

Molecular Docking, Chemical Synthesis, and Characterization of Ciprofloxacin Derivatives as New Antibacterial Agents

Gheith M. ALASADI¹ & Zaid Al-OBAIDI*²⁻⁴

¹ *Department of Pharmaceutical Chemistry, College of Pharmacy, Mustansiriyah University, Baghdad, Iraq*

² *Visiting Research Fellow, Aston University, Birmingham, UK*

³ *Department of Pharmaceutical Chemistry, College of Pharmacy, University of Alkafeel, Najaf, Iraq*

⁴ *Department of Chemistry and Biochemistry, College of Medicine, University of Kerbala, Karbala, Iraq*

SUMMARY. There is an unmet necessity to treat a bacterial infection, reduce bacterial resistance, and hence enhance the therapeutic outcome. Ciprofloxacin is a commonly utilized antibiotic and is prescribed for various conditions. Low water solubility and bacterial resistance are two other limitations of this drug. In this study, the authors designed new derivatives which were examined with a well-established docking software. The best-scored molecules were synthesized and characterized successfully.

RESUMEN. Existe una necesidad insatisfecha de tratar una infección bacteriana, reducir la resistencia bacteriana y, por lo tanto, mejorar el resultado terapéutico. La ciprofloxacina es un antibiótico comúnmente utilizado y se prescribe para diversas afecciones. La baja solubilidad en agua y la resistencia bacteriana son otras dos limitaciones de este fármaco. En este estudio, los autores diseñaron nuevos derivados que se examinaron con un software de acoplamiento bien establecido. Las moléculas mejor puntuadas se sintetizaron y caracterizaron con éxito.

KEY WORDS: chemical synthesis, ciprofloxacin, GOLD software, molecular docking, new derivatives.

* Author to whom correspondence should be addressed. *E-mail:* t-al-obaiz@aston.ac.uk