*Extended Abstract*

# Computational Study of Benzimidazole Derivatives as Potential Antifungal Drugs †

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The infection of fungal diseases has increased in these last years due to the rise in immunodeficient patients, the resistance to current drugs, and the lack of design of new and efficient molecules against those pathogens [1]. On the other hand, benzimidazole derivatives have shown inhibitory activity to Cryptococcus Neoformans fungal with MIC 50 (minimal inhibitory concentration) of 31.2, 15.6, and 7.8 μg/mL for DV, NRE, and ACH type compounds, respectively [2]. In order to find new compounds with benzimidazolic scaffolds by modifying functional chemical groups that can have better antifungal activity, we carried out a computational study using molecular docking, molecular dynamics, and MMGBSA (mechanics generalized born and surface area continuum solvation) to screen the affinity of benzimidazolic ligands with two *Mycobacterium Turberculosis* enzymes (pdb 1E9X y 3IW2). Those enzymes are involved in the synthesis of ergosterol, which is an important component in the cell membrane wall [3]. The accomplishment of the study presented is a good agreement between the computational model and the experimental results and delivered promising compounds as candidate inhibitors based on benzimidazolic scaffold. Furthermore, other studies have reported that compounds with inhibitory capacity to enzyme 1E9X are also potent inhibitors of mycobacterial growth [4]. For this reason, the new benzimidazole derivatives found in this work can be used as effective drugs against infections caused by fungal and Mycobacterium Turberculosis at the same time. Our proposal is based on the fact that ligands have a tight bind with the pocket of enzyme 3IW2.

## References

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