

## 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<sub>f</sub> 0.71<sup>a</sup>. Yield 74%. m.p. 127-130 °C. IR (KBr) cm<sup>-1</sup>: 3248, 1644, 1593. <sup>1</sup>H-NMR (CDCl<sub>3</sub>, 300 MHz,  $\delta$ ): 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<sup>+</sup>).

**1-(3'-Hydroxyphenyl)-3-(2-hydroxyphenyl)-2-propen-1-one (2)** R<sub>f</sub> 0.23<sup>b</sup>. Yield 55%. m.p. 152 °C. IR (KBr) cm<sup>-1</sup>: 3364, 1652, 1606. <sup>1</sup>H-NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ : 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<sup>+</sup>).

**1-(3'-Hydroxyphenyl)-3-(3-hydroxyphenyl)-2-propen-1-one (3)** R<sub>f</sub> 0.18<sup>b</sup>. Yield 54%. m.p. 182 °C. IR (KBr) cm<sup>-1</sup>: 3409, 1644, 1585. <sup>1</sup>H-NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ : 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<sup>+</sup>).

**1-(3'-Hydroxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one (4)** R<sub>f</sub> 0.16<sup>b</sup>. Yield 51%. m.p. 194-195 °C. IR (KBr) cm<sup>-1</sup>: 3339, 1653, 1561. <sup>1</sup>H-NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ : 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<sup>+</sup>).

**1-(3'-Hydroxyphenyl)-3-(2-methoxyphenyl)-2-propen-1-one (5)** R<sub>f</sub> 0.68<sup>a</sup>. Yield 57%. m.p. 128 °C. IR (KBr) cm<sup>-1</sup>: 3347, 1651, 1555. <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$ : 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<sup>+</sup>).

**1-(3'-Hydroxyphenyl)-3-(3-methoxyphenyl)-2-propen-1-one (6)** R<sub>f</sub> 0.62<sup>a</sup>. Yield 55%. m.p. 143 °C. IR (KBr) cm<sup>-1</sup>: 3361, 1660, 1576. <sup>1</sup>H-NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ : 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<sup>+</sup>).

**1-(3'-Hydroxyphenyl)-3-(4-methoxyphenyl)-2-propen-1-one (7)**  $R_f$  0.65<sup>a</sup>. Yield 61%. IR (KBr)  $\text{cm}^{-1}$ : 3350, 1651, 1546.  $^1\text{H-NMR}$  ( $\text{DMSO-d}_6$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-3-(3,4-dimethoxyphenyl)-2-propen-1-one (8)**  $R_f$  0.46<sup>a</sup>. Yield 63%. m.p. 135 °C. IR (KBr)  $\text{cm}^{-1}$ : 3447, 1648, 1567.  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-3-(4-hydroxy, 3-methoxyphenyl)-2-propen-1-one (9)**  $R_f$  0.57<sup>c</sup>. Yield 59%. m.p. 210 °C. IR (KBr)  $\text{cm}^{-1}$ : 3462, 1627, 1535.  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-2-(2-fluorophenyl)-2-propene-1-one (10)**  $R_f$  0.62<sup>c</sup>. Yield 83%. m.p. 96 °C. IR (KBr)  $\text{cm}^{-1}$ : 3362, 1629, 1532.  $^1\text{H-NMR}$  ( $\text{DMSO-d}_6$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-2-(3-fluorophenyl)-2-propene-1-one (11)**  $R_f$  0.64<sup>c</sup>. Yield 87%. m.p. 81-2 °C. IR (KBr)  $\text{cm}^{-1}$ : 3435, 1657, 1553.  $^1\text{H-NMR}$  ( $\text{DMSO-d}_6$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-2-(4-fluorophenyl)-2-propen-1-one (12)**  $R_f$  0.63<sup>c</sup>. Yield 91%. m.p. 136 °C. IR (KBr)  $\text{cm}^{-1}$ : 3297, 1647, 1568.  $^1\text{H-NMR}$  ( $\text{DMSO-d}_6$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-3-(2-chlorophenyl)-2-propen-1-one (13)**  $R_f$  0.64<sup>a</sup>. Yield 84%. m.p. 150 °C. IR (KBr)  $\text{cm}^{-1}$ : 3327, 1652, 1585.  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-3-(3-chlorophenyl)-2-propen-1-one (14)**  $R_f$  0.66<sup>a</sup>. Yield 80%. m.p. 127-128 °C. IR (KBr)  $\text{cm}^{-1}$ : 3404, 1661, 1582.  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-3-(4-chlorophenyl)-2-propen-1-one (15)**  $R_f$  0.57<sup>a</sup>. Yield 88%. IR (KBr)  $\text{cm}^{-1}$ : 3317, 1646, 1546.  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-2-(3-bromophenyl)-2-propen-1-one (16)**  $R_f$  0.67<sup>a</sup>. Yield 76%. m.p. 182 °C. IR (KBr)  $\text{cm}^{-1}$ : 3409, 1661, 1584;  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ), 305.0 ( $\text{M}^+ + 2$ ).

**1-(3'-Hydroxyphenyl)-2-(4-bromophenyl)-2-propen-1-one (17)**  $R_f$  0.68<sup>a</sup>. Yield 88%. m.p. 109-11 °C. IR (KBr)  $\text{cm}^{-1}$ : 3398, 1660, 1527.  $^1\text{H-NMR}$  ( $\text{DMSO-d}_6$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ), 305.0 ( $\text{M}^+ + 2$ ).

**1-(3'-Hydroxyphenyl)-3-(2-nitrophenyl)-2-propen-1-one (18)**  $R_f$  0.72<sup>a</sup>. Yield 84%. m.p. 187-189 °C. IR (KBr)  $\text{cm}^{-1}$ : 3259, 1632, 1524.  $^1\text{H-NMR}$  ( $\text{DMSO-d}_6$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-3-(3-nitrophenyl)-2-propen-1-one (19)**  $R_f$  0.64<sup>a</sup>. Yield 87%. m.p. 207-209 °C. IR (KBr)  $\text{cm}^{-1}$ : 3411, 1664, 1553.  $^1\text{H-NMR}$  (DMSO- $d_6$ , 300 MHz)  $\delta$ : 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<sup>a</sup>. Yield 93%. m.p. 160 °C. IR (KBr)  $\text{cm}^{-1}$ : 3400, 1658, 1574.  $^1\text{H-NMR}$  (DMSO- $d_6$ , 300 MHz)  $\delta$ : 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<sup>c</sup>. Yield 67%. m.p. 169-171 °C. IR (KBr)  $\text{cm}^{-1}$ : 3447, 1567.  $^1\text{H-NMR}$  (DMSO- $d_6$ , 300 MHz)  $\delta$ : 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<sup>a</sup>. Yield 55%. m.p. 119-120 °C. IR (KBr)  $\text{cm}^{-1}$ : 3412, 1653, 1566.  $^1\text{H-NMR}$  (DMSO- $d_6$ , 300 MHz)  $\delta$ : 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<sup>c</sup>. Yield 63%. m.p. 142-143 °C. IR (KBr)  $\text{cm}^{-1}$ : 3438, 1647, 1566.  $^1\text{H-NMR}$  (DMSO- $d_6$ , 300 MHz)  $\delta$ : 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<sup>a</sup>. Yield 60%. m.p. 146 °C. IR (KBr)  $\text{cm}^{-1}$ : 3400, 1628, 1571.  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 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<sup>a</sup>. Yield 59%. m.p. 187-190 °C. IR (KBr)  $\text{cm}^{-1}$ : 3412, 1643, 1555.  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 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<sup>a</sup>. Yield 54%. m.p. 175-177 °C. IR (KBr)  $\text{cm}^{-1}$ : 3404, 1659, 1541.  $^1\text{H-NMR}$  (DMSO- $d_6$ , 300 MHz)  $\delta$ : 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<sup>c</sup>. Yield 62%. m.p. 197 °C. IR (KBr)  $\text{cm}^{-1}$ : 3412, 1661, 1571.  $^1\text{H-NMR}$  (Acetone- $d_6$ )  $\delta$ : 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<sup>c</sup>. Yield 51%. m.p. 152 °C. IR (KBr)  $\text{cm}^{-1}$ : 3423, 1656, 1544.  $^1\text{H-NMR}$  (DMSO- $d_6$ , 300 MHz)  $\delta$ : 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<sup>c</sup>. Yield 50%. m.p. 196-199 °C. IR (KBr)  $\text{cm}^{-1}$ : 3400, 1627, 1537.  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz,)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-3-(thien-2-yl)-2-propen-1-one (30)**  $R_f$  0.67<sup>c</sup>. Yield 76%. m.p. 123 °C. IR (KBr)  $\text{cm}^{-1}$ : 3466, 1642, 1535.  $^1\text{H-NMR}$  ( $\text{DMSO-d}_6$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-3-(5-methylthien-2-yl)-2-propen-1-one (31)**  $R_f$  0.66<sup>a</sup>. Yield 69%. m.p. 114-115 °C. IR (KBr)  $\text{cm}^{-1}$ : 3402, 1624, 1537.  $^1\text{H-NMR}$  ( $\text{DMSO-d}_6$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-3-(5-bromothien-2-yl)-2-propen-1-one (32)**  $R_f$  0.58<sup>a</sup>. Yield 66%. m.p. 133-136 °C. IR (KBr)  $\text{cm}^{-1}$ : 3458, 1665, 1557.  $^1\text{H-NMR}$  ( $\text{DMSO-d}_6$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).

**1-(3'-Hydroxyphenyl)-3-(5-nitrothien-2-yl)-2-propen-1-one (33)** Yield 49%. m.p. 169-171 °C. IR (KBr)  $\text{cm}^{-1}$ : 3412, 1637, 1535.  $^1\text{H-NMR}$  ( $\text{DMSO-d}_6$ , 300 MHz)  $\delta$ : 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 ( $\text{M}^+$ ).