INTERTWINED DEPENDENCE OF PHARMACEUTICAL RESEARCH AND BASIC SCIENCES

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Abstract

Drug discovery and development is a complex and lengthy procedure, which may take at least 10 to 12 years. Besides, it is an extremely expensive process, which may cost up to billions of dollars to discover a new molecular or biological entity. Although pharmaceutical sciences are considered a branch of applied sciences, the procedure consists of pre-clinical and clinical stages from start to marketing, where basic sciences play a critical role, particularly in the pre-clinical stage. In fact, designing a bioactive molecule to become a lead or hit compound as a possible drug candidate, needs an extensive knowledge and background in chemical and biological sciences. Consequently, biological targets such as genes and proteins (enzymes, receptors, structural proteins) are among the most important ones to elucidate and explain the molecular mechanism of pharmacological action of any drug candidate. A comprehensive understanding of diseases threatening human health requires input from basic sciences at the molecular level since pharmaceutical research relies on the data acquired from basic research. Therefore, the role of basic sciences in pharmaceutical research cannot be ignored at all. In this sense, the discovery of antibiotics can be presented as the best and one of the first examples in the 1900s. Since not only pharmacotherapy and pharmacobiotechnology but also other therapeutic applications such as gene therapy are quite intertwined with basic sciences. In this chapter, the essential role of chemical and biological sciences, as well as basic medical sciences, will be highlighted in drug discovery supported by examples.

Keywords

Basic sciences, pharmaceutical sciences, drug research, drug discovery

Introduction

Drug discovery and development is a time-consuming, expensive, multistage, and complex process that involves a wide range of scientific disciplines and technologies. To develop a new drug may take up to 10-15 years (Drews, 2000). The first step in drug discovery is the identification of a potential drug target, which is typically a specific protein, enzyme or other biological molecule that is involved in the development or progression of a disease (Sams-Dodd, 2005; Swinney & Anthony, 2011). Once a target is identified, researchers begin to screen large libraries of chemical compounds to identify molecules that have the potential to bind to and modify the target in a way that will treat or prevent the disease (Overington et al., 2006).

The screening process typically involves a combination of high-throughput screening (HTS) techniques, computer modeling, and other methods to identify molecules that are most likely to be effective and safe (Wu et al., 2023). Once a promising compound is identified, it undergoes further testing and optimization to improve its safety, efficacy, and other properties (Wu et al., 2019).

The next stage of drug discovery involves preclinical testing, which includes testing the safety and efficacy of the drug in animal models (Kaitin, 2010). Preclinical testing helps to identify any potential safety issues and determine the appropriate dosage and administration methods for the drug (Paul et al., 2010). If the preclinical testing is successful, the drug can then proceed to clinical trials, which involve testing the drug in humans to define its safety and efficacy (Moffat et al., 2017). Clinical trials typically involve three phases of testing, with each phase designed to test different aspects of the drug's safety and efficacy (Arrowsmith & Miller, 2013). If a drug successfully completes clinical trials, it can then be submitted to regulatory agencies for official approval. Once approved, the drug can be marketed and made available to patients, who need it. The clinically available drug is also followed after approval as phase 4 monitoring.

Overall, as aforementioned, drug discovery is a complex and challenging process that requires a significant investment of time, resources, and expertise. However, the development of new drugs can have a significant impact on the treatment and prevention of diseases, improving the health and well-being of millions of people around the world. During drug research, basic sciences play a crucial role as they provide a strong foundation for the discovery, development, and testing of new drugs (Bhogal & Balls, 2008; Mohs & Greig, 2017). Here are some of the ways in which basic sciences contribute to drug research:

- Identification of drug targets: Basic sciences help identify and understand the biological processes that are involved in the development and progression of diseases. By studying the underlying mechanisms of diseases, researchers can identify potential targets for drug development.
- Drug design: Basic sciences provide the knowledge and tools necessary to design potential drugs that target specific molecular pathways or biological processes. For example, researchers may use computer modeling and simulation to design drugs that bind to specific enzymes or receptors in the body.
- Preclinical testing: Basic sciences provide the foundation for preclinical testing of drugs, which involves testing the safety and efficacy of new drugs in animal models before they are tested in humans. This testing helps researchers determine the appropriate dosage, safety, and potential side effects of a drug.
- Clinical trials: Basic sciences also play a role in clinical trials, which are the final stage of drug development. Clinical trials involve testing drugs in humans to determine their safety and efficacy. Basic sciences provide the knowledge necessary to design clinical trials, develop appropriate measures of efficacy and safety, and interpret the results.

Results and Discussion

Basic science has a critical function in medicine, as it provides the fundamental knowledge and understanding of how biological systems work at the molecular, cellular, and organismal levels (Mello & Brennan, 2011). Basic scientific research is focused on identifying the underlying mechanisms of diseases, developing new diagnostic tools as well as discovering new treatments and therapies (Patani & LaVoie, 1996). For example, research relevant to basic sciences has been instrumental in the discovery of new drug targets and the development of new drugs and therapies for various diseases.

Scientists use basic science research to understand the molecular pathways involved in diseases and to identify new targets for drug development. By understanding the mechanisms of disease, researchers can develop new drugs and therapies that target specific molecular pathways and help prevent or treat diseases.

- For instance; molecular biology owns a crucial role in drug targeting as it allows researchers to identify specific molecular targets in the body that are involved in disease processes. After identifying these targets by basic science researchers, pharmaceutical researchers can design drug candidates that specifically interact with and modulate the activity of these targets.
- The points associated with molecular biology contributes to drug targeting can be presented as below:
- Identification of drug targets: Molecular biology techniques such as gene expression analysis and protein profiling can help identify specific molecular targets that are involved in disease processes (Gross & Piwnica-Worms, 2006). These targets can then be used to design drugs that specifically interact with and modulate the activity of these targets (Al-Lazikani et al., 2012).
- Understanding drug mechanisms: Molecular biology techniques can also be used to understand how drugs interact with their targets and how this interaction affects cellular and molecular pathways in the body. This understanding is critical for optimizing drug design and developing new drugs with improved efficacy and fewer side effects.
- Personalized medicine: Molecular biology techniques can be used to identify genetic variants that influence drug response in individual patients (Savoia et al., 2017). This information can be used to develop personalized medicine approaches that consider individual genetic differences and tailor drug treatments to individual patients.
- Drug resistance: Drug resistance is a major challenge in the field of medicine, particularly in the treatment of infectious diseases and cancer. Basic sciences play a critical role in understanding the underlying mechanisms of drug resistance and developing strategies to overcome it (Gottesman et al., 2002; Davis & Davis, 2010). Molecular biology techniques can be used to study drug resistance

mechanisms and identify ways to overcome drug resistance. For example, by identifying the specific genetic mutations that lead to drug resistance, researchers can design drugs that are less susceptible to these mutations or develop combination therapies that target multiple pathways to prevent drug resistance.

Overall, molecular biology plays a critical role in drug targeting by providing a deeper understanding of disease mechanisms, identifying specific drug targets, and optimizing drug design and development.

On the other hand, chemistry has been an essential part of in drug discovery process by enabling the design, synthesis, and optimization of molecules with the desired therapeutic properties (Lipinski et al., 2001). The importance of chemistry in drug discovery, including the development of methods to predict drug solubility and permeability, the use of novel chemical reactions for drug design, and the optimization of drug candidates based on their structureactivity relationships is very clear. Chemical sciences possess a vital position in drug development, including the identification of druggable targets, the design and optimization of drug candidates based on their physical and chemical properties, the use of computational methods to predict drug-target interactions, and the targeting of multiple binding sites on proteins for improved efficacy and selectivity. In addition, the findings emphasize the need for interdisciplinary collaboration and integration of multiple disciplines, such as biology, chemistry, and computational sciences. to achieve successful drug development (Lipinski, 2004; Chen & Shoichet, 2009). Thus, pharmaceutical sciences and chemistry are inseparable parts of each other.

Virtual screening is a computational technique used in drug research to identify potential drug candidates from a large database of compounds. It should also be noted that virtual screening has great potential in drug research as well as the challenges and limitations of this approach (Lavecchia, 2013). Virtual screening can be a useful tool in identifying potential drug candidates, particularly in cases, where experimental screening is not feasible or practical (Kitchen et al., 2004; McGaughey et al., 2007). However, the accuracy of virtual screening results depends on the quality of the input data, the choice of screening method, and the selection of appropriate evaluation criteria. In addition, the success of virtual screening in drug discovery often requires a combination of different computational and experimental approaches.

Relevantly, bioinformatics is an essential part of drug discovery from the initial identification of potential drug targets to the optimization of drug candidates (Jorgensen, 2004). Bioinformatics tools can be used to identify for assorted purposes including potential drug targets, predict drug-target interactions, and optimize drug candidates. In addition, bioinformatics methods can be employed to analyze large datasets generated in drug discovery research, such as genomic and proteomic data, to gain insights into disease mechanisms, and to identify potential drug targets (Li et al., 2017). The use of bioinformatics in drug discovery has greatly facilitated the process of drug development and helped to accelerate the discovery of new drugs.

Molecular biology owns a central role in all stages of the drug discovery and development process, from target identification and validation to lead optimization, preclinical testing, and clinical translation (Lazo, 2010; Vamathevan et al., 2019). Molecular biology techniques are used to identify and validate molecular targets implicated in diseases as well as translational biomedicine (Zou et al., 2013). This involves studying the genetic, biochemical, and signaling pathways associated with diseases to identify proteins, nucleic acids, or other molecules that could serve as potential drug targets. Advances in molecular biology continue to drive innovation in drug discovery, leading to the development of novel therapeutics for a wide range of diseases. Molecular biology techniques underpin the development of gene therapies and personalized medicine approaches (Belfield & Delaney, 2015). Molecular biology assays are used in high-throughput screening campaigns to identify potential drug candidates from large compound libraries (Patel, 2013). These assays measure the activity of compounds against specific targets or biological pathways, allowing researchers to identify lead compounds with desired pharmacological properties (Eder & Herrling, 2016). Gene editing technologies such as CRISPR-Cas9 enable precise modification of the genome to correct disease-causing mutations or modulate gene expression, while molecular diagnostics enable the molecular profiling of patients to guide treatment decisions (Robert et al., 2017). It also enables the discovery of biomarkers—molecular signatures associated with disease diagnosis, prognosis, and treatment response. Biomarkers help stratify patient populations, monitor disease progression, and evaluate the efficacy and safety of drug candidates in clinical trials. On the other hand, molecular modeling and computational biology techniques are used in rational drug design to predict the interactions between drugs and their targets at the atomic level (Nero et al., 2018; Brogi, 2019). This approach facilitates the design of novel drug candidates with improved potency, selectivity, and pharmacokinetic properties. These techniques help characterize drug targets at the molecular level, including their structure, function, expression patterns, and subcellular localization. This information is essential for understanding how drugs interact with their targets and for optimizing drug efficacy and selectivity.

Genomic and proteomic approaches enable the comprehensive analysis of genes, proteins, and their interactions in health and disease (Finan et al., 2017; Heilbron et al., 2021). Genome-wide association studies (GWAS) and next-generation sequencing (NGS) technologies identify genetic variations associated with diseases, while proteomics techniques such as mass spectrometry identify and quantify proteins involved in disease pathways (Wu et al., 2019; Andrews et al., 2020).

It should also be mentioned that systems biology is an interdisciplinary field that aims to understand complex biological systems by analyzing their components and interactions at a holistic level. It combines experimental and computational approaches to study how biological molecules and networks function together to regulate cellular processes and maintain homeostasis (Berg, 2014). In the context of drug research, systems biology offers valuable insights into the mechanisms of disease and drug action, facilitating the identification of novel drug targets, optimization of therapeutic strategies, and prediction of drug responses (Butcher et al., 2004). Systems biology approaches enable the comprehensive analysis of molecular pathways and networks underlying diseases, such as cancer, neurodegenerative disorders, By integrating omics data and metabolic diseases. (genomics, transcriptomics, proteomics, and metabolomics) and computational modeling, researchers can identify key molecular drivers of disease progression and potential therapeutic targets (Russell et al., 2013). It facilitates the discovery of novel drug targets by providing insights into the complex interactions between biological molecules and pathways involved in disease pathogenesis. Network-based analyses and computational modeling can prioritize candidate targets based on their centrality, connectivity, and relevance to disease modules (Pujol et al., 2010). Besides, systems biology approaches are valuable for identifying new therapeutic indications for existing drugs through drug repurposing. By analyzing drug-gene interaction networks and molecular signatures associated with different diseases, researchers can uncover unexpected connections between drugs and diseases, leading to the discovery of novel therapeutic uses for approved drugs. Systems biology contributes to the development of personalized medicine approaches by integrating multi-omics data with clinical information to characterize individual variability in drug responses (Azmi, 2014). By identifying biomarkers and molecular signatures associated with drug efficacy and adverse reactions, personalized treatment strategies can be tailored to individual patients, maximizing therapeutic benefits and minimizing side effects. Overall, systems biology plays a pivotal role in drug research by providing a comprehensive understanding of disease mechanisms, facilitating target identification and validation, enabling drug repurposing, supporting personalized medicine approaches, and accelerating the drug development process through predictive modeling and simulation (Pearlstein et al., 2017). By harnessing the power of systems biology, researchers can advance our understanding of complex diseases and develop more effective and personalized therapies.

Conclusion

In summary, basic sciences are essential to drug research, providing the foundation for drug discovery, design, testing, and development. Without a solid understanding of the biological processes involved in diseases and the mechanisms of drug action, it would be difficult to develop safe and effective drugs.

Overall, basic science research is essential for improving our understanding of diseases and for developing new and more effective treatments and diagnostic tools. Without basic science research, many of the advances in pharmaceutical sciences that we have today would not be possible.

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