

AI-Driven Insights: Paving the Path to Next-Generation Therapeutics

Prof. Dhiraj S. Kalyankar¹, Mr. Chaitanya G. Bhagat², Mr. Ayush D. Kadu³,
Ms. Anjali P. Tambade⁴, Mr. Kaustubh S. Dhoran⁵

Department of Computer Science and Engineering¹⁻⁵

Dr. Rajendra Gode Institute of Technology & Research, Amravati, Maharashtra, India
dhiraj.kalyankar50@gmail.com, chaitanyabhagat143@gmail.com, ayushkadu993@gmail.com,
anjalitambade51@gmail.com, kaustubhdhoran24@gmail.com

Abstract: *This chapter thoroughly examines the critical role of artificial intelligence (AI) in drug discovery and development, covering its potential, methodologies, real-world applications, and the challenges it presents. It begins with a comprehensive introduction to AI and its subfields, including machine learning (ML), deep learning (DL), and natural language processing (NLP). The chapter then outlines various AI algorithms such as regression, support vector machines, and neural networks. It also explains approaches for optimizing and validating AI models, with a focus on metrics used for their quantitative assessment.*

Next, the chapter highlights the impact of AI across different stages of the drug discovery and development process, showcasing examples of its use in AI-driven drug discovery companies and their innovative platforms. Challenges such as limited data availability, ethical concerns, and integrating AI with traditional methods are discussed, along with potential solutions like data augmentation and explainable AI (XAI). It also explores regulatory perspectives, particularly from the United States Food and Drug Administration (FDA), illustrating the growing relationship between AI and regulatory science.

The chapter concludes with a forward-looking view on AI's future in drug discovery. AI is revolutionizing the field by automating tasks such as image analysis in pathology and radiology, improving diagnostic accuracy, and reducing human error. In clinical trials, AI is used to optimize trial design, select appropriate patient groups, and monitor real-time data, leading to faster decision-making. AI also plays a key role in analyzing scientific literature, helping researchers stay current with new advancements.

Keywords: natural language processing