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Cheminformatics-Guided Profiling of Anthraquinone Derivatives: Insights into Drug-Likeness, ADME, and Toxicity

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Anthraquinones exhibit a diverse range of pharmacological activities, including laxative, antitumor, anti-inflammatory, antioxidant, and antimicrobial effects. Cheminformatics approaches provide rapid and cost-effective strategies to evaluate various parameters of small molecules prior to experimental validation. In this study, fourteen anthraquinone derivatives (AQ1–AQ14) with diverse substituents were investigated using SwissADME, ADMETlab, ProTox 3.0, and MolPredictX to assess their physicochemical characteristics, pharmacokinetic behaviour, toxicity, and drug-likeness. All compounds complied with Lipinski's Rule of Five, suggesting good oral bioavailability. LogP values (1–3) indicated a favourable balance between lipophilicity and solubility, while Caco-2 predictions showed moderate permeability, except for AQ2 and AQ14, which were limited by high polarity. Hydroxylated and sulfonated derivatives displayed enhanced solubility but reduced passive diffusion, whereas chlorinated derivatives (e.g., AQ3, AQ6) showed improved permeability, though with potential toxicity concerns. Most compounds were predicted to be non-inhibitors of P-gp, reducing efflux risks. High plasma protein binding (94–99%) suggested prolonged circulation with limited free drug availability. Several derivatives were predicted to cross the blood–brain barrier, indicating potential CNS activity. CYP interaction profiling revealed broad CYP1A2 inhibition, with AQ2 uniquely inhibiting CYP3A4. Clearance rates were generally moderate, although AQ2, AQ3, AQ13, and AQ14 exhibited slower elimination and longer half-lives. Overall, AQ3 emerged as the most promising candidate due to favourable permeability, metabolic stability, and drug-likeness scores. These results highlight the utility of cheminformatics in guiding the optimisation of anthraquinone scaffolds for future drug development.

Keywords: SwissADME, ADMETlab, Pharmacokinetic behaviour, 1,5- dichloroanthraquinone

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