Volume 76, February 2018, Pages 437-448

Design, synthesis, antibacterial evaluation and molecular docking studies of some new quinoxaline derivatives targeting dihyropteroate synthase enzyme

El-Attar, M.A.Z.[a],Elbayaa, R.Y.[a,b], Shaaban, O.G.[a,b],

Habib, N.S.[a], Abdel Wahab, A.E.[c],Abdelwahab, I.A.[d],

El-Hawash, S.A.M.[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 12.5 μg/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.

Volume 76, February 2018, Pages 437-448

Reference:

https://08105wgjn-1104-y-https-www-scopus-com.mplbci.ekb.eg/record/display.uri?eid=2-s2.0-85038836736&origin=resultslist&sort=plf-f&src=s&nlo=&nlr=&nls=&sid=8ebe03d38e22915dbdccf6561a7abf57&sot=aff&sdt=cl&cluster=scosubjabbr%2c%22PHAR%22%2ct%2bscopubyr%2c%222018%22%2ct&sl=49&s=AF-ID%28%22Pharos+University+in+Alexandria%22+60011287%29&relpos=14&citeCnt=4&searchTerm=#