



REVIEW ARTICLE

# ACCELERATING DRUG DISCOVERY: THE ROLE OF NEW MOLECULES AND SOFTWARE TOOLS

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**New drug molecules are needed for several reasons, including targeting mutated proteins in diseases, reducing side effects, and treating currently untreatable diseases like Alzheimer's. Desirable properties for new drug molecules include high selectivity, affinity, low toxicity, good pharmacokinetic properties, manufacturability, and intellectual property protection. Key guidelines from the ICH and FDA govern the development, manufacturing, and safety of new drug molecules. Plant-based medicines offer promising therapeutic compounds, such as artemisinin for malaria and taxol for cancer. Synthesis sources have produced drugs like ruxolitinib, ibrutinib, nivolumab, pembrolizumab, and ocrelizumab for various diseases. Software tools like molecular modeling, computational chemistry, cheminformatics, virtual screening, and machine learning aid in drug discovery and development by improving efficiency, accuracy, collaboration, creativity, and cost-effectiveness. Advantages of using software tools in drug discovery include increased efficiency, improved accuracy, facilitated collaboration, enhanced creativity, reduced costs, and increased safety. However, there are some potential disadvantages, such as limitations in accuracy, dependence on data quality, high software costs, complexity, lack of transparency, and ethical concerns. Overall, new drug molecules are essential for addressing various diseases, and software tools play a crucial role in accelerating the drug discovery process by providing predictive capabilities and aiding in decision-making.**

**Key words:** Drug discovery, Mutated proteins, Side effects, Machine learning, Collaboration, Creativity.

## INTRODUCTION

"Novel" drugs are new drugs never before approved or marketed. Innovative drugs often mean new treatment options for patients and advances in health care. In the fields of medicine, biotechnology and pharmacology, drug discovery is the process by which new candidate medications are discovered. A new molecule is developed by the innovator company/organization in the early drug discovery stage, which after undergoing clinical trials could translate into a drug that could be a treatment

for some disease. Synthesis of a new chemical entity is the first step in the process of drug development [1].

### *The need for new drug molecules*

There are a number of reasons why new drug molecules are required. First, many diseases, such as cancer, are caused by mutations in proteins that are essential for cell function. These mutations can make the proteins more active or less active, which can lead to disease.