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# Chapter 3: Fundamentals of Artificial Intelligence in Drug Discovery

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**Abstract:** The field of drug discovery and development has turned into a disruptive technology with artificial intelligence (AI) that has changed the way pharmaceutical research was conducted traditionally by making it more efficient, accurate, and predictive. Some of the applications of AI discussed in this chapter are target selection, virtual screening, lead optimisation, preclinical review, clinical trials, medicine repurposing, and post-market surveillance. Computational biology and chemical analysis of complex biological and chemical data enabled by AI-based techniques such as machine learning, deep learning, natural language processing, and graph neural networks have been useful in de novo drug development, multi-target therapy, and personalised medicine. Some of the challenges that AI has had to face despite its potential are problems with data quality and availability, limitations in its algorithms, interpretability problems, legal issues and ethical concerns such as bias in the algorithms and the privacy of patients. New areas of interest include multi-omics integration, digital twins, AI-biologics synergy, federated learning, and quantum computing integration highlight the promise of making the process of drug development more efficient and predictive, and more patient-centered. The chapter underscores that the successful transformation of AI developments into clinically viable medicines would require responsible application, interdisciplinary collaboration and compliance with the ethical and legal regulations. Everything said and done, AI can radically transform the paradigms of pharmaceutical research and speed up the process of the global search of efficient, safe, and personalised treatment methods.

**Keywords:** Artificial Intelligence, Machine Learning, Deep Learning, Drug Discovery, Computational Drug Design, Target Identification

## 3.1 Introduction:

The goal of the computer science field of artificial intelligence (AI) is to develop machines that can carry out tasks that normally call for human intelligence. AI offers computational frameworks that allow machines to learn from data, identify patterns, and make predictions or well-informed decisions without explicit programming for every potential circumstance in the context of pharmaceutical research. The use of AI in drug