Chapter 14
Convergence of Data Science–AI–Green Chemistry–Affordable Medicine: Transforming Drug Discovery

B. Rebecca
Department of Computer Science and Engineering (Data Science), Marri Laxman Reddy Institute of Technology and Management, Hyderabad, India

K. Pradeep Mohan Kumar
Department of Computing Technologies, SRM Institute of Science and Technology, Chennai, India

S. Padmini
https://orcid.org/0000-0001-8133-3453
Department of Computing Technologies, SRM Institute of Science and Technology, Chennai, India

Bipin Kumar Srivastava
Department of Applied Sciences, Galgotias College of Engineering and Technology, India

Shubhajit Halder
https://orcid.org/0000-0001-7958-4667
Department of Chemistry, Hislop College, Nagpur, India

Sampath Boopathi
https://orcid.org/0000-0002-2065-6539
Mechanical Engineering, Muthayammal Engineering College, India

ABSTRACT

The drug discovery and design process has been significantly transformed by the integration of data science, artificial intelligence (AI), green chemistry principles, and affordable medicine. AI techniques enable rapid analysis of vast datasets, predicting molecular interactions, optimizing drug candidates, and identifying potential therapeutics. Green chemistry practices promote sustainability and efficiency, resulting in environmentally friendly and cost-effective production processes. The goal is to develop affordable medicines that are not only efficacious but also accessible to a wider population. This chapter explores case studies and emerging trends to highlight the transformation of the pharmaceutical industry and innovation in drug discovery.

DOI: 10.4018/978-1-6684-9999-3.ch014

INTRODUCTION

The field of drug discovery and design has embarked on a remarkable journey of transformation, catalyzed by the powerful convergence of data science, artificial intelligence (AI), green chemistry principles, and the overarching objective of providing affordable medicine to a broader populace. This chapter embarks on an exploration of the synergistic interplay among these factors and their profound impact on the landscape of pharmaceutical research and development. In the contemporary era, scientific advancements have led to an explosion of molecular data, which, when harnessed effectively, can unlock a treasure trove of insights into disease mechanisms, molecular interactions, and potential therapeutic interventions (Blakemore et al., 2018). Enter data science and AI—tools that have proven indispensable in deciphering the intricate language of molecules. These technologies empower researchers to sift through vast datasets, predict molecular behaviors, and guide the design of novel drug candidates with unprecedented precision and efficiency.

The echoes of this revolution reverberate across the spectrum of drug discovery, from virtual screening to de novo drug design. Our journey will encompass the applications of data science and AI that have revolutionized lead optimization, compound selection, and even the prediction of a drug candidate's pharmacokinetic and toxicity profiles. Through illuminating case studies, we will showcase how these tools have not only accelerated the discovery process but have also influenced the economics of drug development (Glicksberg et al., 2019). As we delve deeper into the chapters that follow, the spotlight will shift to green chemistry—an ethos that echoes the growing societal call for sustainability and environmental stewardship. Green chemistry's principles resonate strongly with the pharmaceutical industry, where the optimization of production processes to minimize waste, reduce hazardous materials, and conserve energy aligns seamlessly with the broader goals of ethical pharmaceutical manufacturing (Arshad et al., 2016). We will explore how these principles have reshaped synthetic routes, solvent selections, and manufacturing strategies, resulting in not only ecologically friendly processes but also in cost savings that can trickle down to the end consumer.

However, the narrative doesn't end there. An underpinning theme woven throughout this exploration is the pursuit of affordable medicine. As the cost of healthcare continues to challenge global economies, the need for cost-effective drug discovery and development becomes more pressing. In tandem with the advancements in data science and green chemistry, the chapter will underscore the importance of these methodologies in reducing the economic barriers to healthcare access (Jensen et al., 2015). Through the intricate dance of data science, AI, green chemistry, and affordability considerations, the pharmaceutical landscape is undergoing a renaissance of innovation. This chapter's voyage through case studies, trends, and future prospects seeks to illuminate the interwoven tapestry of these elements, offering a glimpse into a world where cutting-edge science converges with ethical responsibility to transform drug discovery, production, and distribution.

The pharmaceutical industry stands on the threshold of a new era—one marked by the seamless integration of data science, artificial intelligence (AI), green chemistry, and the quest for affordable medicine. The symbiotic relationship among these elements holds the potential to reshape drug discovery, addressing critical challenges faced by both researchers and patients alike (Bountra et al., 2017). Traditionally, drug discovery has been a lengthy and resource-intensive process. The identification of potential drug candidates often involved a trial-and-error approach, leading to high attrition rates and exorbitant costs. Enter data science and AI—the dynamic duo that has revolutionized the field. The exponential growth of molecular data, coupled with computational prowess, has unleashed the ability