



J. Serb. Chem. Soc. 79 (1) S1–S5 (2014)

SUPPLEMENTARY MATERIAL TO
**Synthesis, enzyme inhibition and anticancer investigations of
unsymmetrical 1,3-disubstituted ureas**

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J. Serb. Chem. Soc. 79 (1) (2014) 1–10

YIELDS, PHYSICAL, ANALYTICAL AND SPECTRAL DATA FOR THE PREPARED
UREAS

N-(3-Methylphenyl)-2-oxo-1-pyrrolidinecarboxamide (1). Yield: 70 %; m.p.: 229 °C; Anal. Calcd. for C₁₂H₁₄N₂O₂: C, 66.11; H, 6.47; N, 12.85 %. Found: C, 66.10; H, 6.43; N, 12.81 %; IR (KBr, cm⁻¹): 3233 (NH), 1638 (C=O); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 8.56 (1H, *br.s*, NH), 7.28 (1H, *br.s*, Ar-H), 7.19 (1H, *d*, *J* = 8.0 Hz, Ar-H), 7.13 (1H, *t*, *J* = 7.2, Ar-H), 6.76 (1H, *d*, *J* = 7.2 Hz, Ar-H), 3.28 (2H, *br.s*, CH₂), 2.49 (4H, *br.s*, 2CH₂), 2.26 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 173.55, 145.48, 138.78, 135.55, 131.61, 121.16, 119.73, 116.48, 43.70, 31.84, 21.00, 20.95; EI MS (*m/z* (relative abundance, %)): 218 (M⁺, 2) 161 (4), 133 (8), 134 (4), 107 (BP, 100).

N-Mesityl-N'-(3-methylphenyl)urea (2). Yield: 71 %; m.p.: 271 °C; Anal. Calcd. for C₁₇H₂₀N₂O: C, 76.18; H, 7.52; N, 10.45 %. Found: C, 76.15; H, 7.51; N, 10.47 %; IR (KBr, cm⁻¹): 3293 (NH), 1646 (C=O); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 8.26 (2H, *br.s*, NH), 7.31 (2H, *d*, *J* = 4.8 Hz, Ar-H), 7.19 (1H, *s*, Ar-H), 7.07 (1H, *t*, *J* = 7.2 Hz, Ar-H), 6.68 (1H, *d*, *J* = 7.2 Hz, Ar-H), 6.56 (1H, *d*, *J* = 7.2 Hz, Ar-H), 3.31 (6H, *s*, 2CH₃), 3.28 (3H, *s*, CH₃), 2.21 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 155.42, 143.30, 140.28, 137.12, 136.61, 136.04, 132.10, 129.95, 120.76, 120.71, 117.51, 20.95, 20.50, 18.89; EI MS (*m/z* (relative abundance, %)): 268 (M⁺, 21) 161 (6), 135 (85), 107 (BP, 100).

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N-(3-Methylphenyl)-*N'*-(1-phenylethyl)urea (**3**). Yield: 72 %; m.p.: 123 °C; Anal. Calcd. for C₁₆H₁₈N₂O: C, 75.65; H, 7.14; N, 11.02 %. Found: C, 75.67; H, 7.13; N, 11.04 %; IR (KBr, cm⁻¹): 3317 (NH), 1634 (C=O); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 7.56 (2H, *br.s*, NH), 7.26 (1H, *br.s*, Ar-H), 7.19 (1H, *br.d*, *J* = 8.0 Hz, Ar-H), 7.10 (1H, *t*, *J* = 8.0 Hz, H-5), 6.86 (5H, *br.s*, Ar-H), 6.72 (1H, *br.d*, *J* = 8.0 Hz, Ar-H), 2.23 (1H, *br.s*, CH-CH₃), 2.21 (3H, *br.s*, CH-CH₃), 2.14 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 156.82, 140.71, 138.98, 135.68, 131.70, 127.62, 126.64, 126.63, 120.46, 120.37, 117.12, 47.73, 20.95; EI MS (*m/z* (relative abundance, %)): 254 (M⁺, 10) 196 (2), 120 (3), 107 (BP, 100).

N-(3-Methoxyphenyl)-*N'*-(3-methylphenyl)urea (**4**). Yield: 90 %; m.p.: 202 °C; Anal. Calcd. for C₁₅H₁₆N₂O₂: C, 70.37; H, 6.30; N, 10.94 %. Found: C, 70.35; H, 6.31; N, 10.95 %; IR (KBr, cm⁻¹): 3284 (NH), 1629 (C=O); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 8.63 (1H, *br.s*, NH), 8.54 (1H, *br.s*, NH), 7.28 (1H, *br.s*, Ar-H), 7.18 (2H, *m*, Ar-H), 7.15 (2H, *t*, *J* = 8.0 Hz, Ar-H), 6.90 (1H, *dd*, *J* = 8.0, 1.6 Hz, Ar-H), 6.77 (1H, *d*, *J* = 8.0 Hz, Ar-H), 6.53 (1H, *dd*, *J* = 8.0, 2.4 Hz, Ar-H), 3.71 (3H, *s*, OCH₃), 2.26 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 160.62, 155.57, 140.01, 136.04, 135.86, 132.10, 129.82, 120.76, 120.71, 118.27, 113.39, 112.41, 109.13, 55.22, 20.95; EI MS (*m/z* (relative abundance, %)): 256 (M⁺, 22) 149 (4), 123 (65), 107 (BP, 100).

N-(4-Methylphenyl)-2-oxo-1-pyrrolidinecarboxamide (**5**). Yield: 70 %; m.p.: 263 °C; Anal. Calcd. for C₁₂H₁₄N₂O₂: C, 66.11; H, 6.47; N, 12.85 %. Found: C, 66.10; H, 6.43; N, 12.81 %; IR (KBr, cm⁻¹): 3309 (NH), 1634 (C=O); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 7.18 (2H, *d*, *J* = 8.1 Hz, Ar-H), 7.08 (2H, *d*, *J* = 8.1 Hz, Ar-H), 6.32 (1H, *br.s*, NH), 4.19 (2H, *br.s*, CH₂), 2.29 (2H, *d*, *J* = 7.8 Hz, CH₂), 1.77 (2H, *br.s*, CH₂), 1.52 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 173.55, 145.48, 136.44, 129.24, 126.86, 116.19, 43.70, 31.84, 21.00, 20.45; EI MS (*m/z* (relative abundance, %)): 218 (M⁺, 21) 167 (1), 149 (10), 133 (BP, 100).

N-Mesityl-*N'*-(4-methylphenyl)urea (**6**). Yield: 71 %; m.p.: 270 °C; Anal. Calcd. for C₁₇H₂₀N₂O: C, 76.18; H, 7.52; N, 10.45 %. Found: C, 76.15; H, 7.51; N, 10.47 %; IR (KBr, cm⁻¹): 3293 (NH), 1646 (C=O); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 7.57 (1H, *br.s*, NH), 7.30 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.03 (2H, *d*, *J* = 8.0 Hz, Ar-H), 6.85 (2H, *br.s*, Ar-H), 4.76 (1H, *br.s*, NH), 2.28 (6H, *s*, 2CH₃), 2.21 (3H, *s*, CH₃), 2.14 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 155.42, 143.30, 139.72, 137.12, 136.61, 129.95, 129.73, 126.42, 117.23, 20.50, 20.45, 18.89; EI MS (*m/z* (relative abundance, %)): 268 (M⁺, 12) 146 (1), 135 (55), 107 (BP, 100).

N-(4-Methylphenyl)-*N'*-(1-phenylethyl)urea (**7**). Yield: 72 %; m.p.: 164 °C; Anal. Calcd. for C₁₆H₁₈N₂O: C, 75.65; H, 7.14; N, 11.02 %. Found: C, 75.67; H, 7.13; N, 11.04 %; IR (KBr, cm⁻¹): 3293 (NH), 1629 (C=O); ¹H-NMR (400 MHz,

DMSO- d_6 , δ / ppm): 8.23 (2H, *br.s*, NH), 7.30 (4H, *s*, Ar-H), 7.22 (2H, *d*, J = 8.0 Hz, Ar-H), 6.99 (2H, *d*, J = 8.0 Hz, Ar-H), 6.53 (1H, *d*, J = 7.6 Hz, Ar-H), 4.78 (1H, *q*, J = 7.2 Hz, CH-CH₃), 2.19 (3H, *s*, CH₃), 1.36 (3H, *d*, J = 7.2 Hz, CH-CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 156.82, 140.71, 138.43, 129.32, 127.62, 126.64, 126.36, 126.17, 116.83, 47.73, 20.95, 20.45; EI MS (m/z (relative abundance, %)): 254 (M^+ , 8) 149 (1), 132 (2), 107 (BP, 100).

N-(3-Methoxyphenyl)-*N'*-(4-methylphenyl)urea (**8**). Yield: 90 %; m.p.: 183 °C; Anal. Calcd. for C₁₅H₁₆N₂O₂: C, 70.37; H, 6.30; N, 10.94 %. Found: C, 70.35; H, 6.31; N, 10.95 %; IR (KBr, cm⁻¹): 3293 (NH), 1638 (C=O); ¹H-NMR (400 MHz, DMSO- d_6 , δ / ppm): 8.60 (1H, *br.s*, NH), 8.51 (1H, *br.s*, NH), 7.31 (2H, *d*, J = 8.0 Hz, Ar-H), 7.16 (1H, *br.s*, Ar-H), 7.14 (1H, *m*, Ar-H), 7.06 (1H, *d*, J = 8.0 Hz, Ar-H), 6.89 (1H, *d*, J = 8.0 Hz, Ar-H), 6.52 (1H, *d*, J = 8.0 Hz, Ar-H), 3.71 (3H, *s*, OCH₃), 2.23 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 160.62, 155.57, 138.73, 135.86, 129.82, 129.73, 126.42, 119.96, 113.39, 112.41, 109.13, 55.22, 20.45; EI MS (m/z (relative abundance, %)): 256 (M^+ , 15) 149 (5), 123 (44), 107 (BP, 100).

N-(1,3-Benzothiazol-2-yl)-*N'*-(3-methylphenyl)urea (**9**). Yield: 90 %; m.p.: 319 °C; Anal. Calcd. for C₁₅H₁₃N₃OS: C, 63.65; H, 4.63; N, 14.84 %. Found: C, 63.67; H, 4.61; N, 14.86 %; IR (KBr, cm⁻¹): 3396 (NH), 1695 (C=O); ¹H-NMR (400 MHz, DMSO- d_6 , δ / ppm): 9.07 (1H, *br.s*, NH), 8.81 (1H, *br.s*, NH), 8.13 (1H, *d*, J = 8.0 Hz, Ar-H), 7.90 (1H, *br.s*, Ar-H), 7.81 (1H, *d*, J = 8.0 Hz, Ar-H), 7.65 (1H, *br.s*, Ar-H), 7.38 (1H, *d*, J = 7.6 Hz, Ar-H), 7.25 (1H, *t*, J = 7.6 Hz, Ar-H), 7.20 (1H, *t*, J = 7.6 Hz, Ar-H), 6.85 (1H, *t*, J = 8.0 Hz, Ar-H), 2.29 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 161.12, 150.43, 148.77, 139.76, 135.63, 131.70, 127.30, 126.07, 122.99, 121.37, 120.46, 119.74, 118.84, 116.63, 20.95; EI MS (m/z (relative abundance, %)): 283 (M^+ , 4) 240 (1), 176 (20), 150 (BP, 100).

N-(2-Acetylphenyl)-*N'*-(3-methylphenyl)urea (**10**). Yield: 90 %; m.p.: 182 °C; Anal. Calcd. for C₁₆H₁₆N₂O₂: C, 71.70; H, 6.01; N, 10.45 %. Found: C, 71.68; H, 6.02; N, 10.42 %; IR (KBr, cm⁻¹): 3297 (NH), 1683 (C=O); ¹H-NMR (400 MHz, DMSO- d_6 , δ / ppm): 8.87 (1H, *br.s*, NH), 8.62 (1H, *br.s*, NH), 8.06 (1H, *br.s*, Ar-H), 7.65 (1H, *d*, J = 8.0 Hz, Ar-H), 7.57 (1H, *d*, J = 7.6 Hz, Ar-H), 7.43 (1H, *t*, J = 8.0 Hz, Ar-H), 7.31 (1H, *br.s*, Ar-H), 7.21 (1H, *d*, J = 8.0 Hz, Ar-H), 7.16 (1H, *t*, J = 7.6 Hz, Ar-H), 6.79 (1H, *d*, J = 7.6 Hz, Ar-H), 2.56 (3H, *s*, OCCH₃), 2.27 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 200.60, 152.74, 140.27, 140.03, 138.70, 136.04, 132.64, 132.10, 121.91, 120.76, 120.71, 119.34, 117.51, 117.07, 26.80, 20.95; EI MS (m/z (relative abundance, %)): 268 (M^+ , 16) 146 (9), 135 (44), 120 (59), 107 (BP, 100).

N-(1,3-Benzothiazol-2-yl)-*N'*-(4-methylphenyl)urea (**11**). Yield: 90 %; m.p.: 328 °C; Anal. Calcd. for C₁₅H₁₃N₃OS: C, 63.65; H, 4.63; N, 14.84 %. Found: C, 63.67; H, 4.61; N, 14.86 %; IR (KBr, cm⁻¹): 3440 (NH), 1691 (C=O); ¹H-NMR

(400 MHz, DMSO- d_6 , δ / ppm): 9.04 (1H, *br.s*, NH), 8.46 (1H, *br.s*, NH), 7.89 (1H, *br.s*, Ar-H), 7.65 (1H, *br.s*, Ar-H), 7.38 (1H, *t*, $J = 7.8$ Hz, Ar-H), 7.30 (1H, *d*, $J = 7.8$ Hz, Ar-H), 7.24 (1H, *t*, $J = 7.8$ Hz, Ar-H), 7.13 (2H, *d*, $J = 7.2$ Hz, Ar-H), 7.06 (1H, *d*, $J = 7.8$ Hz, Ar-H), 2.23 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 161.12, 150.43, 148.77, 139.21, 129.32, 127.30, 126.17, 126.07, 121.37, 119.46, 118.84, 116.63, 20.99; EI MS (m/z (relative abundance, %)): 283 (M⁺, 4) 176 (25), 150 (BP, 100).

N-Mesityl-N'-(2-methylphenyl)urea (**12**). Yield: 90 %; m.p.: 279 °C; Anal. Calcd. for C₁₇H₂₀N₂O: C, 76.18; H, 7.52; N, 10.45 %. Found: C, 76.15; H, 7.51; N, 10.47 %; IR (KBr, cm⁻¹): 3297 (NH), 1642 (C=O); ¹H-NMR (400 MHz, DMSO- d_6 , δ / ppm): 7.95 (2H, *br.s*, NH), 7.77 (1H, *d*, $J = 7.6$ Hz, Ar-H), 7.14 (1H, *d*, $J = 7.6$ Hz, Ar-H), 7.09 (1H, *t*, $J = 7.6$ Hz, Ar-H), 6.90 (1H, *t*, $J = 7.6$ Hz, Ar-H), 6.87 (2H, *s*, Ar-H), 2.23 (3H, *s*, CH₃), 2.22 (3H, *s*, CH₃), 2.16 (6H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 156.88, 143.30, 137.63, 137.12, 136.61, 132.58, 129.95, 127.43, 125.94, 122.88, 119.96, 20.95, 18.89, 17.49; EI MS (m/z (relative abundance, %)): 268 (M⁺, 23) 161 (1), 135 (69), 107 (BP, 100).

N-(2-Methylphenyl)-N'-(1-phenylethyl)urea (**13**). Yield: 90 %; m.p.: 179 °C; Anal. Calcd. for C₁₆H₁₈N₂O: C, 75.65; H, 7.14; N, 11.02 %. Found: C, 75.67; H, 7.13; N, 11.04 %; IR (KBr, cm⁻¹): 3374 (NH), 1646 (C=O); ¹H-NMR (400 MHz, DMSO- d_6 , δ / ppm): 7.82 (1H, *d*, $J = 8.0$ Hz, Ar-H), 7.60 (2H, *br.s*, NH), 7.34 (5H, *s*, Ar-H), 7.09 (1H, *t*, $J = 7.6$ Hz, Ar-H), 7.04 (1H, *d*, $J = 7.6$ Hz, Ar-H), 6.83 (1H, *t*, $J = 7.6$ Hz, Ar-H), 4.80 (1H, *q*, $J = 7.2$ Hz, CH-CH₃), 2.16 (3H, *s*, CH₃), 1.38 (3H, *d*, $J = 7.2$ Hz, CH-CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 156.28, 140.71, 136.33, 132.17, 127.62, 127.03, 126.64, 126.63, 125.54, 122.62, 119.56, 47.73, 20.95, 17.49; EI MS (m/z (relative abundance, %)): 254 (M⁺, 11) 196 (1), 120 (3), 107 (BP, 100).

N-(3-Methoxyphenyl)-N'-(2-methylphenyl)urea (**14**). Yield: 90 %; m.p.: 163 °C; Anal. Calcd. for C₁₅H₁₆N₂O₂: C, 70.37; H, 6.30; N, 10.94 %. Found: C, 70.35; H, 6.31; N, 10.95 %; IR (KBr, cm⁻¹): 3301 (NH), 1638 (C=O); ¹H-NMR (400 MHz, DMSO- d_6 , δ / ppm): 9.00 (2H, *br.s*, NH), 7.88 (1H, *s*, Ar-H), 7.81 (1H, *d*, $J = 8.0$ Hz, Ar-H), 7.17 (1H, *br.s*, Ar-H), 7.15 (1H, *t*, $J = 8.0$ Hz, Ar-H), 7.10 (1H, *d*, $J = 7.6$ Hz, Ar-H), 6.93 (2H, *t*, $J = 7.6$ Hz, Ar-H), 6.53 (1H, *d*, $J = 7.6$ Hz, Ar-H), 3.72 (3H, *s*, OCH₃), 2.22 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 160.62, 157.03, 137.23, 135.87, 132.58, 130.00, 129.82, 125.94, 122.88, 119.96, 113.39, 112.41, 109.13, 55.20, 20.93; EI MS (m/z (relative abundance, %)): 256 (M⁺, 42) 149 (7), 123 (84), 107 (BP, 100).

N-(2-Methylphenyl)-2-oxo-1-pyrrolidinecarboxamide (**15**). Yield: 70 %; m.p.: 263 °C; Anal. Calcd. for C₁₂H₁₄N₂O₂: C, 66.11; H, 6.47; N, 12.85 %. Found: C, 66.10; H, 6.43; N, 12.81 %; IR (KBr, cm⁻¹): 3313 (NH), 1646 (C=O); ¹H-NMR (400 MHz, DMSO- d_6 , δ / ppm): 8.22 (1H, *br.s*, NH), 7.78 (1H, *d*, $J =$

= 7.6 Hz, Ar-H), 7.16 (1H, *d*, *J* = 7.6 Hz, Ar-H), 7.11 (1H, *t*, *J* = 7.6 Hz, Ar-H), 6.93 (1H, *t*, *J* = 7.6 Hz, Ar-H), 3.28 (2H, *br.s*, CH₂), 2.49 (4H, *br.s*, 2CH₂), 2.26 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 173.55, 146.93, 136.14, 132.08, 126.39, 125.45, 123.32, 118.92, 43.70, 31.84, 21.00, 17.49; EI MS (*m/z* (relative abundance, %)): 218 (M⁺, 1) 161 (1), 133 (2), 107 (BP, 100).

N-(1,3-Benzothiazol-2-yl)-N'-(2-methylphenyl)urea (**16**). Yield: 90 %; m.p.: 329 °C; Anal. Calcd. for C₁₅H₁₃N₃OS: C, 63.65; H, 4.63; N, 14.84 %. Found: C, 63.67; H, 4.61; N, 14.86 %; IR (KBr, cm⁻¹): 3472 (NH), 1695 (C=O); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 11.11 (1H, *br.s*, NH), 8.65 (1H, *br.s*, NH), 7.91 (1H, *d*, *J* = 7.6 Hz, Ar-H), 7.84 (1H, *d*, *J* = 7.6 Hz, Ar-H), 7.65 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.38 (1H, *t*, *J* = 7.6 Hz, Ar-H), 7.22 (2H, *m*, Ar-H), 7.02 (1H, *t*, *J* = 7.6 Hz, Ar-H), 2.27 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 161.12, 151.88, 148.77, 137.12, 132.17, 129.65, 127.30, 126.07, 122.62, 122.54, 122.19, 121.37, 118.84, 116.63, 20.88; EI MS (*m/z* (relative abundance, %)): 283 (M⁺, 6) 176 (12), 150 (BP, 100).

N-(2-Acetylphenyl)-N'-(4-methylphenyl)urea (**17**). Yield: 90 %; m.p.: 235 °C; Anal. Calcd. for C₁₆H₁₆N₂O₂: C, 71.70; H, 6.01; N, 10.45 %. Found: C, 71.68; H, 6.02; N, 10.40 %; IR (KBr, cm⁻¹): 3378 (NH), 1674 (C=O); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 8.84 (1H, *br.s*, NH), 8.58 (1H, *br.s*, NH), 8.04 (1H, *br.s*, Ar-H), 7.65 (1H, *d*, *J* = 8.0 Hz, Ar-H), 7.56 (1H, *d*, *J* = 8.0 Hz, Ar-H), 7.42 (1H, *t*, *J* = 8.0 Hz, Ar-H), 7.33 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.08 (1H, *d*, *J* = 8.0 Hz, Ar-H), 2.55 (3H, *s*, OCCH₃), 2.24 (3H, *s*, CH₃); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 200.60, 152.73, 140.03, 139.72, 138.70, 132.64, 129.76, 126.42, 121.91, 119.34, 117.23, 117.07, 26.80, 20.45; EI MS (*m/z* (relative abundance, %)): 268 (M⁺, 21) 146 (7), 135 (33), 120 (46), 107 (100).