

Bis-(1-phenyl-5-nitro-6-methylthio-1,2,3,4-tetrahydropyrimidinyl)ethane and Bis-(1-phenyl-5-nitro-6-methylthio-1,2,3,4-tetrahydropyrimidinyl)butane

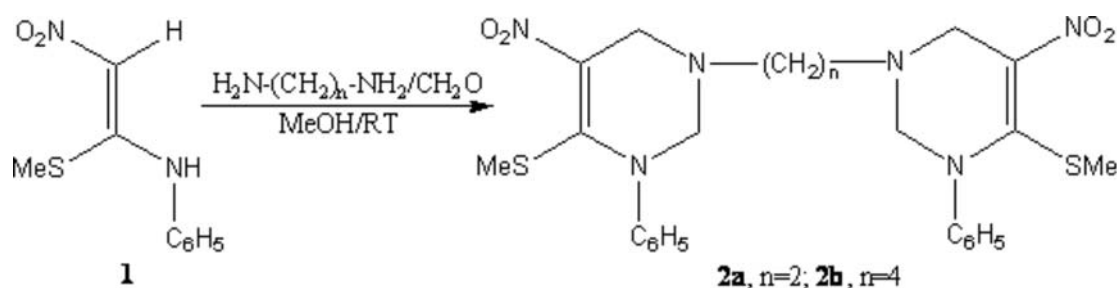
Kaushik Chanda, Milan C. Dutta, Kaushal Kishore, J.N. Vishwakarma*

Organic Research Lab, Department of Chemistry, St. Anthony's College,
Shillong-793 001 (India).

Phone: 0364.2229928, Fax: 0364.2229558, E-mail: jnvishwakarma@rediffmail.com

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5-Nitro-1,2,3,4-tetrahydropyrimidine derivatives [1, 2] are known to possess important biological properties. However, bis-5-nitro-1,2,3,4-tetrahydropyrimidines are unknown in the literature. In continuation with our on-going program on the synthesis of tetrahydropyrimidines [3, 4], we herein report the synthesis of the title compounds. A mixture of ethylenediamine (30 mg, 0.5 mmol) and formaldehyde (60mg, 2 mmol, 40% solution) was stirred in methanol (2 mL) for 5 minutes and to this a solution of 1-nitro-2-anilino-2-methylthioethene **1** [5] (210 mg, 1mmol) in methanol was added and the resulting mixture was stirred at room temperature for 2 hours, when a yellow solid precipitated out. After the completion of the reaction (monitored by tlc), the reaction mixture was cooled in ice water and the solid filtered, washed with MeOH (2X2 mL) to give pure **2a** (150 mg, 57%), which was recrystallized from methanol. The product **2b** was obtained in 81% yield by the same procedure by replacing ethylenediamine by butylenediamine.

Bis-(1-phenyl-5-nitro-6-methylthio-1,2,3,4-tetrahydropyrimidinyl)ethane (**2a**).

Mp: 135-136⁰C (methanol, uncorrected).

IR (KBr, cm^{-1}): 1493, 1530, 1590, 1659.

¹*H*-NMR (300 MHz, CDCl_3) δ : 1.82 (s, 6H, SCH₃), 2.53 (s, 4H, N-CH₂CH₂-N), 3.75 (s, 4H, N-CH₂C=), 4.21 (s, 4H, N-CH₂-N), 7.14-7.39 (m, 10H).

MS (*m/z*): 529 (M^+), 308, 307.

Bis-(1-phenyl-5-nitro-6-methylthio-1,2,3,4-tetrahydropyrimidinyl)butane (**2b**).

Mp: 134-135⁰C (methanol, uncorrected).

IR (KBr, cm⁻¹): 1447, 1531.

¹H-NMR (300 MHz, CDCl₃) δ: 1.55-1.80 (m, 4H, N-CH₂CH₂CH₂CH₂-N), 1.84 (s, 6H, SCH₃), 2.30-2.45 (m, 4H, N-CH₂CH₂CH₂CH₂-N), 3.78 (s, 4H, N-CH₂C=), 4.21 (s, 4H N-CH₂-N), 7.18-7.39 (m, 10H).

MS (m/z): 557 (M⁺), 335, 264.

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