propen-1-one (33) Yield 49%. m.p. 169-171 °C. IR (KBr) cm^{-1} : 3412, 1637, 1535. $^1\text{H-NMR}$ (DMSO-d_6 , 300 MHz) δ : 10.00 (1H, bs), 7.66 (1H, d, $J=15.5$ Hz), 7.55 (1H, d, $J=15.3$ Hz), 3.0 (6H, s). MS (m/z): 275.1 (M^+).