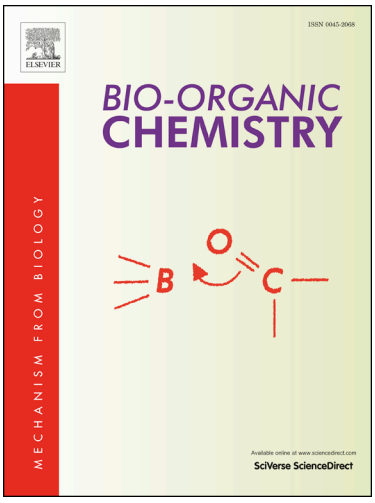

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Design, Synthesis, Antibacterial Evaluation and Molecular Docking Studies of Some New Quinoxaline Derivatives Targeting Dihyropteroate Synthase Enzyme

Maryam A.Z. El-Attar [a], Omaima G.Shaaban[a,b], Rasha Y. Elbayaa*[,a,b], Nargues S. Habib[a], Abeer E. Abdel Wahab[c], Ibrahim A.Abdelwahab[d] and Soad A. M. El-Hawash[a]

[a]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Alexandria University, Alexandria 21521, Egypt

[b]Department of Pharmaceutical Chemistry, Faculty of Pharmacy & Drug Manufacturing ,Pharos University in Alexandria, 21311, Egypt

[c]Genetic Engineering and Biotechnology Research Institute (GEBRI), the City for Scientific Research and Technology Application, Borg El-Arab, Alexandria, Egypt

[d]Department of Microbiology and Immunology, Faculty of Pharmacy& Drug Manufacturing ,Pharos University in Alexandria, 21311, Egypt

Abstract

Development of new antimicrobial agents is a good solution to overcome drug-resistance problems. From this perspective, new quinoxaline derivatives bearing various bioactive heterocyclic moieties (thiadiazoles, oxadiazoles, pyrazoles and thiazoles) were designed and synthesized. The newly synthesized compounds were evaluated for their *in-vitro* antibacterial activity against nine bacterial human pathogenic strains using the disc diffusion assay. In general, most of the synthesized compounds exhibited good antibacterial activities. The thiazolyl **11c** displayed significant antibacterial activities against *P. aeruginosa* (MIC, 12.5 µg/mL vs levofloxacin 12.5µg/mL).Molecular docking studies indicated that the synthesized compounds could occupy both *p*-amino benzoic acid (PABA) and pterin binding pockets of the dihydropteroate synthase (DHPS), suggesting that the target compounds could act by the inhibition of bacterial DHPS enzyme. The results provide important information for the future design of more potent antibacterial agents.

Key words