THE ROLE OF SYNTHETIC CHEMISTRY IN THE RESEARCH AND DEVELOPMENT OF NOVEL MEDICINES AND PESTICIDES

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Abstract

Synthetic chemistry plays a critical role in the invention and development of new drugs and pesticides. His involves the formation and synthesis of new composite with selected properties like selectivity, strength, and safety. Moreover, this process starts with the recognition of the leading compound or composite, which can be a chemical-free, natural or completely synthetic composite that indicates an activity without any particular target. It has been observed that medicinal chemists apply this technique of synthetic chemistry for modifying the leading compound with the help of SAR or structure-activity relationship as it helps to optimize its activities, and any kind of pharmacokinetic properties. Along with this, this process involves the formation and combination of analogues of the leading composite with the changes and modifications to the molecular form for improving its properties.

Keywords- Synthetic chemicals, drug design, Organic synthesis, Green chemistry, Structure-activity relationship (SAR), Bioassays

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1. Introduction

HTS or High-throughput screening is mainly used to specify the potential and leading composite from the chemical libraries. However, after the screening process, synthetic chemists optimize the leading composite through the modification of chemical bodies, applying different synthetic chemistry processes including, fragment-related drug and pesticide formation, combinatorial chemistry and molecular composition or docking [1]. Other than this, toxicology, drug metabolism and pharmacological medicines are also crucial elements of drug formation or drug discovery.

Objectives

- To critically evaluate the critical key factors of synthetic chemicals that are influencing new Pesticides and Drugs
- To analyze the role of synthetic chemistry in the discovery of new pesticides and drugs
- To identify the significant ways in which synthetic chemistry affects the drug and pesticide design
- To describe the challenges of synthetic chemistry in drug design

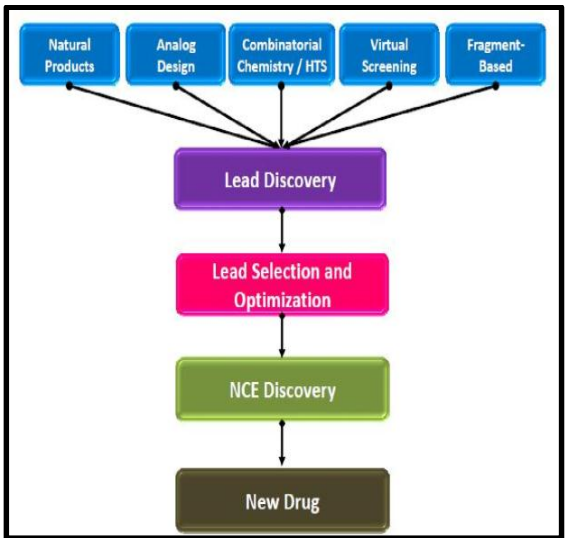

Figure 1: Drug discovery

2. Methodology

In the present day, the usage of synthetic chemistry can help the drug design process in the pharmaceutical sector, and for scientific purposes. Synthetic chemistry works by providing provide new molecules and completely natural compounds based on semi-synthesis in a drug design [2]. The suite uses thematic analysis on molecule formation under synthetic chemistry and the use of drug properties in the human body is also discussed here. The approach used in this research paper is descriptive and a secondary qualitative method has been used here.

Drug Design in Synthetic Chemistry

Drug design through synthetic chemistry is a process of creating and developing new drugs or refining the existing ones with the help of chemical synthesis. Synthetic chemistry is an important tool that helps in the process of drug design and drug discovery and it enables chemists to make new composites that be examined for their possible therapeutic effects [3]. The procedure of drug discovery by synthetic chemistry includes different stages. In the first stage, this process involves determining a particular molecule like a protein or enzyme that is implicated in a specific disease. In the second stage, chemists and scientists use computational tools, different types of screening processes or many other methods for identifying a set of compounds and molecules that have the possibility to bind to the targeted molecules and optimize their activity.

For	Against
Direct substituents in any direction without compromising MW or LogP	Unnecessary with targets for which no hit/lead molecules exist – start simple
Create unique structures that do not infringe upon existing patents	Increased production costs
Discovery of new syntheses, methodologies and reagents	Increased pre-clinical and clinical trial costs
Intricate, interesting and challenging syntheses	Difficult, tedious and laborious syntheses
Create molecules that resemble natural products with drug-like properties	No guarantee that highly 3-dimensional leads will pass clinical trials

Figure 2: Arguments for and against the use of diversity-oriented synthesis

Figure 2 shows different arguments related to diversity-based synthesis and the flexibility of the drug design and formation of complex molecules indicates that the products of such chemical processes are frequently unique. There are many arguments among scientists and chemists about the complexity of the process and how new drugs are discovered, and how diversity-oriented synthesis supports the creation of diverse molecules or composites [4].In the third stage, after the identification of the leading composite, chemists use the techniques of synthetic chemistry for modifying its structure and improving its pharmacological properties, such as its selectivity, strength, and potency.

In the fourth stage, when the promising composites have been completely synthesized and optimized, it is examined for determining their safety, efficacy and pharmaceutical properties [5]. It has been observed that when a composite pass the phase of preclinical testing, it can proceed through the other clinical tests for evaluating its safety in the human body. Overall, synthetic chemistry is a critical part of the process of drug design as it enables chemists to make new molecules with good properties and trial them for therapeutic effects. Thus, drug design is an intricate and challenging chemical process that needs a multidisciplinary process, computational tools, biochemistry, and pre-clinical and clinical tests.

Computer-Aided Drug Design

Computer-aided drug design combines computational methods, tools and synthetic chemistry processes for designing and optimizing new drug molecules. This process allows chemists to screen huge datasets of the composites, predict their properties, and create new molecules with ameliorated pharmacological properties [6]. This process involves several stages, including molecular modelling, virtual screening, lead composite optimization, toxicity predictions, and pre-clinical and clinical trials. In the molecular modelling stage, chemists use different types of computational tools for the targeted molecules as well as their interactions with other potential drug candidates [7]. This enables the chemists to signify the binding affinity and other important properties of the composites. With the help of molecular modelling data, chemists can screen huge databases for understanding the possible drug candidates with desired properties. In the stage of virtual screening, chemists can use the techniques of toxicity predictions, chemists can predict the toxicity properties of the composites and can identify the safety concerns of the compounds and optimize them for any further process [8]. Therefore, computer-aided drug design is still an intricate process that needs multidisciplinary competence and validation through different types of experimental testing.

Molecular Dynamics

The process of molecular dynamics in drug discovery contains several steps, including molecular

modelling, stimulation of molecular dynamics, and analysis and optimization.

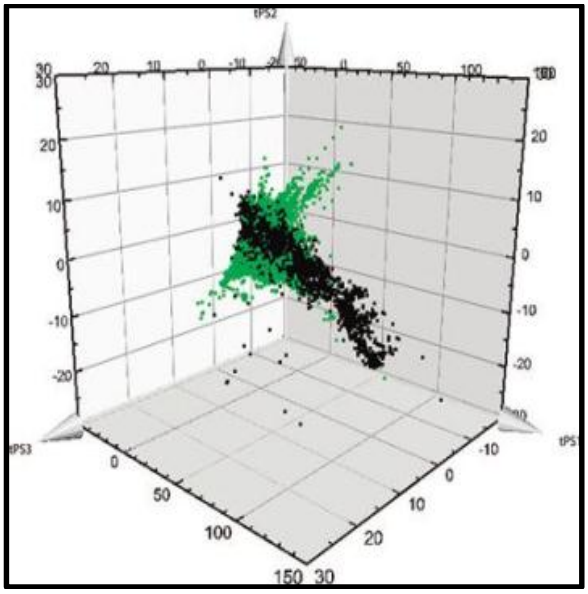

Figure 3: Chemical diversity for drug discovery purposes

Figure 3 is showing the unravelling of natural chemical or molecular diversity for drug design or drug discovery purposes. The figure seems that synthesizing has some difficulties in drug discovery strategies. This process allows chemists and scientists to monitor how the molecules react, interact, and also help them to understand the possible binding sites as well as drug interactions. After the stimulation stage, chemists examine the data for identifying the probable drug molecules that have suitable properties [10]. Therefore, molecular dynamics work as a powerful tool in drug discovery as this can accelerate the process of drug discovery and it requires ample computational tools and resources for validated and experimental testing.

In the stage of molecular modelling, chemists create a computational model for the targeted molecules like protein and other potential drug candidates [9]. In the state of molecular dynamics simulation, the chemist stimulates the activity of the targeted compounds and different drug candidates over time.

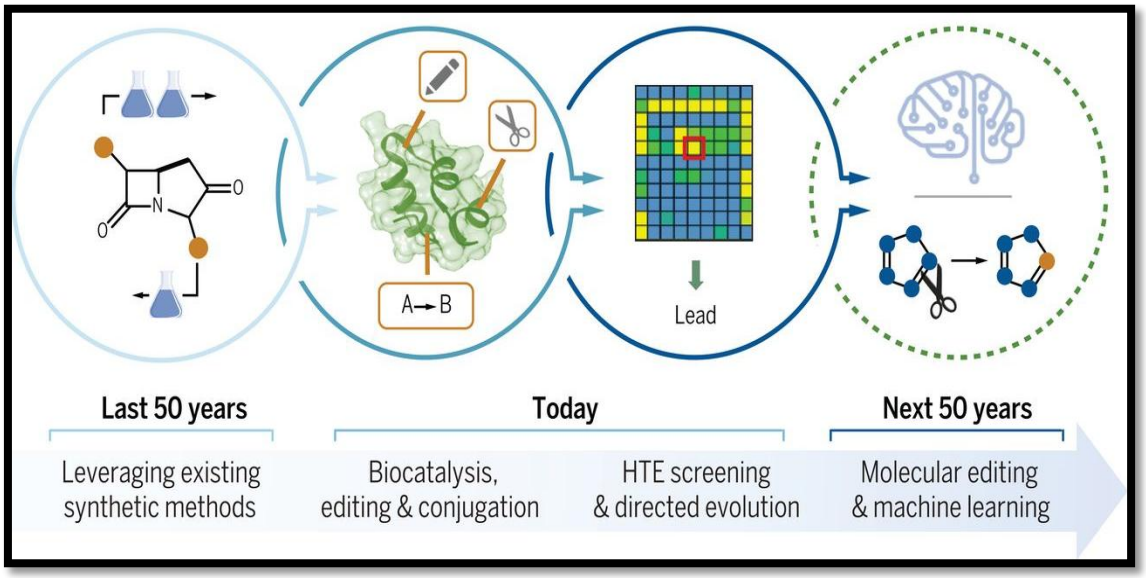

Figure 4: Steps taken for drug designing processes
(Source: 6)

Mathematical Model in Drug Design

Mathematical modelling plays a critical role in the drug discovery process as it enables chemists to predict the nature of the drug in the human body. Along with this, it helps to optimize the selectivity, safety and efficacy of the molecules. There are several types of mathematical models that can help in the drug design process such as the pharmacokinetic model, quantitative structure-activity relationship model, molecular docking model and systems pharmacology model [11]. Pharmacokinetic models are used in the drug discovery process for predicting how a drug moves to the human body. This model can help to predict the levels of drug exposure in the tissues and organs over time and also can provide the guideline for drug usage, drug dosage, efficacy and safety. Along with this, this model assumes that the drug molecules can be distributed in the body uniformly and also optimizes the dosing regimens, and minimizes the chances of toxicity by understanding the safe dose and the frequency of drug administration [12]. Other than this, the model can also be used to know more about the different drug candidates and choose the most optimistic composites for further development.

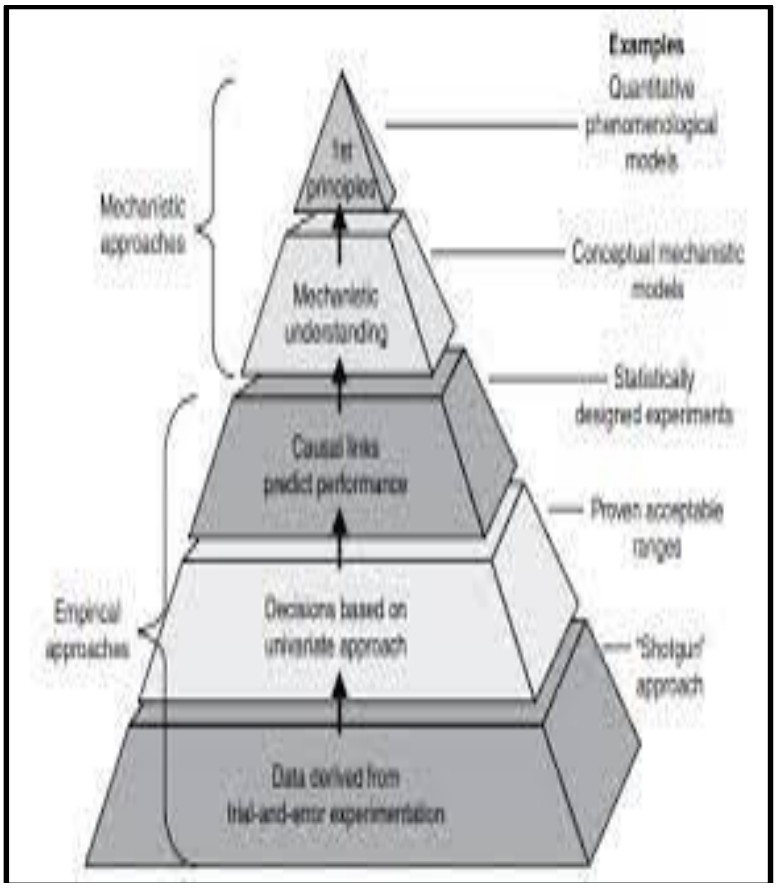

Figure 5: Mathematical model in drug design

Therefore, it can be deduced that the pharmacokinetic model provides important ideas about drug design, providing valuable insights into how the drugs react when it comes to the human body and helping to advance the drug development process.

Problem Statement

Drug discovery by synthetic chemistry can create common problems such as the complexity of biological targets, different synthesis challenges, safety-related concerns and many other issues [13]. To identify these issues, researchers or scientists in drug discovery often use computational models, tools for predicting the activities of drug molecules.

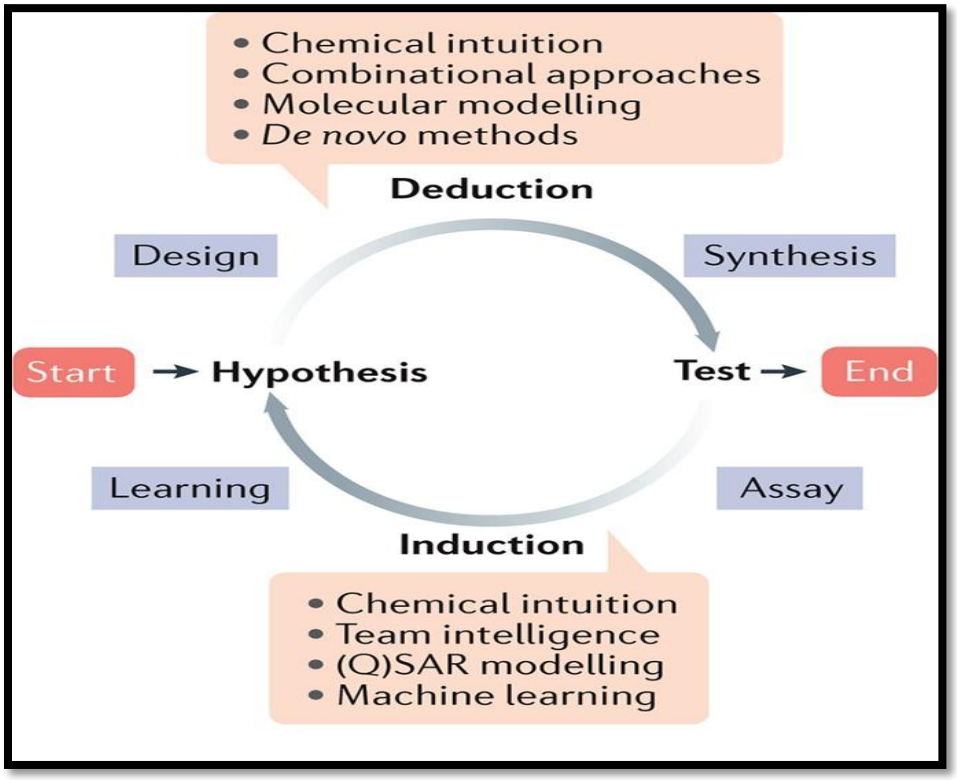

Figure 6: Relation between deduction and induction in drug designing

3. Conclusion

From the overall study, it can be concluded that drug formation and synthetic chemists mainly help in the optimization of leading composites for these properties. However, the aim of this process is to develop new composites with good pharmacological properties which are safe and also make proper pharmacokinetic profiles for use. Overall, this process of chemical science plays a vital role in drug discovery and pesticide development and its influence on the modern pharmaceutical process as well as agriculture is completely inestimable.

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