EXPLORING THE CHEMICAL SPACE OF BILIRUBIN ANALOGUES: VIRTUAL SCREENING AND EVALUATION OF PHARMACOKINETICS AND DRUG-LIKENESS PROFILES

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Abstract
Bilirubin is widely recognized as an important endogenous molecule, offering significant benefits in the context of chronic diseases, although it may become toxic at high concentrations [1]. Based on this premise, our study aimed to identify novel compounds that reproduce the beneficial effects of bilirubin while potentially exhibiting improved safety profiles. Using the Pharmit [2] platform for pharmacophore virtual screening, we identified nine candidate molecules that were further assessed for their pharmacokinetic behavior and drug-likeness using OSIRIS Property Explorer [3], SwissADME [4], and Molinspiration [5]. From these, five compounds were selected based on ADME/Tox parameters and according to established drug-likeness criteria. This work presents an *in silico* framework for the rational selection of bilirubin-based scaffolds in the design of new, safer analogues. .Further experimental investigations will be necessary to verify their *in vivo* effectiveness and safety profile.

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