Synthesis, analgesic activity and computational study of new isothiazolopyridines of Mannich base type.

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Streszczenie

A series of new 4-arylpiperazine derivatives of isothiazolopyridine of Mannich base type and their non-4-arylpiperazine analogues (3 and 4) were synthesized and assayed as potential analgesic agents. Pharmacological assay demonstrated that all the compounds prepared, without exception, displayed significant activity in the mouse writhing assay. The analgesic action, expressed as ED50, was found to be 2-10 times more potent than that of acetylsalicylic acid and 1.5-10 times weaker than that of morphine, these being used as standards. The toxicities (LD50) of the investigated derivatives varied and ranged from 250 to 2000 mg/kg. Additionally, the computational investigations were performed in order to find correlation between molecular structure and biological effects (toxicity, analgesic action) of discussed compounds. Useful model was found for toxicity assessment.

Adres publiczny

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