

(4Z)-1-Propargyl(1,3-Dipropargyl)-4-(2-oxopropylidene)-1,3,4,5-tetrahydro-2H-1,5-benzodiazepin-2-one

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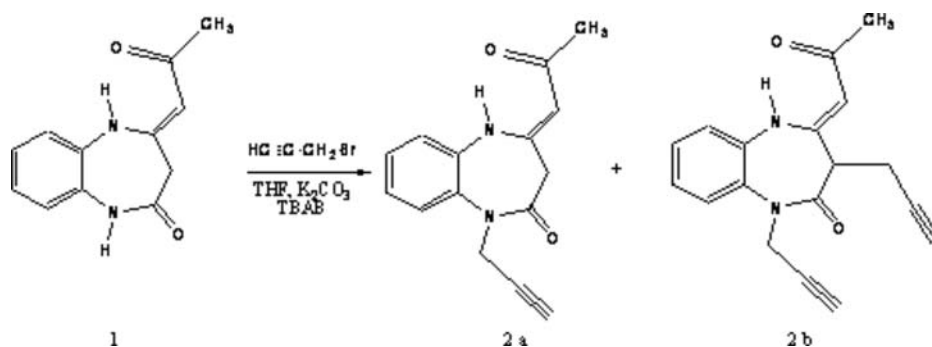
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We describe in this work the synthesis of new benzodiazepine derivatives susceptible to possess various pharmacological activities.



To a solution of (4Z)-2-oxopropylidene-1,5-benzodiazepin-2-one **1** [1,2] (0,01 mole, 2,16 gm in tetrahydrofuran 60 mL, was added K₂CO₃ (0,02mole, 2,76 gm), propargylbromid (0,02 mole, 2,36 gm) and tetra n-butylammonium bromid TBAB (0,001 mole, 0,321 gm). The mixture was stirred at room temperature for 48 hours. The solution was filtered by suction filtration. The solvent was removed under reduced pressure. The residue was chromatographed on silica gel column using hexane and ethyl acetate (80/20) as eluent to afford the products **2a** and **2b** as white solids.

(4Z)-1-Propargyl-4-(2-oxopropylidene)-1,3,4,5-tetrahydro-2H-1,5-benzodiazepin-2-one, 2a

This compound was obtained in 50% yield;

Melting Point: 172-174 °C

¹H-NMR (250 MHz, CDCl₃): δ= 2.1 (s, 3H, CH₃), 2.3 (t, 1H, ⁴J=2.4 Hz, C≡CH), 3.1 (HAHB, J=11.8 Hz, OC—CH₂), 4.7 (HAHB, ²J=17.17 Hz, ⁴J=2.4 Hz, N—CH₂), 5.3 (s, 1H, =CH—), 7.1-7.3 (m, 4H, HArom)

¹³C-NMR (62.9 MHz, CDCl₃): δ= 29.4, 38.5, 41.2, 72.5, 79.0, 96.6, 122.6, 123.2, 125.6, 126.7, 132.4, 134.5, 155.0, 166.7, 198.1

Elemental analysis: Calculated for C₁₅H₁₄N₂O₂: C, 70.85 %; H, 5.55 %; N, 11.02 %; Found: C, 70.67 %;

H, 5.46 %; N, 11.13 %;

(4Z)-1,3-Dipropargyl)-4-(2-oxopropylidene)-1,3,4,5-tetrahydro-2H-1,5-benzodiazepin-2-one, 2b

This compound was obtained in 25% yield;

Melting Point: 173-176 °C

$^1\text{H-NMR}$ (250 MHz, CDCl_3): δ = 1.9(t, 1H, $^4J=2.6$ Hz, $\text{CCH}_2\text{C}\equiv\text{CH}$), 2.1 (s, 3H, CH_3), 2.3 (t, 1H, $^4J=2.4$ Hz, $\text{NCH}_2\text{C}\equiv\text{CH}$), 3.3 (t, 1H, $^4J=7$ Hz, $\text{HC}-\text{CH}_2$), 4.2($\text{H}_\text{A}\text{H}_\text{B}$, $^2J=17.4$ Hz, $\text{HC}-\text{CH}_2$), 4.7 (d, 2H, $^2J=2.5$ Hz, $\text{N}-\text{CH}_2$), 5.21(s, 1H, $=\text{CH}-$), 7.1-7.3(m, 4H, H_Arom), 12.6(s, 1H, NH).

$^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3): δ = 16.0, 29.9, 38.6, 44.7, 93.5, 122.7, 123.3, 125.8, 125.8, 127.0, 131.9, 134.2, 156.2, 166.9, 198.1

Elemental analysis: Calculated for $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_2$: C, 73.95 %; H, 5.52 %; N, 9.58 %; Found: C, 73.82 %; H, 5.58 %; N, 9.66 %;

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