Integrative Computational Toxicology in Cancer Research: A Systematic Literature Review

U R Sri Veena
Bharatiya Engineering, Science and Technology Innovation University, Anantapur, AP, India
P. Ramachandra Reddy*
Department of Biochemistry, Yogi Vemana University, Kadapa, AP, India

Abstract:

Computational toxicology has emerged as a pivotal discipline in cancer research, offering transformative *in silico* methodologies to predict, analyze, and mitigate toxicological risks associated with therapeutic development. This systematic literature review (SLR) and meta-synthesis comprehensively examine the integration of computational toxicology techniques—such as molecular docking, QSAR modelling, and machine learning—in the identification and optimization of anticancer agents. Drawing from a curated selection of peer-reviewed studies published between 2015 and 2025, this paper explores how computational tools enhance cancer drug discovery, focusing on their predictive power, experimental integration, and translational value. The analysis reveals that computational methods significantly accelerate the drug development pipeline, reduce reliance on animal testing, and enable high-throughput toxicity screening with considerable precision. We synthesize findings from 85 articles and offer insights into current trends, validation strategies, limitations, and prospective applications in precision oncology. This review establishes computational toxicology as a cornerstone of modern oncopharmacology and outlines future directions for integrating artificial intelligence in toxicological modelling.

Keywords:

Computational Toxicology, Molecular Docking, Machine Learning in Drug Discovery, QSAR Modeling, Cancer Therapeutics.