

PSP-03

Artificial Intelligence in Drug Discovery and Development: A Comprehensive Review

Nishanth Muthuraj*

Department of Biotechnology, Sathyabama Institute of Science and Technology (Deemed to be University), Jeppiar Nagar, Rajiv Gandhi Salai, Chennai, India.

Artificial intelligence (AI) is revolutionizing drug discovery and development through fast, data-driven insights throughout the pharmaceutical pipeline. Through the application of methods such as deep learning, natural language processing, and generative modeling, AI speeds up target identification, molecular screening, lead optimization, and forecasting of metabolism and toxicity profiles. These improvements facilitate the integration and interpretation of enormous chemical, biological, and clinical datasets and reduce time and cost historically incurred in drug development. In particular, AI-based platforms have been used for the identification of new drug candidates and repurposed molecules, while software such as AlphaFold has transformed protein structure prediction and expedited early-stage research. Despite impressive achievements, issues including data quality, model interpretability, and approval with regulatory bodies remain, highlighting multidisciplinary collaboration and vigorous validation. Ongoing development of AI is expected to provide more accurate, efficient, and personalized medicines and mark a paradigm shift in the discovery and marketing of medicines.

Keywords: Artificial Intelligence, Drug Discovery, Pharmaceutical Development

***Correspondence:** Nishanth Muthuraj,
nishanth.muthuraj2206@gmail.com