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IN SILICO EVALUATION OF SELECTED BENZIMIDAZOLE DERIVATIVES IN THE DISCOVERY OF NEW POTENT ANTIMICROBIAL AGENTS

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Benzimidazoles are heterocyclic compounds that represent pharmacophores of many drugs. Apart from antimicrobial (antibacterial and antifungal) activities, benzimidazole derivatives are remarkably effective compounds possessing a wide spectrum of biological activities. Pharmacokinetic and toxicological properties of forty-two benzimidazole derivatives were calculated using Molinspiration, SwissADME and OSIRIS Data Warrior. The properties of benzimidazoles were compared to those of doxycycline, chloramphenicol and ketoconazole. The compounds met all criteria for satisfying oral bioavailability. The majority of tested benzimidazoles is considered non-toxic, and the irritating behaviour was not observed in any of the cases. Finally, the most promising nine derivatives were selected on the basis of favourable pharmacokinetic parameters and toxicological characteristics. The ability to pass through the hematoencephalic barrier is expected for all components except one, and none of the selected components is a substrate for P-glycoprotein. In addition, metabolic properties are favourable since all the selected components are expected to inhibit not more than three Cytochrome P450 isoenzymes and to be non-toxic.

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