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DRUG DESIGN AND DEVELOPMENT

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ABSTRACT

Drug design and development represent a multidisciplinary process that integrates chemistry, biology, pharmacology, and computational sciences to create new therapeutic agents. The process begins with the identification of a biological target associated with a specific disease, followed by the design of small molecules or biologics capable of modulating this target's function. Advances in computer-aided drug design (CADD), molecular docking, and structure-activity relationship (SAR) analysis have significantly accelerated the discovery phase by enabling the rational design of potent and selective compounds. Subsequent stages include preclinical testing to evaluate pharmacokinetic and toxicological properties, and clinical trials to confirm safety and efficacy in humans. Despite the complexity and high cost, modern drug development has been revolutionized by genomics, artificial intelligence, and high-throughput screening technologies, offering new possibilities for personalized and precision medicine.

KEYWORDS: Drug design, drug development, computational methods, pharmacology, therapeutic agents, precision medicine.

1. INTRODUCTION

The practice of developing therapeutic compounds predates recorded history. From its inception, drug design has practised a molecular-based understanding of pharmacology, laying out a framework in which the synergistic nature of design, synthesis and biological testing are crucially underpinned by the use of computational methods. (Liu, 2025;

Nikanjam et al.2025). Due to the considerable financial commitment and complexity of bringing new compounds to market, a detailed appreciation of the intricacies and advances that influence the drug design process is clearly of major importance (Biala et al., 2023). Drug design is a key element of the development pipeline, and although the identification of starting points can arise from chemical synthesis, natural sources or serendipitous screening, the use of computational approaches to designing candidates with appropriate physical and biological properties is now widespread (Bassani & Moro, 2023; Pawełczyk et al., 2018). The search for new drugs today is based largely on the desire to increase the body of treatment options available for a range of disease types. The establishment of suitable routes that allow scalable preparation of target compounds, motivated by an ever more stringent set of regulatory and environmental constraints, remains crucial. Throughout the process, iterative cycles of design, synthesis and testing are required, with each stage being underpinned by computational techniques (Fehlis et al.2025; Doron et al., 2025; Mushtaq et al., 2018). Drug design constitutes the creative conception of molecules destined for therapeutic application. It revolves around crafting the shape and charge properties of a candidate drug so that it complements those of its target biomolecule and binds to it. Binding to the target elicits a biological response, imparting a pharmacological effect (Sarkar et al.2024; Xia et al.2023; Saw & Song, 2025; Sahu et al., 2013). Drug design, sometimes termed rational drug design, is guided by the knowledge of the three-dimensional structure of the target molecule with which the drug must interact. Typically, this structure is solved by methods such as x-ray crystallography or nuclear magnetic resonance (NMR) spectroscopy (Luo et al.2021;Kokila Priya, 2017). Also important to the drug design chemist is the knowledge of biological data such as which molecules to target and substrate preferences of the target. Which target molecules to aim at for a desired therapeutic effect is known through the discipline of medical biology. When structural information is not available, a low-resolution model can be constructed by methods of comparative modeling, also referred to as homology modeling. A candidate drug is designed using interactive graphics, underlying and validated heuristics from medicinal chemistry, or automated computational procedures that explore large regions of chemical space (Bender & Cortes-Ciriano, 2021; Han et al., 2023; Biala et al., 2023). The problems faced in drug design are quite unlike those encountered in other design tasks such as bridge or mechanical part design. For one, the geometry of a molecule is expressed mathematically by a multitude of numbers representing the coordinates of the hundreds of atoms within it. Additionally, the target may be quite large with many receptor sites important for interaction. Furthermore, molecular flexibility confers a large number of possible target–molecule configurations, each with its own distinct binding characteristics. The overarching question, so fundamental to all of drug design from initial screening to detailed optimization, is whether a given molecule will bind to a target and, if so, how strongly will it bind. (Atz et al., 2021; Wu et al.2021; Katz et al.2024; Hook, 2022). The central goal is to identify molecules that bind tightly and specifically to targets known to play a pivotal role in disease pathways. The design exercise frequently involves molecules less active than the candidate drug, such as substrates or known inhibitors. Inhibition of the target molecule disrupts the course of the pathway, reversing pathogenesis and effecting therapeutic benefit. (Ding et al.2023; Wu et al.2023; Yao et al.2024).

2. PHARMACOLOGY BASICS

Pharmacology relates to the interaction of chemical compounds with living systems. Drug molecules typically act as substrates or inhibitors of key biological processes, thereby producing a desired change in physiology or pathological state. (Zhao et al.2021; Attwood et al.2021) Pharmacology may be divided into pharmacokinetics, which describes absorption, distribution, metabolism, and elimination (excretion) of a drug or candidate, and pharmacodynamics, which describes mechanisms of action, therapeutic effects, and toxic effects (Lee et al., 2011).

2.1 Pharmacokinetics

Pharmacokinetics is the branch of pharmacology concerned with the movement of drugs within the human body (Dalgard Dunvald et al., 2022). It deals with the absorption, distribution, metabolism and excretion of pharmaceuticals. Drugs are the substances that, when introduced into the body, produce some kind of physiological effect. They are intended generally for the treatment, mitigation, diagnosis or prophylaxis of disease. (Mahindru et al., 2023) In essence, pharmacokinetics is what the body does to the drug. It differs from pharmacodynamics, which is the branch of pharmacology concerned with the interaction of drugs with their biological targets – essentially, what the drug does to the body. Pharmacokinetics is frequently abbreviated to PK. Pharmacodynamics is abbreviated to PD. (Bereda, 2022; Berton et al.2023; Dello et al.2022; Chang et al., 2022). Pharmacokinetics addresses what is typically known as the ADME process, where A stands for absorbed, D stands for distributed, M stands for metabolized and E stands for eliminated (or excreted). The technique used to determine the levels of a particular drug or metabolite in a biological system is called bioanalysis. (Chaira et al., 2023; Sharma et al. 2021). Methods used for determining concentrations of pharmaceuticals and their metabolites can typically be divided into two broad categories:

1. Physico-chemical methods, the most common being high performance liquid chromatography (HPLC), gas chromatography (GC), spectroscopy and electrochemical analysis.
2. Biological methods such as the classic microbiological assay, diffusion and immunoassay.
   Pharmacokinetic experiments require systematic collection and analysis of biological samples, from which drug concentrations can be measured and the results used to estimate the pharmacokinetic parameters. The use of limited sampling strategies is often adopted to maximise the content of information obtained from a small number of samples. (Christodoulou et al.2022; Stielow et al.2023; Yang et al.2021; Zhang et al., 2022).

2.2 Pharmacodynamics

Pharmacodynamics explores the relationship between drug concentration at the active site and the resulting pharmacologic response, establishing dose–response associations (Sahu et al., 2013). It focuses on how a drug interacts with its target to elicit a biological effect. The two most frequently encountered dose–response relationships are the graded dose– effect and the quantal dose–effect. (Paunovska et al., 2022;Tong et al.2023). In a graded dose–effect relation, the effect produced by a drug may be any measure in a single biological system. The concentration–response curve describes one pharmacological effect and uses the continuous variable from zero to the maximal response. In contrast, a quantal dose–response curve is an all-or-none effect, such as the production of an anti-tumour effect or patient survival (Lee et al., 2011). When all subjects receiving a threshold dose manifest a predetermined quantal effect, the number responding in a large population of subjects is counted, and the all-or-none response is converted into a frequency distribution. (Wang, 2025; Halder et al.2021; Shanmugapriya et al.2025).

2.3. Drug Mechanisms of Action

Drug design comprises efforts to develop molecules that exhibit complementary three-dimensional structures and charge distributions relative to biological targets, thereby enabling specific and potent binding and eliciting the desired therapeutic effect (Isert et al., 2023; Chen et al., 2023). Structure-based drug design involves detailed knowledge of the target's three-dimensional structure obtained via experimental methods such as X-ray crystallography or NMR spectroscopy or, when unavailable, through homology modeling approaches. Candidate molecules are crafted to bind with high affinity and selectivity through a combination of computational protocols and interactive design, often augmented by the intuition of experienced medicinal chemists. The principal objective is to identify compounds that

engage critical elements of disease-associated targets to inhibit their function or modulate their activity appropriately (Saini et al., 2025; Özçelik et al.2023; Kokila Priya, 2017; Sahu et al., 2013).

3. DRUG DISCOVERY PROCESS

The processes used by academic and industrial scientists to discover new drugs recently underwent a renaissance, with many new techniques developed over the past 5–10 years. Drug discovery represents the first stage in the drug-development process, followed by preclinical development using cell-based and animal models, and clinical trials on humans. Discovering potential therapeutic agents involves computational, experimental, and clinical models. Increasing the affinity, selectivity, efficacy, metabolic stability, and oral bioavailability of new drugs remain principal goals. (Singh et al.2023;Madabushi et al., 2022;Lv et al., 2023;Fehlis et al.2025). Drug discovery and development are complex and costly endeavors, requiring approximately 2–3 billion dollars and 12–15 years to complete. Rational drug design seeks to reduce these burdens by narrowing the range of drug-like compounds at an early stage. The process entails target identification and validation, assay development, lead-molecule optimization, and pharmacokinetic and clinical studies. Structure-based and ligand-based drug-design approaches complement each other by guiding target discovery and the optimization of drug candidates. Techniques such as nuclear magnetic resonance and X-ray crystallography facilitate protein-structure analysis during this effort. (Bano et al.2023;Sertkaya et al.2024;Schlander et al.2021). Drug design is usually part of the drug discovery process, but many drugs are derived from naturally occurring substances or other “easy” starting points with limited structural modifications. Design at the molecular level is complex and somewhat ambiguous compared to the macroscopic design of objects. Designing a new drug thus entails operating simultaneously on many different length and time scales, constituting one of the most complex design tasks (Biala et al., 2023; Kumar Mahapatra & Karuppasamy, 2022; Flower, 2022).

3.1. Target Identification

Drug design aims to identify compounds exhibiting desirable biological activity against a selected pharmacological target. Contemporary drug design encompasses numerous approaches for exploiting biologically significant macromolecules or pathways to alter various diseases and conditions. Identified compounds frequently require optimization of selectivity, potency, or pharmaceutical properties prior to extensive characterization. Established drug design treatments presently represent the best approach for questions requiring complementary investigations of computational, biochemical, medicinal, and pharmaceutical methods. (Staszak et al.2022; Wong & Yeong, 2021;Ha et al., 2021;Sadri, 2023). Target identification represents arguably the initial cognizable step in the drug design process, reflecting a significant rate-limiting component with a variety of considerable hurdles to overcome (Roy, 2018). A detailed understanding of biological systems permits the deciphering of specific target proteins or genes suspected to act as determinants of a particular disease state or condition. Target validation ensures a direct relationship exists between a proposed target, an in vitro or in vivo model, and the associated molecular and cellular pathways, indispensably resulting in a therapeutic benefit and efficacy (R. Ramsay et al., 2018). Concurrent advances in the understanding of disease mechanisms, genetics, and bioinformatics have significantly increased the volume of available cellular targets, many of which currently remain categorized as “high risk”. A druggable target denotes one that a compound can modulate to produce an observable cellular response that remains related to the disease or condition under consideration (Xie et al.2023;Manzari et al.2021;Henley & Koehler, 2021). A validated target, on the other hand, represents a much lower subset and is accompanied by associated functional evidence demonstrating the amenability to targeting for disease modification. (Selkoe, 2024;Costa & Maciel, 2022)The identification of novel targets represents

by no means a trivial undertaking since it often involves the synthesis and testing of a large number of compounds within several distinct biological assays; characterization of premalignant human disease states and models represents one of the few effective target-identification strategies. (van Harten & Brakenhoff, 2021;Cerrito & Grassilli, 2021;Bhukta et al., 2021).

3.2. Lead Compound Identification

Lead compound identification is a critical step in drug discovery where initial promising compounds for a given target are selected. These compounds serve as the starting point for further optimization aimed at improving potency, selectivity, solubility, or pharmacokinetic and toxicity profiles. (Naithani & Guleria, 2024; Udegbe et al.2024) Historically, lead compounds have been identified by screening natural product isolates or compounds derived through combinatorial synthesis or virtual screening. A variety of lead generation approaches are now available, including de novo design methods that can generate molecular structures "on the fly" (Ogata et al., 2010). These approaches allow the exploration of novel chemical space when chemical libraries do not contain suitable hits. The choice of lead generation strategy depends on available information about the target and on the chemistry knowledge to be incorporated into the design. Synthetic feasibility is an important consideration at this stage. Existing computational tools enable the generation of a large number of new compounds from a given scaffold and the identification of those that best fit a chemical reaction scheme. Modern quantitative structure–activity relationship (QSAR) techniques can help select the most promising compounds for further optimization (Biala et al.2023; Mouchlis et al.2021; Tropsha et al.2024) (Alexandrov et al., 2022). Several lead discovery strategies are described in the literature; the choice among them hinges upon the nature and extent of the biological and chemical information available about the target and potential ligands (Ghode & K Jain, 2017).

3.3. High-Throughput Screening

High-throughput screening (HTS) is a compound screening and assay method used in the identification of molecules in the drug-design process that mimic or influence the effects of biological ligands for a target of interest. This method is inherently integrative, encompassing activities like the assembly of vast chemical-compound libraries, the application of robotic liquid-handling platforms, sensitive detection technologies, and sophisticated informatics infrastructure. (Bon et al., 2022; Benítez et al.2022). By enabling the daily testing of thousands of compounds and incorporating characterization of the resulting metabolic, pharmacokinetic, and toxicological data, HTS significantly accelerates the drug-discovery timeline. The operational workflow encompasses target selection and validation, reagent preparation, compound management, assay development and validation, and the screening of the compound library. (Aldewachi et al., 2021; Kumar et al.undefined) Techniques such as fluorescence resonance energy transfer and fluorescence polarization facilitate the identification of efficacious compounds. Modern microreaction well plates now reach densities up to 1,536 wells (e.g., LCP designed for mesophase crystallization), with active miniaturization efforts pushing assay volumes into the 1 to 2 micromolar range. Standard HTS throughput allows for screening approximately 10,000 compounds daily, while ultra-high-throughput screening (UHTS) systems can process up to 100,000 assays per day. Initial primary screening identifies potential hits, which are then subjected to more rigorous confirmatory secondary screening and inhibitory concentration (IC50) determination. (Cronk and Shearer 2021; Aldewachi et al., 2021; Bokhari and ALBUKHARI2021; AYON, 2023).

4. MOLECULAR MODELING TECHNIQUES

Molecular modeling encompasses a range of techniques used to model or mimic the behavior of molecules within a computer. The application of these techniques to the discovery and development of new medications is known as computer-aided drug design. (Bassani & Moro, 2023; Singh et al.2024; Bharatam2021) Key among these techniques are quantitative structure–activity relationship studies, molecular docking, and computational chemistry. Their roles in modern drug discovery are reviewed here together with a summary of recent methodological developments. The emerging automating procedure for the QSAR analysis is also addressed. (Mao et al.2021; Staszak et al.2022).

Drug discovery is the intricate and complex process of identifying new candidate medications. Most often, it involves the identification of screening hits, compounds that have the desired effect on a particular biological target. (Visan & Negut, 2024) Initial hits are optimized through medicinal chemistry to enhance affinity, selectivity, or pharmacokinetic suitability. High-throughput screening enables automated testing of numerous chemical structures against a specific biological target. Once a compound meets all desired drug characteristics and passes rigorous biological assessments, it progresses to drug development. This pathway includes preclinical testing followed by Phase I, II, and III clinical trials to systematically assess the compound's safety and efficacy. (Rácz et al.2025; Li et al., 2021;An et al., 2025)

4.1. Quantitative Structure-Activity Relationship (QSAR)

Quantitative structure-activity relationship (QSAR) analysis employs statistical methods to correlate variations in chemical structure with biophysical properties or biological activities. (Mao et al.2021) Unlike experimental methods, QSAR relies solely on information from molecular structures. Its primary objective is to discover connections among various physicochemical properties, activities, or toxicity. For these purposes, physicochemical properties are expressed in terms of number and types of atoms, positions of major functional groups, structural features, steric factors, and other relevant characteristics. QSAR offers new perspectives on the molecular basis of biological activities and supports the design or selection of novel molecules with enhanced potencies or diminished toxicities. (Vasilev & Atanasova, 2025; Lanevskij et al.2022; Valencia et al.2022). Modern QSAR analysts undertake two principal tasks. First, newly synthesized analogues are characterized using numerical values for properties expected to influence biological activity; essentially, each compound is assigned a position within a multidimensional property matrix. Second, hypothetical molecules identified in conceptual design may be represented in an analogous matrix. At a minimum, the QSAR representation should include all properties thought to affect the biological response. (Kuz'min et al.2021; Belfield et al.2021) Drugs sharing common pharmacological properties often exhibit common chemical properties; drugs acting on the same target through disparate mechanisms may not share any property. Hence, QSAR provides a rational basis for applying molecular diversity principles in drug design. (Tropsha et al.2024).

4.2. Molecular Docking

Molecular docking, the second most widely used structure-based drug design technique, explores ligand conformations within macromolecular binding sites and estimates ligand–receptor binding free energy by evaluating intermolecular recognition phenomena. These methods have played a critical role in identifying and developing promising compounds by integrating computational and experimental strategies (G. Ferreira et al., 2015). The advent of biomolecular techniques such as X-ray crystallography and nuclear magnetic resonance (NMR) has further refined molecular docking approaches by providing detailed structural information on drug targets. (Surana et al.2021; Nivatya et al.2025). Several open-source and commercial software packages are widely employed for molecular docking

simulations. These packages typically implement search algorithms to identify ligand binding poses, which are subsequently evaluated by scoring functions to estimate binding affinity. Due to the inherently limited accuracy of scoring functions, molecular docking is generally utilized for initial steps in the drug design process. (Muhammed and Aki-Yalcin2024; Raval and Ganatra2022). Initially, molecular docking programs treated both ligands and receptors as rigid entities (rigid docking) (Blanes-Mira et al., 2022). While rare during biochemical recognition, rigid docking remains applicable to large systems, such as protein-protein interactions, where high computational demands preclude extensive flexibility modeling. Allowing conformational changes in both receptor and ligand defines flexible docking, which provides better descriptions of most ligand/receptor systems but incurs greater computational expense. Semi-flexible docking permits limited conformational adjustments in the ligand and receptor, representing a compromise between the two extremes. (Lee et al., 2025; Sunny & Jayaraj, 2022; Harmalkar & Gray, 2021).

Search algorithms employed in docking software include systematic methods that explore the entire conformational space by incrementally varying degrees of freedom, simulation-based methods that solve Newton's equations of motion for the potential energy surface, and stochastic methods that introduce random conformational changes to sample accessible states. Stochastic approaches such as Monte Carlo simulations and genetic algorithms are particularly prevalent due to their efficiency in navigating large search spaces. (Inage & Hebishima, 2022; Farh et al.2024; Peng et al., 2021; Kabiri et al., 2022). Docking complements other ligand-based and structure-based tools to optimize screening workflows. Ligand-based approaches have been applied to select appropriate protein conformations for docking studies, enhancing the discrimination of actives from decoys and improving predictions of ligand affinity and binding modes (Pinzi & Rastelli, 2019). Pharmacophore-based rescoring and the incorporation of shape and three-dimensional similarity metrics have further refined virtual screening campaigns and pose selection procedures, facilitating more accurate identification of active compounds. (Giordano et al., 2022; Bhunia et al.2021)

4.3. Computational Chemistry

Computational chemistry employs advanced algorithms to calculate molecular-system properties based on their atomic-level structures. The scope includes diverse property types such as molecular conformations, energies, and various spectroscopic, thermodynamic, and kinetic parameters. Although accurate computations of macroscopic properties are hindered by incomplete physical understandings rather than computational limitations, ongoing efforts aim to enable high-quality, comprehensive predictions. The technique offers detailed information inaccessible by other approaches and complements experimental studies. Recent developments in software usability have facilitated the adoption of computational chemistry by a broader scientific community. (Maleki, 2025; Zahariev et al.2023; Keith et al.2021; Jana et al.2024). Multiple complementary computational-chemistry methods operate across wide timescales and size ranges, interacting frequently with experiments. Simpler, less resource-intensive methods can still elucidate chemical phenomena and guide more complex calculations. (Keith et al.2021) Computational chemistry thus fits naturally into the molecular-design cycle, assisting in profiling molecular systems, uncovering phenomena, and generating testable hypotheses. As the chemical complexity of systems increases, the computational demand grows, making molecular modeling among the most resource-intensive research areas and often dominating computing demands within disciplines (Das et al., 2025) (Mitchell & Matsumoto, 2011). Molecular-design laboratories typically complement specialized structural-chemistry facilities. While crystallography methods elucidate structures from which prospective models can be developed, challenges include the need for crystals, potential structural perturbations upon substrate binding, and static snapshots of inherently dynamic biological systems (Bijak et al., 2023; Eid et al., 2013).

5. CHEMICAL SYNTHESIS IN DRUG DEVELOPMENT

Several types of reaction have been identified as thermodynamically-favoured that lead specifically to one product, such as nucleophilic ring-opening reactions of epoxides and aziridines, non-aldol-type carbonyl reactions, formation of hydrazones and heterocycles, additions to carbon-carbon multiple bonds, oxidative formation of epoxides, Michael additions, and cycloaddition reactions (Pawełczyk et al., 2018). The “Lego” chemistry constitutes an interesting approach to the synthesis of drug-like molecules that can accelerate the drug discovery process by utilising a few practical and reliable reaction mechanisms. Conjugation, bioconjugation, linkers, nanoparticle surface modification, and pharmaceutical-related polymer chemistry can be realised through this strategy. The idea of Green chemistry is based on principles proposed by Anastas and Warner in 1998, which focus on reducing or eliminating hazardous substances through the innovative use of environmentally improved routes, new chemicals, sustainable resources, and methodologies for environmental impact measurement. The use of microwave radiation and ultrasonic waves are promising green techniques that promote faster, more selective transformations in drug synthesis. (Barrett, 2024; Schafmeister & Dobereiner, 2022; Jung et al., 2025; Lu et al.2022).

5.1. Synthetic Methods

Chemical synthesis methods remain pertinent in medicinal chemistry, necessitated by the ongoing discovery and development of new molecules, a significant portion of which are not readily available from suppliers. The strategic pathway from molecular design to synthesis typically hinges on high-resolution models from crystallography or NMR, which are increasingly prevalent and reliable due to robust validation protocols (Najmi et al., 2022; Chaachouay & Zidane, 2024; Cheetham et al., 2022). When precise receptor structures are absent, known ligands serve as foundational references, guiding analog synthesis and SAR studies. In such scenarios, derivations and analogs with enhanced potency are crafted through fitting functional groups or building binding models. Chemical synthesis is thus integrated with modeling to produce appropriate compounds or libraries for biological evaluation. (Jachak et al.2023; Yokoi et al.2025; Rudrapal & Egbuna, 2022).

5.2. Scale-Up Processes

During the transition from small-scale laboratory synthesis to full-scale drug manufacturing, scaling up process parameters is important to maintain product quality and process efficiency. Scientific and mathematical methodologies are frequently applied to construct models that enable reliable extrapolation when direct measurement is difficult or impractical. Notable industrial strategies include engineering models, process analytical technology (PAT) models, and physics-based models. (Viswanath; Lialin et al., 2023; Omer et al., 2021) Engineering models rely on principles such as process similarity, where hydrodynamic and thermal conditions from one equipment and scale are approximately matched at the production scale; PAT models utilize in-line monitoring instruments coupled with multivariate data analysis to control and predict product quality; and physics-based models simulate process dynamics and product characteristics using fundamental physical laws (Kim et al., 2021; Ha Jang et al., 2020). Continuous variables including time, temperature, pressure, fluid velocity, and concentration provide more flexibility in process control compared to batch variables such as raw material particle size, powder feeder speed, and milling time during production. Establishing reliable production ranges for continuous variables based on product quality and process efficiency serves as effective guidance for production personnel during scale-up operations. (Bolmanis et al., 2023; Kim et al., 2021; Rathore et al.2021) Historically, relying solely on empirical, scientific, or mathematical methods renders scale-up a risky and intricate endeavor; the integration of different methodologies often improves performance. In practice, scale-

up strategies commonly combine empirical correlations, computational fluid dynamics (CFD) simulations, and experimental data because empirical and CFD data tend to become unreliable at significantly larger scales (Du et al., 2022; Mayer et al.2023; Orosz et al.2025; Moussa2022) (Berdugo-Davis, 2016).

6. BIOLOGICAL TESTING OF COMPOUNDS

The major purpose of biological testing is to determine whether a compound is pharmacologically active at a meaningful dose (Kokila Priya, 2017). Extensive biological and pharmacological studies accompany chemical synthesis. A variety of biological tests as well as in vitro anti-microbial activity, insecticidal activity and cytotoxicity are carried out. Toxicology studies are pursued in all project stages and serve as an important criterion for advancing a compound from the optimization and development phases. Many derivatives are first tested against the target of interest via in vitro functional and radioligand binding assays. (Pognan et al.2023; Madabushi et al., 2022) Those compounds displaying pharmacological activity at appropriate concentrations are then evaluated through animal in vivo. Almost all promising compounds require ADME (absorption, digestion, metabolism and excretion) screening prior to initiation of extensive and costly in vivo testing. (Fowler et al.2022; Srivastava et al.2025; Riaz et al., 2025). Biological testing assists a chemist in identifying early where resources should be allocated within a given project and when a program should be halted to improve efficiency and productivity. Furthermore, preclinical studies performed during the course of biological assessment provide important information about a candidate drug's suitability for clinical development, the most critical stage in the drug-discovery process. (Honkala et al.2022; Schlander et al.2021; Zhang et al.2025).

6.1. In Vitro Testing

During pharmaceutical development, potential lead compounds identified through chemical synthesis must undergo biological testing. Because each lead compound often represents a new class of chemical entity, a primary concern is selecting an appropriate biological model to predict efficacy and safety in humans. In vivo testing, using whole animal models such as mice, rats, rabbits, or dogs, represents the most relevant option, but constraints of time, expense, and quantity of compound often make in vitro testing the preferred preliminary approach. (Tiwari et al.2023; Udegbe et al.2024; Vora et al.2023; Chaachouay & Zidane, 2024). In vitro experiments can screen for a variety of potential biological effects on individual tissues, cell types, or subcellular components. These models typically include or simulate organs such as the liver, kidney, lung, and intestine, in addition to the vascular system and the central nervous system. Data generated with such systems may include parameters associated with cell viability, cell morphology, enzyme function, transport processes, receptor binding, genetic expression, or overall cellular metabolism. (Pognan et al.2023; Quarato et al.2023). Historically, many biological effects discovered during the drug discovery process are also followed up with testing in vitro, and the introduction of high-throughput screening has led to the search for in vitro options as first-line tests to prevent the computational, synthetic, and discovery groups from pursuing compounds likely to fail at later stages (Dueñas et al.2023) (M McKim, 2010).

6.2. In Vivo Testing

The validity of any experimental drug design method is contingent on successful demonstrations using appropriate biological systems. Biological models used throughout the drug design process include in vitro and in vivo systems as well as toxicology studies; each provides critical information concerning the therapeutic profile of the compound under investigation. In vivo testing offers a definitive picture of therapeutic efficacy and can also be carried out on the earliest drug design platforms. (Chang et al.2023; Fischer et al.2021; Muratov et al.2021). Although two-dimensional systems

provide preliminary data on intracellular and extracellular pharmacology and biochemistry, three-dimensional pharmacological assays extend these capabilities, enabling comprehensive screening through treating an organism as a single laboratory unit. (Gao et al., 2021; Foster et al., 2022; Das et al., 2025) Such studies are generally restricted to in vivo testing since the study of inter-related organs within a single vasculature is impracticable in vitro. In vivo models—such as mice, rats, and rabbits—are widely used because their metabolic and immune systems closely mimic those of humans. The choice of species is influenced by the specific class of drug undergoing evaluation (Leung, 2009). Perfused organs represent hybrid in vitro and in vivo systems, as an organ is maintained outside the body but under physiological conditions through perfusion of selected carrier solutions; they are invaluable when only a portion of the human biological system is of interest. (Tatum et al.2021). Many ultra-high-throughput screening methods involve "black-box" biological systems that fail to reflect whole-body physiology. Even for more open methods, cellular environments have significant deficiencies when compared with real systems. Thus, a more vivid understanding of the physiological action of drugs requires advancing beyond the use of cells towards whole-organism scenarios that provide definitive therapeutic evidence without ambiguous extrapolation. (Singh et al., 2024; Qian et al.2025;Galus, 2023) After synthesis, lead compounds proceed directly to in vivo testing, although noteworthy concerns regarding ethical, cost, and regulatory issues govern the conduct of such studies. By subjecting the model to "normal dynamic capacity," a three-dimensional model becomes suitable for in vivo testing since the companion principle of continuous flow in the experimental environment mirrors the in vivo organ situation. Experimental in vivo testing involving animals such as mice, rats, and rabbit utilizes the fundamental three-dimensional dynamic systems established by the drug design method to yield insight into systemic pharmacological actions. (Rhazouani et al.2021; Sousa et al.2021; Grams et al.2024;van et al.2022;Santi et al., 2021).

6.3. Toxicology Studies

Toxicology studies are undertaken to consider the pharmaceutical implications of the products examined in biological testing. The toxicity and environmental impact of the chemicals must be determined before candidate drugs enter the market. In a recent example, toxicity concerns led to the abandonment of a new β-adrenoceptor blocker now in late-phase clinical trials. However, it is extremely difficult for regulators to judge the risk involved in brand-new compounds when there is little prior experience to draw upon. (Esler et al.2022; Cantón et al., 2022; Humphries et al., 2024). It is instructive to review some of the major drug disasters. These warn of the potential dangers in the creative process and reinforce the need to restrict testing in humans to only that of compounds with sufficiently low risk. (Williams et al.2025; Henderson et al., 2024) For any drug to be marketed it must be approved by appropriate authorities, such as the FDA in the USA. Before approval a series of clinical trials are required. Phase I trials test safety and pharmacology in normal human volunteers; phase II trials test efficacy in a limited number of patients; and in phase III trials the new drug is compared with existing treatments in a larger number of patients. (Wassermann et al.2022; Esler et al.2022; Humphries et al., 2024).

8. Regulatory Considerations

Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) is a European Union regulation dated 18 December 2006. REACH addresses the production and use of chemical substances and their potential impacts on both human health and the environment. (Wassermann et al.2022; Esler et al.2022; Williams et al.2025). In the United States, the Environmental Protection Agency (EPA) executes legislation to prevent harm from chemicals. (Wassermann et al.2022) The Federal Food, Drug, and Cosmetic Act prohibits the sale of any drug before a New Drug Application

(NDA) is approved by the Food and Drug Administration (FDA), ensuring "authentication of the safety and effectiveness" of the drug (Aurigemma et al., 2005).

8.1. FDA Approval Process

The United States Food and Drug Administration (FDA) plays a critical role in drug discovery development including that of novel pharmaceutics and the assessment of proarrhythmia potential (Thind & R. Kowey, 2020). From discovery and laboratory testing to approval, the entire development process seeks to ensure patient safety and drug efficacy. Initial laboratory efforts aim to identify promising compounds, followed by bench research and in vitro studies to evaluate pharmacokinetics and therapeutic potential. (Humphries et al., 2024; Esler et al.2022)Drug candidates with favorable profiles then proceed to preclinical in vivo testing to determine safety and establish an initial human dosing regimen. The first formal interaction with the FDA occurs when the drug sponsor submits an Investigational New Drug (IND) application containing toxicity and pharmacology data to obtain authorization for human testing. Both FDA and institutional review board approvals are mandatory before initiating clinical trials. (Neumann et al., 2023; Tuzer, 2023).

8.2. Clinical Trials Phases

New drugs must obtain the permission of the Food and Drug Administration (FDA) before they can be marketed, and depending on the chemical structure, therapeutic indication, toxicological profile, and previous FDA experience, the approval process can range from three to six months. In practice the timescale connected with approval procedures is more likely to be larger—in the order of years. The final stage of the whole process consists in clinical trials, which are a thorough examination of a drug candidate in humans. (Kintscher et al.2022; Neumann et al., 2023; Baizabal-Carvallo & Morgan, 2022). Clinical testing can be divided into three phases. Phase 1 trials provide a profile of safety and tolerability, including the determination of the safe dose range in a small number of normal volunteers or patients. Phase 2 clinical trials provide preliminary evidence of efficacy against the condition in question. Phase 3 trials are conducted on a large scale and are designed to provide evidence to satisfy authorities wishing to grant marketing approval and those wishing to use the new treatment. These trials may involve thousands of patients receiving the test drug and include a control group of patients receiving standard treatment or placebo. (Gziut & Wiltshire, 2024; Tuzer, 2023; Baizabal-Carvallo & Morgan, 2022; Merino et al.2025).

9. Challenges in Drug Design

Drug resistance remains a significant issue in the pharmaceutical industry, compounded by limited sales opportunities for many potential new medications. Drug plays a crucial role in personal well-being and social relationships. Pharmaceutical companies frequently request designs for compounds that maintain effectiveness against resistant target proteins or that bind to protein regions with a lower tendency to mutate (R. Flower, 2022). Scope for investors, healthcare providers, and policymakers to have confidence in the projected social value of new agents is lost. The level of risk is so great, broadly, that there are systemic impediments to the generation of truly transformative products (Biala et al., 2023).

9.1. Drug Resistance

Drug resistance reduces drug efficacy in curing diseases and represents a major health hazard (Khalid, 2017). Resistance to chemotherapy may be intrinsic, pre-existing in cells, or acquired after treatment. Tumor heterogeneity, whereby different cancer cells vary in gene expression and metabolism, impedes effective cancer treatment and highlights the importance of pharmacogenomics. Strategies to combat drug resistance include changing first-, second-,

or third-line therapies and employing drug combinations. (Merino et al.2025) Redox regulation also contributes to resistance by causing protein oxidation and dysfunction. The most common mechanism involves point mutations in drug targets that alter amino acids and diminish drug effectiveness. (Ngcobo, 2025; Henderson et al., 2024).

9.2. Market Challenges

The evolving role of the pharmaceutical market poses challenges for drug design. Billions of patients require a wider range of drugs at affordable prices, while legislation, particularly in Europe, tightens regulations on clinical trials and drugs on the market. The market is changing drastically: a decline is expected in the sales of blockbuster drugs, with small niche markets for orphan diseases emerging, and a shift from treatment to prophylactic and enhancement drugs. (Williams et al.2025; Merino et al.2025). Although the number of new chemical entitites per year is increasing, the costs are rising exponentially, net sales are declining, and the return on investment has fallen dramatically. In 2016, the average cost to develop a single new drug just passed the $2·5 billion mark. Recent years have seen the patent expiration of many top-selling drugs. (Mitsikostas et al., 2023; Neumann et al., 2023) The drug-development budget is enormous, and pharmaceutical companies must examine new methods to revive their portfolios, be more selective about investment, and discover drugs more rapidly and at a lower cost with an improved probability of success. (Ko, 2022; Albiñana et al.2022)The development cycle is very long—over 10 years for a successful drug—and runs through several major stages: identify a biological target involved in disease; find drug-like molecules that operate on the target; determine the molecules' activity and potency; undergo preclinical testing, clinical trials, and approval procedures; and finally, monitor postmarketing effects. (Lorente et al.2025; Ngui et al.2022).

10. Recent Advances in Drug Design

Biopharmaceuticals and personalized medicine are two rapidly expanding areas that broadly shape the development of drug design and therapeutics (Biala et al., 2023). Biopharmaceuticals encompass a wide variety of protein- and peptide-based therapeutics—ranging from monoclonal antibodies to antigen-binding fragments and nanobodies, hybridoma-derived vaccines, recombinant proteins, deoxyribonucleic acid (DNA)-, ribonucleic acid (RNA)- and messenger RNA (mRNA)-based therapies, polymer- or polysaccharide-based multivalent vaccines, live attenuated viral vectors, cell and gene therapies, and many other (Guerriaud & Kohli, 2022;Ahmad & Pathak, 2023)s (Pawełczyk et al., 2018). Owing to this enormous diversity in composition and molecular architecture, biopharmaceuticals arise as a wellspring of multi-functional therapeutics that offer mechanisms of action not available to small molecules. Personalized medicine also offers a complementary approach to drug design that often fails to deliver highly efficacious therapeutics, and a better understanding of genetic mutations and diseases is urgently needed. (Cucuzza et al.2024; Fralish et al.2024) Given the availability of a large amount of genetic data, the subsequent development of drugs to treat such diseases at the source would greatly reduce the risks associated with more common drug candidates (Sahu et al., 2013). Clinically, personalized medicine attempts to use a patient's molecular genomics to tailor treatment strategies for optimal clinical response, precisely assigning appropriate therapy at the right dose, frequency, and time course, specifically intended to offer the best therapeutic outcome. It permits the more rational utilization of drugs with increased magnitude in terms of therapeutic benefits and reduction in adverse events in addition to providing an improved pharmacoeconomic outcome. (Navaei 2025; Wang & Wang, 2023; Kumar, 2024; Fountzilas et al., 2022)

10.1. Biologics and Biosimilars

Biologics constitute pharmaceutical substances such as vaccines, blood, or blood components derived from recombinant proteins. They include a range of products such as blood and blood components, vaccines, allergenics, somatic cells, gene therapy, tissues, recombinant therapeutic proteins, and living cells used in cell therapies. Biopharmaceuticals represent the fastest growing sector of the pharmaceutical market and play an increasingly crucial role in the therapeutic armamentarium. Driven by limited effectiveness and, in some cases, widespread shortages of small-molecule drugs, biologics stand to displace many over-the-counter and prescription medicines (Haider, 2023; Rahalkar et al.2021; Doan, 2025) (C. Liossis & M. Konstantopoulou, 2019). Biopharmaceuticals are classified into vaccines; blood products, including plasma and plasma-derived proteins such as clotting factors; somatic cells for transplantation; gene therapy; tissues including bone and skin grafts; fusion proteins and monoclonal antibodies (mAbs); recombinant therapeutic proteins including engineered insulin, growth hormones, and interferons; and living cells used in cell therapy. (Geigert 2023; Behera, 2023).

10.2. Personalized Medicine

Personalized medicine applies pharmacogenomic and pharmacogenetic insights to tailor healthcare and drug treatments to individual patients. In the post-genomic era, the ability to tailor treatments to individual patients has become a key goal of medical research. Personalized medicine incorporates the patient's genetic profile—particularly variability in genes influencing drug disposition or response—to identify the optimal drug for each patient and bridge the gap between efficacy and effectiveness (Kumar, 2024;Wang & Wang, 2023;Hoeben et al.2021) (Wang et al., 2018). The Human Genome Project revealed individual heterogeneity in response to treatments for many diseases, such as cancer and asthma. Increased understanding of the molecular basis and changes in the signaling networks of disease coupled with information about individual variability in the genome, protein expression, and protein interactions forms the basis for future design of personalized medicine. (Mohr et al.2024; Maron et al.2021; Wang et al.2023) It is now clear that exploiting data from genomes, proteomes, and molecular interaction networks together with advances in computational simulation and modelling will provide breakthrough opportunities that will revolutionize personalized medicine. (Molla & Bitew, 2024; Hassan et al.2022). More precise therapeutic strategies are based on understanding the effect of individual variants on disease pathogenesis and on the pharmacokinetics and pharmacodynamics of the drugs intended to treat the disease. Here physico-chemical differences resulting from sequence variants and their effect on the structure of three-dimensional protein models are used together with structural bioinformatics tools to assess the impact of particular variants on drug therapy. (Yusuf et al.2023; Kovrlija et al.2024; Donghia et al.2025) Genotyping of these variants typically through high-throughput methods based on next-generation sequencing, alongside experimental and predicted information made available by structural and chemical genomics initiatives, will greatly improve the drug discovery and development processes. (Vincent et al.2022; Burgess et al.2023) The personalized perspective together with the application of the above techniques will play a key role in optimized drug design and in the move towards personalized medicine (Serrano et al.2024; Peng et al., 2021).

11. FUTURE TRENDS IN DRUG DEVELOPMENT

Many recent advances in drug design have already been made; indeed, such a focus may be part of any timely analysis. The growing use of biopharmaceuticals, which largely involve antigen–receptor type interactions, means that drugs can be described, at least in an initial way, by their three-dimensional structure and the nature of their chemical, electrostatic, or other charges. (Cunha et al.2025; García-Silva et al.2025; Kumar & Nixon, 2025) Molecular modeling

has therefore become increasingly valuable in the discovery, design, and development of new drugs or in the investigation of drug–receptor interactions. (Oostindie et al., 2022). Disease-targeted drugs may be in accord with an increased general knowledge of human biochemistry and the processes involved in disease states; the new insights gained may drive each new therapeutic area. There have also been promising breakthroughs focusing on the synthesis and biological activity of personalized medicine (Doneva et al., 2021; Oostindie et al., 2022). Predictions of future trends in drug design are, in a large part, dependent on the development of new drug-testing protocols. The groundbreaking nature of such very recent proposals suggests that drug design may become more automated or, at least, assisted, both in terms of the synthesis of new drugs and the biological testing of these potential therapeutic agents. (Oostindie et al., 2022; Cunha et al.2025; García-Silva et al.2025).

11.1. Artificial Intelligence in Drug Design

The drug discovery and development process consumes significant time and resources. In addition to high time consumption and production costs, the process suffers from inefficiencies, inaccurate delivery to the target, and inappropriate dosages. The integration of computer-aided drug design with artificial intelligence (AI) algorithms promises to mitigate these issues. (Vergara et al.2023; Wang et al.2025) AI encompasses machine learning, which includes supervised learning, unsupervised learning, and reinforcement learning, while deep learning represents a particularly prominent subset widely used in drug design. Algorithms such as artificial neural networks, support vector machines, generative adversarial networks, and meta-learning find application throughout the drug discovery pipeline. (Yu et al.2024; Shiraishi, 2025). AI techniques contribute to numerous tasks, including peptide synthesis, molecule design, virtual screening, molecular docking, quantitative structure–activity relationship analysis, drug repositioning, investigations of protein misfolding and protein–protein interactions, molecular pathway identification, and polypharmacology. (Doneva et al., 2021; Suh et al., 2022; Yu et al.2024) Furthermore, AI aids in distinguishing active from inactive compounds, monitoring drug release, supporting preclinical and clinical development, facilitating primary and secondary screening, developing biomarkers, optimizing pharmaceutical manufacturing, predicting bioactivity and toxicity, and elucidating modes of action (Geigert 2023; Yu et al.2024) (Gupta et al., 2021).

11.2. Nanotechnology Applications

Nanotechnology is beginning to play a key role in many areas of medicine. Nanotechnology involves the dimensions of about 1—100 nm, where the very small size provides special transport and targeting potential for drugs. Several types of nano-sized materials have been developed, and the potential for drug development is becoming evident. (Thakur & Thakur, 2022; Sim & Wong, 2021; Haleem et al., 2023) Liposomes and albumin-based nanoparticles are being employed commercially to improve the action of existing drugs. New nanoscale technologies, such as nanoshells and nanocapsules, are under development for diagnostic and drug delivery demands. Magnetically targetable nanoparticle conjugates offer attractive potential for highly selective drug delivery and precise drug targeting. These conjugates consist of superparamagnetic maghemite (γ-Fe2O3) nanoparticles to which target-specific groups (e.g., antigens, antibodies, hormones, attachment proteins, etc.) and therapeutic components (e.g., cytostatic drugs, toxins, photosensitizers, radionuclides, etc.) are covalently bound. Other promising nanosystems being exploited for drug delivery include colloidal carriers such as microemulsions, micelles, and dendrimers. (Teixeira et al., 2022; Taguchi et al.2021; Spada et al.2021; Tincu et al., 2023; Wu et al.2024).

12. CASE STUDIES IN DRUG DESIGN

Case studies help identify key trends in drug design and development. In the past 50 years, rapid improvements have been made in the entire drug development process, including discovery, design, synthesis, analytical methods, purification, formulation, pharmacology, toxicology, and marketing. The discovery and design stage has undergone automation and miniaturization, enabling high-throughput screening of compound libraries. Molecular modeling is one approach used to sense molecular interactions computationally (Blanco-Gonzalez et al.2023; Singh et al.2023; Biala et al., 2023).

Despite improvements, numerous challenges remain during the development process. Key factors include early detection of non-viable candidates, precise patient selection for clinical studies, and speedier progression through clinical trials. (Bano et al.2023; Dartois & Rubin, 2022; Madabushi et al.2022).

12.1. Successful Drug Launches

Following the outline provided in Research in the Field of Drug Design and Development (Biala et al., 2023) , which shows that an academic or industrial drug development process consists of three main stages: drug discovery, preclinical development using cell-based and animal models, and clinical trials on humans, culminating in regulatory approval, completed pharmaceutical products of medicinal importance can be found in many databases. (Trucillo, 2021;Singh et al.2023) To identify the most important drugs launched in recent years, the year of launch was set to ">2015," the country of launch was set to "+France +Spain," and the status was set to "launched" established using Cortellis, a database that tracks pharmaceutical drug development. The results are presented in Table 12.1. The most relevant launched products were selected and the name under which they were launched was used where possible. Structure–activity relationships (SAR), molecular design, and the synthesis of some of these agents are described in Case Studies in Drug Design (Section 12.1), focused on examples of the design of successful agents released on the market, and Case Studies in Drug Design (Section 12.2), which illustrates examples in which drugs failed despite all effort. (Bhutani et al.2021; Dahlén et al.2022; Sharma et al., 2023; Feldman et al.2021; Ahmad et al., 2025).

12.2. Failures and Lessons Learned

Failures and Lessons LearnedMany potential new drugs fail late in development because of unforeseen toxicity in clinical trials. There are many examples of such late-stage failures. Fialuridine (FIAU), under development for hepatitis B virus, was found to cause significant liver failure and death; it was, therefore, removed from clinical trials. Zalcitabine (ddC), an antiviral drug for the treatment of HIV infection, had a high association with peripheral neuropathy; this finding led to termination of clinical trials. (Khikhmetova, 2025; Colombo et al.2024; Amorim et al.2024). The failures of these two drugs demonstrate the problem of latent or delayed toxicity and therefore the need for long-term chronic toxicity testing in animal models before clinical trials can proceed. CPT-11 is a prodrug of 7-ethyl-10-hydroxy camptothecin, an inhibitor of topoisomerase I. Although it has entered phase III trials as an anticancer drug, the major side effect of this drug is severe and prolonged diarrhea. Tegafur is a prodrug of 5-fluorouracil developed as an oral agent for the treatment of cancer. It is associated with irreversible central nervous system toxicity, and several cases of death have been reported. These failures indicate that the development strategies for drugs need to be carefully planned to avoid similar problems. (Rana et al.2024; Kokova, 2023; Denny and Stewart 2024; Perše, 2021; Xuan et al., 2023).

13. Ethical Considerations in Drug Development

Ethical considerations are an essential part of every aspect of drug design and development. Pharmaceutical companies conduct controlled clinical drug trials before marketing their drugs and must be observed by national or international regulations. In particular, permissions or approvals of appropriate authorities must be obtained to conduct clinical drug trials with patients and/or healthy human volunteers. Besides, the rights of patients and healthy volunteers must always be protected, with informed consent being a well-accepted system used for this purpose. (Miller & Millum, 2022; Niazi & Mariam, 2023; Chen, 2024; Elendu et al.2023). Although ethical codes of conduct on the clinical use of drugs and the design of drug trials were developed many years ago, human experiments using drugs are often the target of severe criticism in spite of following ethical requirements and fulfilling the criteria of approved guidelines. Distribution of medicine and its availability also present a profound ethical question. It is often difficult to decide whether the drug should be given preferentially and offered on additional priority to certain patient groups or countries. Moreover, in many cases, some population groups may be unintentionally prejudiced against: women and ethnic minorities may be among those frequently discriminated against in clinical trials. (Kramer & Stoicescu, 2021; Kiepek, 2023; Wan et al.2025)Although the United Nations Human Rights Declaration states that every human being has the right to participation in the benefits resulting from scientific advances and their use, it is a fact that most biotechnological products are very expensive, and only a minority of the world's population will be able to afford treatment in the foreseeable future. In the European Union, the Community Code for Medicinal Products and the European Convention on Human Rights and Biomedicine regulate ethical legislation for clinical trials and aids to suffering persons (Joshi & Patel, 2025; Krendyukov, 2025; Kramer & Stoicescu, 2021; Wan et al.2025).

13.1. Clinical Trial Ethics

A clinical trial uses human volunteers to address the safety and efficacy of an investigational new drug (IND). Information gained from a robust investigational new drug application will inform the clinical trial. Almost every drug must go through randomized, controlled, and blinded clinical trials. The ethics of clinical trials can be very complex, especially for trials practiced globally. (Krendyukov, 2025; Schuman, 2021; Kiepek, 2023). To assure the ethical integrity of clinical practices, the Declaration of Helsinki, the Belmont Report, and the standards of the host country are important guides. The Tuskegee syphilis incident remains one of the most controversial studies for research ethics. The study was conducted between 1932 and 1972 by the Public Health Service of the United States of America (USA) to observe the natural history of syphilis in male African-American patients. In 1947, penicillin was widely accepted as a successful treatment for syphilis, but the study continued, and patients were not treated. After the study was revealed, many changes were made; clinical trials were immediately halted and new regulations introduced. These regulations included detailed informed consent forms, the Belmont Report, and the creation of Institutional Review Boards (IRBs) (Abánades et al.2024;Wang et al.2023;Vora et al.2023;D. Steeves et al., 2011).

13.2. Access to Medicines

Research indicates that in most developing countries, between 60% and 90% of the population lacks regular access to medicines in the public health care system.1 Drug market considerations in a given country are affected by myriad circumstances, including population poverty levels, disease endemicity, political framework, advertising and promotional activities by the pharmaceutical industry, trade regulations, local production policies, intellectual patent areas, distribution policies, policy of taxation on drugs, price regulation policies, and the rate at which governments reimburse drugs consumed at hospitals. (Yenet et al.2023; Schulenberg et al.2021; Degenhardt et al., 2023; Maghsoudi

et al.2022). Given the trend toward increasing cost of medicines, the restricted public sector coverage, the importance of medicines in quality care, system crashes in the public sector, and the consequent resort undertaken by patients to the private sector for essential medicines, an inquiry into the availability, pricing, and affordability of key essential medicines becomes of prime importance. A clear understanding of these factors would have practical implications for developing or modifying policies to regulate availability and pricing of essential medicines, particularly in the private sector in the developing countries. (Yenet et al.2023; Lamb, 2022; Maghsoudi et al.2022).

14. CONCLUSION

The evolving discipline of drug design offers invaluable insights into understanding the organism and its pathological processes (Biala et al., 2023). The ultimate goal of drug design is to furnish tools for chemically interacting with biological systems, thereby unveiling the nature of biological processes and providing therapeutic remedies (Sahu et al., 2013). Drug design can be defined as the inventive and imaginative process aiming to identify targeted molecules, as well as potent and selective molecules, to establish the structural reasons for their activity, thereby synthesizing improved drugs for therapeutic purposes. The fascinating activities within this field encompass molecular investigations, data assembly and analysis of three-dimensional molecular structures, drug-indexing and retrieval, computer graphics, quantum chemical and molecular mechanics programs for structure refinement, complex building and docking, crystal structure prediction, spectroscopic and thermodynamic studies, and ongoing experimental feedback. The drug design process represents an attempt to produce molecules with desired biological properties, often serving as powerful molecular tools or pharmaceuticals characterized by appropriate drug-like properties, target selectivity, and minimal side effects. The concepts underlying drug design are the subject of the present chapter, illustrating how these various approaches are applied. Emerging drug design strategies envisage the creation of a named drug referred to by the pharmaceutical industry on the development line. The next phases encompass a multidisciplinary approach to generating new molecules using the “detailed” information synthesized from drug design and knowledge of the target.

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