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Artificial Intelligence: Driven Predictive Modelling of Pharmacokinetics, Pharmacodynamics, and Drug-Drug Interactions

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ABSTRACT

Pharmacokinetics (PK) and pharmacodynamics (PD) constitute the scientific foundation for understanding drug disposition and therapeutic response. While PK characterizes absorption, distribution, metabolism, and excretion (ADME), PD elucidates drug–receptor interactions and subsequent biological effects. A major challenge in drug development and clinical therapeutics is the occurrence of drug–drug interactions (DDIs), which may compromise efficacy, induce adverse reactions, or necessitate market withdrawal. Early and accurate prediction of DDIs is therefore critical for enhancing drug safety, reducing attrition rates, and optimizing therapeutic regimens. This study explores the application of Artificial Intelligence (AI) and network-based computational modelling to predict DDIs by integrating both PK and PD parameters. Structural similarity analysis using two-dimensional (2D) molecular descriptors is combined with interaction network frameworks to identify potential interaction patterns. The underlying hypothesis is that structurally analogous compounds with known interaction profiles are likely to exhibit comparable pharmacological behaviours. Additionally, AI-enhanced mathematical and compartmental modelling approaches, including one-, two-, and multi-compartment models are employed to simulate drug concentration–time profiles and mechanistic interactions. These computational strategies enable improved prediction of systemic exposure, interaction risk, and therapeutic outcomes. The integration of AI with PK/PD modelling represents a next-generation approach in predictive pharmacology, facilitating safer drug development, personalized dosing strategies, and precision therapeutics.

Keywords: *Artificial Intelligence, Pharmacokinetics, Pharmacodynamics, Drug–Drug Interactions, Predictive Modelling*

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