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Design, Synthesis, SAR, Docking and antibacterial evaluation: Aliphatic amide bridged 4-aminoquinoline clubbed 1,2,4- triazole derivatives

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Abstract: A series (7a-7k) of aliphatic amide bridged 4-aminoquinoline clubbed 1,2,4- triazole derivatives were designed on the basis of field alignment and mapping and finally synthesized via six step synthesis protocol. The antibacterial activities of all the synthesized molecules were performed on different gram positive and gram negative bacterial strains. Compound 7a, 7d and 7h were found most active against all the strains in comparison with reference ciprofloxacin. Molecular docking studies of most active compounds were performed on DNA gyrase protein pdb: 1ZI0 and results revealed that functional groups and its positions seems to be critical for their antibacterial activities.
Key words : 4-aminoquinoline, 1, 2, 4- triazole, antibacterial activity, Molecular docking, DNA gyrase, Field analysis.

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