

A Review: Uses of Artificial Intelligence in Formulation and Drug Design

^{1*}Om R. Arsul, ¹Gajanan D. Mogal, ¹Akshay B. Makhar

Raosahab Patil Danve College of Pharmacy, Badnapur¹

Dr. Babasaheb Ambedkar Technological University, Lonere, Raigad MS

E-mail id.: arsulom85@gmail.com

Corresponding Author: Om Rajendra Arsul

Abstract: *Artificial intelligence (AI) has become a transformative force in pharmaceutical sciences, significantly enhancing drug design and formulation development. Conventional drug discovery and formulation approaches are often costly, time-consuming, and reliant on extensive experimentation. AI-based techniques, including machine learning, deep learning, neural networks, natural language processing, and advanced computational algorithms, provide efficient data-driven solutions that improve accuracy and reduce development timelines. In drug design, AI supports target identification, virtual screening, molecular docking, de novo drug design, QSAR modeling, and prediction of pharmacokinetic and pharmacodynamic properties, thereby accelerating lead identification and optimization. In pharmaceutical formulation, AI aids in predicting physicochemical properties, selecting excipients, optimizing dosage forms, and implementing quality-by-design strategies by modeling complex relationships between formulation variables and critical quality attributes. Despite challenges related to data quality, interpretability, and regulatory acceptance, ongoing advances in big data analytics, automation, and computational power continue to expand AI applications. Overall, AI enhances decision-making, minimizes trial-and-error experimentation, improves product quality, and drives innovation across pharmaceutical drug development.*

Keywords: Artificial Intelligence, Drug Design, Pharmaceutical Formulation, Machine Learning, Computer-Aided Drug Design, Drug Development

