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Transformation of Drug Discovery towards Artificial Intelligence: An *in Silico* Approach

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Abstract

Computational methods play a key role in the design of therapeutically important molecules for modern drug development. With these “*in silico*” approaches, machines are learning and offering solutions to some of the most complex drug related problems and has well positioned them as a next frontier for potential breakthrough in drug discovery. Machine learning (ML) methods are used to predict compounds with pharmacological activity, specific pharmacodynamic and ADMET (absorption, distribution, metabolism, excretion and toxicity) properties to evaluate the drugs and their various applications. Modern artificial intelligence (AI) has the capacity to significantly enhance the role of computational methodology in drug discovery. Use of AI in drug discovery and development, drug repurposing, improving pharmaceutical productivity, and clinical trials will certainly reduce the human workload as well as achieving targets in a short period of time. This chapter elaborates the crosstalk between the machine learning techniques, computational tools and the future of AI in the pharmaceutical industry.

Keywords: Conceptual Density functional theory, drug discovery, Artificial Intelligence, Machine learning, pharmaco-kinetic parameters

1. Introduction

Computer-aided drug design [1, 2] has the potential to lower the cost, decrease the failure rates and speed up the discovery process. Computational tools play various roles in medicinal chemistry ranging from optimization of protein-ligand interactions for drug discovery to the design of new drugs. These methods are broadly classified as structure based and ligand based methods. For structural methods the computational studies are carried out for molecular dynamics, protein–ligand docking and calculation of free binding energies. For the ligand based methods, the computational calculations help to predict the biological response about known active and inactive ligands which include quantitative structure–activity relationships, activity cliffs analysis, and similarity search. In recent years, discovery of new molecules that could be more effective with fewer unwanted side effects is a constant concern of pharmaceutical industry. So, new developed research methods are used to predict the properties and activities of molecules even before they are synthesized. The significant development of computational tools as well as theoretical studies of quantum chemistry allow

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