

Synthesis of 1-[3-(2-methyl-5-nitro-1*H*-imidazol-1-yl)propyl]-1*H*-1,2,3-benzotriazole and 1-[3-(2-methyl-5-nitro-1*H*-imidazol-1-yl)butyl]-1*H*-1,2,3-benzotriazole

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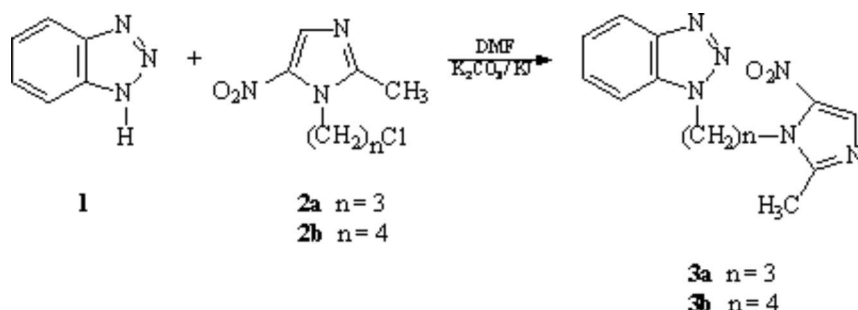
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The title compounds were obtained in reaction 1,2,3-benzotriazole (1) with 1-(3-chloropropyl)- (2a) and 1-(4-bromobutyl)-2-methyl-5-nitro-1*H*-imidazole (2b) [1].

The derivatives of 5-nitroimidazole show various interesting biological properties. They have good chemotherapeutic activity [2], are potent anti-bacterial agents [2] and are very effective against various infections especially antiprotozoic [3].

1-[3-(2-methyl-5-nitro-1*H*-imidazol-1-yl)propyl]- 1*H*-1,2,3-benzotriazole (3a)

A mixture of 1,2,3-benzotriazole (1) (commercial product) (0.76 g, 6.38 mmol), 1-(3-chloropropyl)-2-methyl-5-nitro-1*H*-imidazole (1.58 g, 7.76 mmol) (2a) [1] and powdered anhydrous K₂CO₃ (2 g) and a catalytic amount of KI in dry DMF (25 mL) was stirred at room temperature for 24 h. The resulting solution was poured into water (100 mL) and precipitated solid was filtered off and washed with water. The crude product was purified by recrystallization from isopropyl alcohol giving 1-[3-(2-methyl-5-nitro-1*H*-imidazol-1-yl) propyl]-1*H*-1,2,3-benzotriazole (3a) as colorless needles (1.45 g, 79.5%).

Melting point: 167-169°C

¹H-NMR (CDCl₃, 80 MHz): δ= 8.10 (dd, 1H, aromatic H, *J* = 8.96 Hz, *J* = 1.21 Hz), 7.80 (s, 1H, CH imid.), 7.32-7.57 (m, 3H, aromatic H), 4.70 (t, 2H, CH₂ CH₂ -N-benzotriazole, *J* = 6.40 Hz), 4.04 (t, 2H, CH₂ CH₂ -N-imid., *J* = 7.12 Hz), 2.66-2.35 (m, 2H, CH₂ CH₂ CH₂), 2.34 (s, 3H, CH₃),

MS, (70eV) *m/z* (%): 286 (7.0), 269 (5.0), 171 (100).

IR (KBr, cm⁻¹): 1537 and 1336 (NO₂), 1495 (CH₂), 1292 (C-N).

Elemental Analysis: Calculated for C₁₃H₁₄N₆O₂ (286.29): C 54.54, H 4.93, N 29.36; found C 54.23, H

4.87, N 29.02.

1-[3-(2-methyl-5-nitro-1*H*-imidazol-1-yl)butyl]-1*H*-1,2,3-benzotriazole (3b)

A mixture of 1,2,3-benzotriazole (**1**) (commercial product) (0.38 g, 3.19 mmol), 1-(3-bromo-butyl)-2-methyl-5-nitro-1*H*-imidazole (0.85 g, 3.43 mmol) (**2b**) [1] and powdered anhydrous K₂CO₃ (0.65 g) and a catalytic amount of KI in dry DMF (20 mL) was stirred at room temperature for 19 h. The resulting solution was poured into water (60 mL) and precipitated solid was filtered off, and washed with water. The crude product was purified by recrystallization from isopropyl alcohol giving 1-[3-(2-methyl-5-nitro-1*H*-imidazol-1-yl) butyl]-1*H*-1,2,3-benzotriazole (**3b**) as colourless needles (0.72 g, 75.2%).

Melting point: 168-170°C

¹H NMR (CDCl₃, 80 MHz): δ= 7.93-7.34 (m, 4H, aromatic H), 7.66 (s, 1H, CH imid.), 4.81 (t, 2H, CH₂ CH₂-N-benzotriazole, *J* = 6.32 Hz), 3.91 (t, 2H, CH₂ CH₂-N-imid., *J* = 7.36 Hz), 2.43-1.71 (m, 4H, CH₂ CH₂ CH₂ CH₂), 2.37 (s, 3H, CH₃).

IR (KBr, cm⁻¹): 1539 and 1330 (NO₂), 1496 (CH₂) 1289 (C-N).

Elemental Analysis: Calculated C₁₄H₁₆N₆O₂ (300.32): C 55.99, H 5.37, N 27.98; found C 55.82, H 5.36, N 27.84.

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Sample Availability: Available from MDPI.

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