Latin American Journal of Pharmacy
(formerly *Acta Farmacéutica Bonaerense*)
Lat. Am. J. Pharm. **40** (12): 2914-9 (2021)

Received: October 1, 2021
Accepted: October 25, 2021

Design, Docking and ADME Study of Benzimidazole Derivatives as Potential Antibacterial Agents

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***SUMMARY*. To combat bacterial resistance, we designed a series of benzimidazole derivatives as inhibitors of bacterial DNA gyrase and tested them as potential antibacterial agents through an *in silico* approach. Thirty-two compounds were designed based on the pharmacophore of ciprofloxacin. Their antibacterial activity was assessed through docking against bacterial DNA gyrase. The pharmacokinetics of the compounds was also investigated by SwissADME. Two of the designed compounds managed to score better than ciprofloxacin in the docking study and many were able to generate a docking pose similar to that of ciprofloxacin. In terms of the ADME study, all the designed compounds were predicted to have good permeation, oral absorption and drug likeness. They showed differences in the topological polar surface area (TPSA), and those differences were in line with the best compounds in the docking study. In summary, these compounds could be progressed to synthesis and *in vitro* evaluation as potential antibacterial agents.**

RESUMEN. Para combatir la resistencia bacteriana, diseñamos una serie de derivados de bencimidazol como inhibidores de la ADN girasa bacteriana y los probamos como posibles agentes antibacterianos mediante un enfoque *in silico*. Se diseñaron 32 compuestos basados en el farmacóforo de ciprofloxacinoa. Su actividad antibacteriana se evaluó mediante acoplamiento contra ADN girasa bacteriana. SwissADME también investigó la farmacocinética de los compuestos. Dos de los compuestos diseñados lograron obtener una puntuación mejor que la ciprofloxacina en el estudio de acoplamiento y muchos pudieron generar una postura de acoplamiento similar a la de la ciprofloxacina. En términos del estudio ADME, se predijo que todos los compuestos diseñados tendrían una buena permeabilidad, absorción oral y similitud con el fármaco. Mostraron diferencias en el área de superficie polar topológica (TPSA), y esas diferencias estaban en línea con los mejores compuestos en el estudio de acoplamiento. En resumen, estos compuestos podrían progresar hacia la síntesis y evaluación *in vitro* como posibles agentes antibacterianos.

KEY WORDS: benzimidazole, ciprofloxacin, DNA gyrase, GOLD docking, SwissADME

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ISSN 0326 2383 (printed ed.)
ISSN 2362-3853 (on line ed.)