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Synthesis, Characterization, Biological evaluation and Computational study for Prediction of Molecular Properties of Some Novel N-{(1,3-benzo[d]thiazol-2-yl)carbamothioyl}-2/4-substituted benzamides

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Abstract : As a part of systematic investigations a series of novel N-{(1,3-benzo[d]thiazol-2-yl)carbamothioyl}-2/4-substituted benzamides **3a-g** were synthesized by the reaction of 2-aminobenzothiazole **1** with benzoyl isothiocyanates **2a-g**. The structure elucidation of these compounds was completed by means of chemical tests, elemental (C, H, N and S) and spectral (IR, ¹H NMR and mass) analysis. All of them were screened for their antibacterial activity against Gram positive and Gram negative bacteria showing promising results, and have shown moderate to potent antibacterial activity comparable to standard drugs. Physicochemical parameters, toxicity profiles and drug likeness properties were studied using bioinformatics tools like molinspiration.

Keywords : Benzothiazoles, 2-Aminobenzothiazoles, Benzamides, Benzoylisothiocyanates.

