Modern Trends in Medicinal Chemistry: Techniques, Applications, and Innovations (VOLUME-1)

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About the Book

Modern Trends in Medicinal Chemistry: Techniques, Applications, and Innovations (Volume-1) is a timely and comprehensive compilation of peer-reviewed chapters that collectively reflect the evolving landscape of modern medicinal chemistry. With the convergence of traditional synthetic methods and emerging interdisciplinary technologies, this book provides a scholarly platform for understanding the significant innovations shaping the pharmaceutical sciences today.

This volume features twelve well-researched chapters authored by reputed academicians and scientists. The topics span across advanced drug design, green chemistry applications, natural product-based drug discovery, targeted drug delivery systems, nanotechnology in medicine, and the application of artificial intelligence and computational tools in drug development. Each contribution provides critical insights into the challenges and future directions within its thematic focus, while offering practical perspectives for academic research, clinical translation, and industry relevance.

Designed for postgraduate students, researchers, educators, and professionals in the pharmaceutical and biomedical sectors, this book bridges theoretical frameworks and applied science. It encourages interdisciplinary thinking and highlights global research efforts aimed at enhancing therapeutic outcomes and achieving innovation-driven healthcare solutions. As the first volume of an ongoing series, this book lays a strong foundation for subsequent explorations in the field of medicinal chemistry.

Preface

Medicinal chemistry, once defined narrowly by synthetic organic methodologies and traditional pharmacological approaches, has today blossomed into an expansive, interdisciplinary field at the intersection of chemistry, biology, materials science, and digital technology. The increasing complexity of diseases, the demand for safer and more effective therapeutics, and the pursuit of precision medicine have all fueled the need for innovation at every stage of drug discovery and development. The integration of green chemistry, computational modeling, nanotechnology, and artificial intelligence has not only broadened the scientific toolkit of medicinal chemists but has also redefined the paradigms of modern pharmaceutical research.

This edited volume, Modern Trends in Medicinal Chemistry: Techniques, Applications, and Innovations (Volume-1), brings together a collection of scholarly works that capture the current momentum in this transformative era of medicinal chemistry. The twelve chapters included herein are written by eminent scholars and research professionals who delve into key developments such as targeted drug delivery systems, structure-based drug design, green synthesis, nano-enabled therapies, and AI-driven screening methodologies. Each chapter offers both foundational knowledge and forward-looking perspectives, addressing critical challenges while exploring new frontiers.

One of the key strengths of this volume lies in its thematic diversity. It explores not only the theoretical and experimental aspects of drug development but also presents the strategic relevance of natural products and sustainable practices. Special attention is given to cancer therapeutics, an area of intense global research, with multiple chapters focusing on nanotechnology-based interventions and anticancer drug development. Additionally, the inclusion of chapters on artificial intelligence and computational chemistry reflects the shift toward data-driven discovery models in pharmaceutical sciences.

The primary aim of this book is to serve as a comprehensive academic reference for students, researchers, educators, and industry professionals. It is intended to foster critical thinking, inspire innovative approaches, and provide a panoramic view of the evolving research methodologies and applications in medicinal chemistry. The interdisciplinary nature of the content also encourages collaboration across scientific domains and promotes the advancement of translational research.

We extend our sincere appreciation to all contributing authors for their high-quality research and valuable insights. Their contributions have made this volume a meaningful academic resource. We also acknowledge the reviewers and editorial team whose commitment to scholarly rigor ensured the quality and coherence of the publication.

We hope this book serves as both a reference and an inspiration for further advancements in the fascinating and vital field of medicinal chemistry.

CONTENT

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Modern Trends in Medicinal Chemistry: Techniques, Applications, and Innovations (volume-1)

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Advances in Drug Design: Techniques and Strategies

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Abstract

Drug design is an ancient and intricate pharmaceutical discipline. Since Emil Fisher proposed at the end of the 19th century that the interaction between a medication and its receptor is similar to that between a key and a lock, many advancements have been achieved in the area of drug design. Drug design has steadily evolved into a logical, well-structured discipline with a strong theoretical foundation and real-world applications. Examine the many studies conducted by researchers on drug creation approaches and tactics in this page. According to the review, a number of methods, including metabolomics, genomics, and proteomics, complement other approaches well. Additionally, the most recent drug design techniques can be used to find drug molecules with higher target specificity, accuracy, and safety at a lower cost and in a shorter amount of time. Furthermore, recent drug development efforts across a variety of disorders heavily rely on "Computer-Aided Drug Design (CADD)" methodologies. Computer approaches have significantly accelerated the development and optimisation of potential therapeutic medications.

Keywords: Drug design, Computer-Aided Drug Design (CADD) techniques, Structure-Based Drug Design, Ligand Based Drug Design, Artificial intelligence (AI), drug discovery, etc.

1 Introduction

Medication is a synthetic drug that alters biological functions in order to treat, diagnose, or prevent illness. Drugs may be made synthetically or come from natural sources. In addition to being safe and non-toxic, a drug should have a specific action, minimal side effects, chemical and metabolic stability,

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synthetic feasibility, solubility in water at therapeutic concentrations to avoid bloodstream precipitation, solubility in lipids to facilitate distribution during the body and the ability to cross lipid membranes, and uniqueness [1], [2]. Drugs interact with certain bodily targets to produce their effects. Because of these interactions, two types of impacts are produced: the effects of the drug on the body and the effects of the drug on the body. Pharmacodynamics takes these effects into account, whereas pharmacokinetics does the same [3], [4]. Pharmacodynamics is the study of how drugs work, how concentration and effect are related, and how side effects occur. The study of pharmacokinetics examines the drug's absorption, distribution, metabolism, and excretion over time; these are referred to as ADME processes or ADME characteristics [5], [6].

A. Drug design

The terms "drug design" and "ligand design," which refer to the creation of molecules that will attach firmly to their target, are comparable. Even if design techniques for predicting binding affinity are relatively successful, a number of additional features, such as "bioavailability, metabolic half-life, and side effects", needs to be adjusted before a ligand may become a safe and effective drug [7]. It is often challenging to forecast these additional features using logical design methods. "Drug design," "rational drug design," or simply "rational design" refers to the innovative process of creating new medications by a knowledge of a biological target. In order to provide the patient with a therapeutic advantage, the medication is often a small, organic molecule that stimulates or prevents the function of a biomolecule, such as a protein [8], [9]. In its most basic form, drug design is the process of creating compounds that will attach to a biomolecular target because they are complimentary in shape and charge. Although not always, computer modelling techniques are often utilised in medication design [10]. This kind of modelling is also known as computer-aided drug design. Finally, a technique for developing novel pharmaceuticals, structure-based drug design relies on elucidating the biomolecular target's three-dimensional structure [11]. The class of drugs known as biopharmaceuticals, which includes therapeutic antibodies and peptides in particular, is growing in importance alongside small molecules. Computational techniques have also been developed to increase the stability, selectivity, and affinity of these protein-based treatments [12], [13].

B. Prodrugs and analogues

Analogues and prodrugs are two different kinds of molecules that may be created in drug design to alter the drug molecule.

1. Prodrug

In order to become more active and have effects, prodrugs—inactive or low-activity drug forms—go through chemical or enzymatic transformation in vivo. The prodrug conversion to active is intended to occur at the target location, midway during the absorption phase, or pre-post, depending on the needs. Prodrugs are divided into two categories: bioprecursor prodrugs and carrier-linked prodrugs. During an enzymatic or chemical process, the carrier-linked prodrugs (promoeity) temporarily bind to the active moiety that separates within the body [14]. The bioprecursors are the result of molecular conversion of

an inactivated moiety and do not exhibit promoeity, while these prodrugs primarily consist of ester and amid, phosphate, carbamates, and oximes, among others. Within the organism, metabolic conversion transforms the bio-precursors into the active moiety. Prodrugs enhance medication delivery to the brain and allow the active component to be metabolised naturally. Parkinson's disease is treated with L-dopa, a traditional example of a prodrug. Dopamine is very hydrophilic and vulnerable to enzymes in the brain's epithelial cells, which limits its absorption [9].

2. Analogue design

Creating a new molecule that is physiologically comparable to the original therapeutic molecule is known as analogue design. Analogue molecules have better qualities than native ones. In the field of drug development, this method is useful, straightforward, and widely used. Sixty-six percent of small molecules are made using this technique, and several analogue-based compounds, including as steroids, prostaglandins, anticancer medications, and antibiotics, have been commercially accessible for the last fifty years. Before the project is started, the pharmacokinetic and hazardous aspects are taken into account. Actually, drug-structure repositioning creates new drugs in new fabrics, while analogue design creates new chemical entities [9], [15].

2 Literature Review

(Niazi & Mariam, 2024) [16] Computer-Aided Drug Design (CADD), which bridges the fields of biology and technology, is a revolutionary force in the ever-changing field of drug development. This paper covers the history of CADD, how it was classified in structure-based and ligand-based approaches, and how important it is for expediting and simplifying drug discovery. As CADD develops, protecting data privacy and integrating a variety of biological data become critical. There are still issues that need strong ethical frameworks and algorithm optimisation. In order to create a healthier, more promising future for drug development, this paper's conclusion emphasises the need of taking proactive steps in traversing the ethical, technical, and pedagogical boundaries of CADD.

(Ouma et al., 2024) [17] provides information on computational resources for ab initio and silico approaches and methods, such as AI uses for drug discovery and drug metabolism estimates for drug design. MD, molecular docking, QM, QM/MM, and DFT are computational techniques for drug design and development. Thus, the developing approach of synergistically combining various techniques affects traditional treatments for complicated disorders. We address ligand- and structure-based drug discovery, MD simulation force field models, docking techniques, and subtractive and additive QM/MM coupling. Docking and virtual screening, scoring functions, hit optimisation, and ADMET property assessment will be the focus as computer-aided drug (CADD) approaches improve. Based on recent results, computational tools will help find new molecules with good therapeutic effectiveness.

(Gupta et al., 2024) [18] highlights the many computational methods used in the process of in silico aided drug discovery. “Quantitative Structure-Activity Relationship (QSAR) models”, molecular docking, molecular dynamics simulations, and artificial intelligence-based techniques are all essential

for accelerating drug discovery and optimisation. With a focus on their advantages, disadvantages, and possible future paths, this study critically assesses the status of computational approaches in silico aided drug creation. The field of pharmaceutical research has seen a substantial transformation as a result of the use of computational methods into drug discovery. For the quick and efficient discovery of new therapeutic medicines, the combination of in vitro and in silico techniques offers great potential as these techniques advance, closing the gap between computational predictions and experimental validations.

(Naithani & Guleria, 2024) [19] examines the diverse range of integrated computational approaches used in the assessment and discovery of lead compounds. "Molecular modelling, drug-target interaction analysis, cheminformatics, structure-based drug design (SBDD), molecular dynamics simulations, high-throughput screening, and ADMET (absorption, distribution, metabolism, excretion, and toxicity)" computation are some of the techniques that fall under this category. In order to create new therapeutic agents to address a variety of medical problems, this review reveals the vital role of integrative computational methods and highlights how they can transform drug discovery into a more efficient, cost-effective, and target-oriented endeavour.

(Elizabeth & Amalia, 2022) [20] "Structure-Based Drug Design and Ligand Based Drug Design" are two computational drug discovery techniques that have been shown to speed up and improve the likelihood of discovering novel medications. The purpose of this article is to provide a summary of several methods for developing new drugs, with a focus on the advantages of computational methods. The two computational approaches are discussed in this paper, with a focus on their application, which should help the drug research and development industry become more cost- and time-efficient. The drug discovery stage may be shortened to 9–13 years by using computational approaches, while the usual method to new drug development takes around 11–16 years.

(Dheeraj Bisht et al., 2020) [9] Researchers are working on structure-guided drug design utilising a three-dimensional target structure. The drug molecule found by target-based drug design has a lot of promise to prevent different illnesses, but it also has a lot of negative effects. In order to develop a promising therapeutic candidate, this paper delves deeply into the ways in which a multidisciplinary approach to "combinatorial chemistry, gene expression research, structure-based drug design, and artificial intelligence-based drug design" may be used. In the future, creating new medication candidates would need increasingly advanced computer-based techniques.

(Ferreira et al., 2015) [21] Combining experimental and computational methods has proven very beneficial in the discovery and creation of new, promising molecules. In contemporary drug design, molecular docking techniques are widely used to investigate the ligand conformations that are incorporated into the binding sites of macromolecular targets. The ligand-receptor binding free energy is also estimated using this method by assessing important events related to the intermolecular recognition process. These days, there are many different docking algorithms accessible, so knowing the benefits and drawbacks of each approach is crucial for creating strategies that work and producing results that are pertinent. This review's objective is to analyse current molecular docking techniques used in

medicinal chemistry and drug development, examining the field's advancements and the function of combining structure- and ligand-based approaches.

3 Conclusion

The advancements in drug design have revolutionized pharmaceutical research, enabling the discovery of more precise, safe, and cost-effective therapeutic agents. Techniques such as genome expression profiling, metabolomics, genomics, and proteomics, coupled with high-throughput screening, have enhanced target specificity and reduced drug discovery timelines. Structure-based drug design has significantly improved ligand efficiency, while computational methods, including Computer-Aided Drug Design (CADD), have accelerated drug optimization. By accurately forecasting medication interactions and processes, the combination of deep learning and artificial intelligence (AI) has further revolutionised drug research. Even more computational power might be available with quantum computing, which could improve drug design techniques. These advancements have strengthened the pharmaceutical industry's ability to develop treatments for complex diseases with unprecedented efficiency. The synergistic application of computational tools and AI not only enhances drug development but also aligns with the United Nations' Sustainable Development Goal 3, promoting global health and well-being. As drug design continues to evolve, these cutting-edge approaches will drive the development of novel therapeutics, ultimately improving patient outcomes and advancing medical science.

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Targeted Drug Delivery Systems: Current Trends and Future Prospects

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Abstract

The majority of dosage forms available today have subpar biopharmaceutical and pharmacokinetic qualities. In order to prevent harm to other tissues or organs, a suitable "drug delivery system" that delivers the active drug molecule only to the site of action has to be created. A technique for giving medications to patients at the intended location or site of action is called targeted drug delivery. Targeted drug delivery is one of the most innovative approaches to sickness diagnosis and treatment in the medical sciences. Review the many studies on current developments and potential future directions in targeted drugs delivery systems in this article. The review found that TDD improves treatment effectiveness by reducing side effects and dose requires. To improve medication transport and release, a variety of carriers have been investigated, including as nanoparticles, liposomes, micelles, and biodegradable polymers. Effectively targeting many tumour locations is still a difficulty in cancer therapy, despite attempts to create highly selective delivery methods. It is expected that as TDD systems develop, they will play a bigger part in treating complicated illnesses including cancer, neurological problems, and autoimmune issues, opening up new possibilities in precision medicine.

Keywords: Targeted drug delivery systems (TDD), Diagnosis and treatment of diseases, Nanomaterial-based drug delivery systems (NBDDS), Active and passive targeting, Conventional drug delivery systems (DDS), Nanocarriers, etc.

1 Introduction

The body uses drug delivery systems (DDS) to distribute therapeutic medications as required to safely provide the intended therapeutic effect. These systems are often created to lower adverse effects, boost

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pharmacological effectiveness, and enhance the active compounds' water solubility and chemical stability [1], [2]. The first sustained release version of Dexedrine was produced in the 1950s, and since then, modern drug delivery technologies have continuously advanced. Targeting the biological location with therapeutic medication concentrations and maintaining them is the aim of every drug delivery method. In recent years, nanoparticles have shown significant promise as carriers in current medication delivery methods [3], [4]. Encapsulating medications in nanoparticles, such as liposomes, dendrimers, nanocapsules, nanospheres, and micelles, among others, increases the therapeutic index and lowers the negative side effects [5].

A. Targeted Drug Delivery

A medicine may be delivered to a particular organ, tissue, cell, or receptor using a technique called targeted drug delivery (TDD). By lowering cytotoxicity to healthy cells and increasing the medication's bioavailability and effectiveness, this lowers the dose necessary in comparison to standard drug delivery [6]. In vitro and in vivo, TDD systems should ideally be chemically and physically stable, non-immunogenic, and biochemically inert (non-toxic). In addition to having uniform capillary distribution, they must to have restricted drug distribution to specific cells, tissues, or organs [7]. The pharmacological action of TDD should not be dependent on the release kinetics, and the rate of drug release should be predictable and controlled [8]. It should deliver a therapeutic dose of medication with little to no leaking while in transportation. Utilising carriers that are biodegradable or easily removed from the body is recommended. It should be straightforward or very simple to prepare the distribution system, reproducible, and economical [9][10].

B. Strategies for drug targeting

Drug targeting may be approached in several ways, some of which include [11]:

Passive targeting: Passive targeting is the term used to describe drug delivery techniques that seek to distribute the medication into the systemic circulation. The body responds to the medication's physicochemical characteristics or the drug delivery system's ability to trap the drug until it reaches the target spot by passively targeting it.

Active targeting: With this approach, the medication is targeted once the target group has been identified and affixed to the drug delivery system's surface by the target cells' receptors. Albumin protein, bioadhesive nonionic surfactants, and antibodies are examples of the target group. There are three categories of active targeting: intracellular targeting, cell targeting, and first-order targeting, which is also known as organ targeting.

Inverse targeting: Its objective is to stop the medication delivery technique from being passively absorbed by the reticulum-endothelial system (RES). Large molecules of dextran sulphate or a large quantity of the blank drug delivery system may be injected to block the normal uptake function of RES, resulting in a saturation of RES and the suppression of the defence mechanism. For medication targeting to non-RES organs, inverse targeting is particularly helpful.

Ligand mediated targeting: Both synthetic micro-emulsions of low-density lipoprotein (LDL) particles coated with Apo proteins and natural LDL particle receptor uptake are necessary for this kind of medication targeting.

Physical targeting: In order to target medication delivery systems to a specific place, the physical targeting approach aims to modify them externally. Applying an electric field, altering the pH, and changing the temperature are examples of the physical alterations. This approach has great promise for targeting genes and tumours.

Dual targeting: Through a drug delivery system, the dual targeting mechanism increases the therapeutic efficacy by allowing the carrier to work in concert with the entrapped medication. An antiviral drug placed onto a carrier molecule with antiviral action, for example, increases the therapeutic effect.

C. Applications of targeted drug delivery system

- Treatment of cancerous tumours is the most important use of targeted drug delivery, while it is often employed to treat a variety of diseases, including vascuar disorders, polygenic diseases, etc.
- Drugs may be delivered using liposomes to treat illnesses like TB. TB is traditionally treated using skin-to-chemotherapy, which is not very successful. This might be because the chemotherapy does not reach a high enough concentration at the infection site. Better concentration building at the infection site and improved microphage penetration are made possible by the liposome delivery mechanism [12].

2 Literature Review

(Alshammari et al., 2024) [13] provides a thorough grasp of the architecture and physiological environment of the colon while examining the development and efficacy of colon-targeted medication delivery systems. The evaluation offers information about the benefits and possible drawbacks of each application. The research highlights how crucial it is to conduct regulated in vitro drug testing throughout the development stage. The future directions for effective growth in this discipline are also covered. For researchers navigating the ever-changing area of colonic drug administration, this review is an invaluable resource since it integrates information from anatomy, formulation procedures, and evaluation approaches.

(Tiwari et al., 2023) [14] Either passive or aggressive methods are used to direct the medication to the tumour location. Active targeting uses ligand-coated nanoparticles, while passive targeting uses the tumour microenvironment and improved permeability and retention effect. Nanotechnology is being used to detect cancer early on by identifying cancer-specific biomarkers using tumour imaging. Examples of the use of nanotechnology in cancer therapy include the development of "photoinduced nanosensitizers, the reversal of multidrug resistance, and the efficient transport" of RNA molecules and CRISPR/Cas9 for therapeutic reasons. Nevertheless, more research is required in the area of creating and using nanoparticles for better cancer detection, even with the current developments in nano-oncology.

(Cheng et al., 2023) [15] "Nanomaterial-based drug delivery systems (NBDDS)", which have unique physicochemical and biological properties, are often used to improve the safety and therapeutic efficacy of encapsulated drugs. By integrating "therapeutic drugs with nanoparticles" via logical targeting pathways, nano-targeted delivery systems were created to get around the main drawbacks of conventional drug treatment, including poor stability and solubility, a lack of transmembrane transport, a brief circulation time, and undesirable toxic effects. Here, we examined the latest advancements in therapeutic treatments using a variety of nanomaterial-based systems and targeted design methodologies. The difficulties and viewpoints of smart systems in accurately addressing various intravascular and extravascular disorders were also covered.

(Mumtaz et al., 2023) [16] Drugs for the treatment of acute disorders may now be transported in novel ways thanks to nanotechnology, which has made this work easier to do. However, by using nanoparticles as efficient medication transporters, it has been resolved. The main topics of this research are the types and properties of nanomaterials (NMs) used, the drawbacks of conventional "drug delivery systems (DDS)", and the common ways that drugs are administered via the skin. We have listed the most recent advancements in NMs for drug delivery and their mode of action, such as "carbon-based NMs, inorganic/metal-based NMs, polymeric NMs, and hybrid NMs". The present obstacles and difficulties that hinder the transition of nanomaterials from study to practice are also addressed in this paper, along with recommendations for more efficient use of nanomaterials in a variety of diseases.

(J. Li et al., 2023) [17] Significant oncotherapy discoveries and advancements have been made by several experts in this discipline. Additionally, examine new technology and tailored medication delivery approaches to improve oncotherapy. We also go over two common medication delivery methods based on different nanocarriers for improving tumour therapy: passive and active targeting. The comparison and fusion of active and passive targeting are also conducted in the meanwhile. The related difficulties of targeted drug delivery methods, both active and passive, are also covered, along with the opportunities for future research.

(Prabahar et al., 2021) [11] The purpose of the targeted drug delivery system in the use of chemotherapeutic medications to treat cancer is to guarantee that the pharmacological activity of the therapeutic agent only affects the diseased organs and does not damage the healthy ones. Medication targeting may be achieved by using various carriers that preserve and deliver the complete medication to a predetermined organ or tissue. A variety of carrier types, including "dendrimers, noisomes, ufasomes, virosomes, cubosomes, nanobots, transferosomes, nanotubes, nanowires, nanoshells, quantum dots, nanopores, gold nanoparticles", and more, may be used for drug targeting. There are several therapeutic targeting strategies, including as "ligand-mediated targeting, physical targeting, inverse targeting, double targeting, dual targeting, active targeting, and passive targeting". A realistic way to deliver a therapeutic chemical to a specific place without putting other organs at risk is drug targeting.

(Dunuweera et al., 2018) [9] A complex method of giving patients their prescriptions in a manner that increases the concentration of the drug only in the targeted organs, tissues, or cells is called targeted drug delivery, or TDD. TDD delivers a least necessary therapeutic agent to a sick body location for a long

duration. This prevents drugs from harming healthy tissue by controlling the amounts of drugs in plasma and tissue. "Neutrophils, fibroblasts, artificial cells, lipoproteins, liposomes, inorganic nanoparticles, magnetic nanoparticles, soluble polymers, biodegradable microsphere polymers (natural and synthetic), and immunological micelles" are examples of drug carriers found in advanced delivery systems. When selecting a vehicle, one should take into account side effects or cytotoxicity to healthy cells, the chemical and physical characteristics of pharmaceuticals, the drug delivery route, the intended site, and disease. Thus, TDD formulations take into account target cell features, indicators or transport carriers that deliver drugs to receptors, ligands, and physically regulated components.

(Kumar et al., 2017) [18] Delivering medications to patients at the intended location or site of action is known as targeted drug delivery. By lessening the negative effects of the medication, this increases therapy effectiveness. This method's intrinsic benefit results in the necessary medication being administered at a lower dosage with fewer adverse effects. Lipoproteins, liposomes, and microspheres are among the several drug carriers that may be used in this advanced delivery method. The current review addresses the research update on targeted drug delivery systems, as well as its benefits, drawbacks, and need.

(Thakur et al., 2015) [19] The latest developments in drug delivery systems mostly centre on intelligent drug delivery systems, which address the safe and effective distribution of drugs at the appropriate time and dosage. A smart drug delivery system includes the use of hydrogels, nanoparticles, and microencapsulation methods. Drugs ranging from painkillers to chemotherapy may be delivered using nanoparticles, which can be inserted into the skin, brain, or spinal cord. Because of their connection to self-regulation and controlled time drug monitoring systems, these new developments in drug delivery systems have therefore shown to be methods for improving health in the future.

3 Conclusion

A cutting-edge method in medical research for accurate illness detection and therapy is targeted drug delivery, or TDD. By ensuring drug molecules reach specific sites within the body, TDD minimizes dosage requirements and reduces side effects, enhancing therapeutic efficacy. Various carriers, including nanoparticles, liposomes, micelles, and biodegradable polymers, have been explored to optimize drug transport and release. The advent of advanced technologies such as 3D printing has further enabled personalized medicine by controlling drug release kinetics. In cancer treatment, despite efforts to develop highly selective delivery mechanisms, challenges remain in effectively targeting multiple tumor sites. Nanocomposites and nanoarchitectures offer promising solutions, enabling controlled drug interactions at targeted locations. Moreover, biodegradable nanomaterials facilitate sustained and localized drug release, improving treatment outcomes. The continuous advancements in TDD systems, including dual-drug delivery and bioengineered carriers, present new opportunities for enhanced therapeutic strategies. Future research should focus on refining drug targeting precision, minimizing off-target effects, and exploring novel biomaterials to improve drug stability and efficacy. As TDD systems evolve, their role

in treating complex diseases such as cancer, neurological disorders, and autoimmune conditions is expected to expand, offering a new frontier in precision medicine.

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Green Chemistry Approaches in Medicinal Chemistry

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Abstract

One area of study that has gained global interest in analytical chemistry is "green chemistry." Green analytical innovations have been put forward to reduce toxicity without compromising analytical performance. This could be shown at every stage of the analysis by reducing operational risk and contamination of the environment via reduced chemical use and waste production. In this article, review the various researcher's study on green chemistry approaches in medicinal chemistry. The article concluded that green nanotechnology plays a crucial role in therapeutic advancements, including antidiabetic and anticancer treatments, by facilitating targeted drug delivery with reduced toxicity to healthy tissues. The development of green analytical methodologies, assessed through tools like GAPI and Eco-Scale, further supports sustainable pharmaceutical practices. green chemistry offers a sustainable approach to pharmaceutical R&D, reducing environmental impact while maintaining high efficacy in drug design. With continued innovation and investment, green chemistry is set to transform medicinal chemistry, ensuring safer and more sustainable drug development for the future.

Keywords; Green chemistry approaches, Medicinal chemistry, Drug design, Green solvents, Nanoparticles, Pharmaceutical chemistry, Green nanotechnology, etc.

1 Introduction

To increase environmental protection and the economics of chemical manufacture, new chemistry is needed. For creative chemistry research and applications, chemists, researchers, and industry leaders find the green chemistry notion to be an alluring technology. First and foremost, green

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chemistry is defined as minimising environmental harm when producing materials and minimising and appropriately disposing of waste produced during various chemical processes [1]. A other definition of green chemistry is a novel approach to the synthesis, processing, and use of chemical resources in a way that reduces risks to the environment and people [2]. The concept of green chemistry has given rise to a number of new terms, including eco-efficiency, sustainable chemistry, atom economy or efficiency, process intensification and integration, inherent safety, product life cycle analysis, ionic liquids, alternative feedstocks, and renewable energy sources [3]. Therefore, there is a pressing need to advance synthetic and engineering chemistry, either by employing environmentally benign starting materials or by carefully planning innovative synthesis pathways that leverage contemporary energy sources to produce less harmful compounds [4], [5].

A. Green chemistry

An field of chemical engineering and chemistry known as "green chemistry," or "sustainable chemistry," is concerned with creating goods and procedures that utilise and produce fewer or no hazardous materials. A number of pre-existing concepts and research initiatives (such as atom economy and catalysis) gave rise to green chemistry in the years before the 1990s, when concerns about resource depletion and chemical pollution gained more attention [6]. Green chemistry's rise in both Europe and the US was associated with a change in how environmental issues were approached: from command-and-control regulation and the requirement to cut industrial emissions at the "end of the pipe," to actively preventing pollution by innovatively designing production technologies [7]. In the middle to late 1990s, the group of ideas that are today known as "green chemistry" came together, and the phrase itself gained popularity, defeating rival names like "clean" and "sustainable" chemistry [8]. Through its financing, professional coordination, and pollution control initiatives, the Environmental Protection Agency spearheaded the development of green chemistry in the United States. University of York academics helped launch the journal Green Chemistry and create the Green Chemistry Network inside the Royal Society of Chemistry in the United Kingdom at the same time [4].

B. The impact of green chemistry on the environment and population

By lowering the amount of resources required to perform analytical procedures, including solvents, solutions, water, and organic compounds, as well as their storage, green chemistry makes a significant contribution to the economy. The use of GAC in pharmaceutical analysis makes it possible to replace hazardous compounds with safe and sustainable substitutes, resulting in the transition from waste to clean waste [9]. A significant impact on environmental samples and undesired environmental elements has been seen as a result of the current surge in analytical activity. Pharmaceutical analysis residues must be recycled and pre-treated in order to be released back into the environment with the fewest possible negative consequences. However, these procedures are costly, which raises additional financial concerns that scientists should be mindful of [10]. Thus, it is necessary to recycle both online and offline, with the added advantage of recovering expensive and hazardous chemicals. Recycling shouldn't, however, lower the sample throughput or

compromise the techniques' accuracy and precision. However, the population is affected by pharmaceutical activity in a variety of ways and across a range of fronts. Various analytical methods, reagents, solvents, operators, and strategies that affect the patient are used to make medication [11].

C. Importance of sustainable synthesis of biologically active compounds

Green synthesis uses renewable energy sources to generate electricity while maximising consumption and minimising energy waste. Pharmaceutical companies generate 1.27 trillion dollars a year, making them the top contributors to the world economy. However, they also contribute significantly to the carbon footprint, generating more than 1.9 million tonnes of CO2 yearly. Ten years ago, the concept of environmental preservation was originally put out, but due to a lack of industrial participation, many of the programs failed. Controlling production and identifying processes to reduce their environmental effect have always been goals of the industrial nations, but these industries were never satisfied with the earlier ideas [12].

D. Relevance of Green Chemistry in Medicinal Chemistry

Green chemistry plays a crucial role in medicinal chemistry by promoting environmentally friendly practices in the synthesis, design, and production of pharmaceutical compounds. By using renewable feedstocks and atom economy, the environmental impact of drug production is reduced and efficiency is raised. Additionally, cleaner chemicals and solvents lead to fewer hazardous drugs, improving environmental outcomes and patient safety. Green chemistry helps medicinal chemists create more sanitary synthetic routes for active pharmaceutical agents (APIs). The industry decreases unwanted byproducts by replacing more hazardous chemicals with safer ones and using catalysis to boost reaction efficiency [13].

E. Reduction of hazardous waste in pharmaceutical production

The use of more environmentally friendly synthesis techniques greatly lowers the amount of hazardous waste generated during the manufacturing of pharmaceuticals. For instance, it has been shown that using flow chemistry and microwave-assisted synthesis improves reaction efficiency and reduces waste production. Compared to conventional batch procedures, flow chemistry allows for exact control over reaction conditions, which results in greater yields and fewer byproducts. Furthermore, since enzymes may be extremely selective and usually function in moderate environments, biocatalysis often produces less harmful byproducts, improving atom economy and reducing environmental impact [12].

2 Literature Review

(Gavanaroudi, 2024) [14] To address this significant flaw, the creation of nanoparticles from microbes or plants may be helpful in creating biocompatible nanoparticles. Utilising plant extracts to create nanoparticles simplifies and expedites the synthesis process. In actuality, the production of nanoparticles may be accomplished without the requirement to grow and preserve cells thanks to extracellular synthesis. To date, the production of metal nanoparticles, particularly gold, has been accomplished by

the use of plant extracts. Examples of these plants include cinnamon, eucalyptus black tea, and sweet root.

(KHAN A et al., 2024) [8] As environmental safety becomes more of a concern, green chemistry is growing rapidly, and chemists are finding it more and more challenging to create new goods, processes, and services that satisfy the social, financial, and environmental requirements. Current green chemistry and its use in illness treatments are briefly discussed in this article, along with green chemistry in nanotechnology. The elements influencing the environmentally friendly production of nanoparticles are also covered. An overview of the present state of green chemistry and its application to pharmaceutical chemistry, toxicology, and pharmacology is provided in this study.

(Onagun & Gbenga, 2024) [12] investigates innovative green chemistry techniques, with a focus on waste minimisation, atom economy, and the use of renewable feedstocks to create biologically active chemicals. Safer solvent substitutes, flow chemistry, and biocatalysis are important developments that show the way to effective, less harmful medication manufacturing. These sustainable approaches have a great deal of promise to lessen the environmental toxicity and carbon footprint of pharmaceuticals, while being hindered by industrial and governmental limitations. The industry may enhance public health, solve urgent ecological issues, and promote a paradigm change towards sustainable pharmaceutical manufacture by using green approaches.

(Parvez et al., 2023) [15] Green chemistry has gained traction and been embraced by the organic and pharmaceutical industries. In order to reduce waste, use renewable resources, create biodegradable materials, and use less energy, Green Chemistry was established. Green chemistry examined the different chemical-related catastrophes brought on by toxicity (whether they were cancerous or explosive), physical hazards (whether they were flammable or explosive), and worldwide threats. (Depletion of stratospheric ozone or climate change). Green chemistry's guiding principles fall into two categories: "Reducing Risk" and "Minimising the Environmental Footprint." This particular study offers a succinct overview of current developments and applications of green chemistry concepts to daily tasks, chemical reactions, economics, pharmacy procedures, and analytical chemistry to produce new drug molecules.

(Rubab et al., 2022) [16] By creating environmentally friendly catalysts, green solvents, using microwave and ultrasonic radiation, solvent-free, grinding, and chemo-mechanical techniques, synthetic chemists can overcome the challenges of conventional synthesis, including slow reaction rates, unhealthy solvents and catalysts, and lengthy reaction completion times. A preferred structural motif with a variety of pharmacological and medical uses, 1,2,4-thiadiazole is a member of the class of heterocycles combining nitrogen and sulphur. In order to build various 1,2,4-thiadiazole scaffolds, this thorough review systematises the types of green solvents, green catalysts, ideal green organic synthesis characteristics, and green synthetic approaches like microwave irradiation, ultrasound, ionic liquids, solvent-free, metal-free conditions, green solvents, and heterogeneous catalysis.

(de Marco et al., 2019) [17] An important turning point in the global economic history was the expanding industrialisation process. The development of analytical techniques is one of the most active areas of

research and development in green chemistry, leading to the creation of so-called green analytical chemistry. This paper describes the multifaceted effects of green chemistry on pharmaceutical analysts, the environment, the public, analysts, and companies. Every decision and critical mindset has an impact on the finished product as well as everything around it. This study also considers the future of green chemistry, our future, and the environment.

(Gupta & Mahajan, 2015) [18] The rapidly evolving discipline of "green chemistry" offers a path towards the sustainable advancement of science and technology in the future. It may be used to create synthetic delivery systems that are safe for the environment and can save lives while delivering life-saving medications. Chemical engineers and chemists are anticipated to develop more sustainable and environmentally friendly chemical methods for medication design, and this trend is probably going to keep expanding over the next decades. This study outlines environmentally friendly procedures for using the concepts of green chemistry to synthesise certain FDA (Food and Drug Administration)-approved medications that are in high demand and have stringent chemical and optical purity standards.

3 Conclusion

Green chemistry has revolutionized medicinal chemistry by enabling environmentally friendly synthetic processes with minimal toxic byproducts. The green synthesis of nanoparticles using biological sources such as bacteria, fungi, and plant extracts has demonstrated promising applications in disease diagnosis, drug delivery, medical imaging, and environmental remediation. Green nanotechnology plays a crucial role in therapeutic advancements, including antidiabetic and anticancer treatments, by facilitating targeted drug delivery with reduced toxicity to healthy tissues. The development of green analytical methodologies, assessed through tools like GAPI and Eco-Scale, further supports sustainable pharmaceutical practices. Despite its growing acceptance, the full potential of green chemistry in drug manufacturing requires greater investment in education and research. Additionally, a deeper understanding of technical aspects, such as acoustic power and reactor geometry in ultrasound-assisted synthesis, is needed to optimize reaction mechanisms and enhance efficiency. While challenges remain, green chemistry offers a sustainable approach to pharmaceutical R&D, reducing environmental impact while maintaining high efficacy in drug design. With continued innovation and investment, green chemistry is set to transform medicinal chemistry, ensuring safer and more sustainable drug development for the future.

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Advances in Structure-Based Drug Design: Challenges and Opportunities

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Abstract

Drugs for a range of illnesses have been developed with the help of SBDD. Structure-based medication design uses three-dimensional geometric information about macromolecules, including proteins or nucleic acids, to identify suitable ligands. Examine the many studies conducted by researchers on the prospects and difficulties in structure-based medication discovery in this page. This study comes to the conclusion that because of the flexibility of proteins, solvent effects, and important water molecules in target proteins, the existing scoring methods have difficulty properly estimating binding free energy. Improving predictions of protein-ligand interactions still requires addressing these issues. SBDD has a lot of potential to speed up drug development with cutting-edge computational methods, despite these obstacles. Drug-target interaction prediction, ligand binding site identification, and de novo ligand generation provide practical ways to target unknown macromolecular structures. By improving structural refinement, drug association mapping, and protein structure prediction, the use of deep learning into SBDD has created new opportunities. These developments increase the possibility of finding potent medicinal molecules by enabling a more effective search of chemical space.

Keywords: Structure-Based Drug Design (SBDD), Computational techniques, Therapeutic compounds, Drug discovery, Direct drug design, Molecular docking, etc.

1 Introduction

Drug development is still an experimentally rigorous, expensive, and time-consuming process, despite the fact that high-throughput screening (HTS) and whole-cell screens have traditionally been used to

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identify effects that may be proposed into drug candidates according to a particular target, often an important enzyme [1]. However, in contrast to conventional drug discovery, drug design draws on the existing information for a particular biological target rather than relying just on screening enormous libraries, which is inherently a trial-and-error process [2], [3]. Using the target's three-dimensional structure, structure-based drug design, or SBDD, is a well-known method of drug design that finds or improves compounds that have a high affinity and selectivity for binding to the target [4]. From the early days of structural biology, it was clear that structural information could be used to find potential drugs. However, it took several years before the first successful examples, such as HIV protease inhibitors and carbonic anhydrase inhibitors for glaucoma treatment, were achieved [5].

Therefore, SBDD requires a three-dimensional representation of the target. There are several experimental methods for obtaining the structure, but X-ray crystallography is the most common. The resolution revolution saw a dramatic improvement in the resolution capabilities of single-particle cryo-EM, which piqued interest in "nuclear magnetic resonance (NMR) and, more recently, cryo-electron microscopy (cryo-EM)". Targets with challenging experimental structures are also often subjected to in silico structure prediction. This may be accomplished via homology modelling from a closely related homologous protein when suitable models are available [6].

A. Structure-based drug design

Direct drug design, or structure-based drug design, relies on x-ray crystallography and nuclear magnetic resonance spectroscopy-disclosed three-dimensional structures of biological targets. A homology model of a target protein may be constructed using the experimental data of a similar protein in the event that the target protein's experimental structure is not accessible [7]. A medicinal chemist's intuition combined with interactive visualisations may be used to develop candidate drugs that are expected to attach to the biological target with high affinity and selectivity based on the target's structure. As an alternative, new drug candidates may be proposed using a variety of automated computational processes [8].

There are three major groups into which current structure-based drug design techniques may be broadly classified. The first method uses quick approximation docking tools to search through large datasets of small molecule 3D structures for new ligands that fit the binding pocket of a particular receptor. Virtual screening is the term for this technique [9]. The creation of novel ligands is the subject of a second group. Using this technique, ligand molecules are gradually assembled from tiny fragments to build up inside the binding pocket's limitations. These fragments might be single atoms or pieces of molecules. The capacity to suggest novel structures that aren't included in any database is the primary advantage of this strategy. Optimising existing ligands by assessing suggested analogues within the binding cavity is the third technique [10].

B. “Principles of Structure-Based Drug Design (SBDD)’

The foundation of SBDD is the idea of lock-and-key binding, in which a drug molecule attaches itself to a particular location on the target protein in a manner similar to how a key fits into a lock. Depending on the kind of interaction, the drug molecule's binding to the target protein may either inhibit or stimulate

the protein's function [11]. The first step of SBDD is to get the three-dimensional structure of the target protein. Techniques like as X-ray crystallography, cryo-electron microscopy, and nuclear magnetic resonance spectroscopy are all within the realm of possibility. Finding small molecules that can bind to the desired protein as well as alter its function is the next step after determining the protein's structure [12].

One computer method for predicting how tiny compounds would attach to a target protein is called “molecular docking”. The goal of molecular docking is to identify potential ligands for a target protein by searching a database of small molecules for their binding sites. After that, the molecules with the greatest match are chosen for further examination [13]. "Structure-activity relationship (SAR)" study is performed to maximise the specific drugs' interaction to the target protein. In SAR analysis, the compounds' chemical structures are changed, and their ability to interact with the target protein is tested. By comparing the activity of the modified molecules to that of the primary molecule, SAR analysis may help identify the crucial molecular properties required for binding to the desired protein [6].

C. Applications of SBDD

Drugs for a variety of ailments have been successfully developed via SBDD. The creation of protease inhibitors to treat HIV is a prominent example. One enzyme that is essential to the virus's reproduction is HIV protease. Small compounds that could attach to the protease's active site and stop its activity were created using SBDD in order to stop the virus from replicating. Because of this strategy, medications like ritonavir and saquinavir, which are often used to treat HIV, have been developed. Additionally, SBDD has been used in the creation of cancer medications [14]. DNA mutations often seen in cancer cells cause overexpression of certain proteins, which may promote the formation of tumours. In order to delay or halt the development of tumours, SBDD has been utilised to create tiny compounds that can attach to these overexpressed proteins and block their function. "Imatinib, which targets the Bcr-Abl protein in chronic myeloid leukaemia, and vemurafenib", which targets the BRAF protein in melanoma, are two of the cancer drugs developed by SBDD [12].

2 Literature Review

(Batista-Silva et al., 2024) [15] The prognosis for prostate cancer (PCa), one of the most common tumours in males, is dismal due to a lack of appropriate biomarkers or their modulators. In addition to playing a significant part in the initiation and spread of PCa, membrane proteins (MPs) might make appealing therapeutic targets. The successful finding of biomarkers and inhibitors is hampered by experimental difficulties in targeting MPs. Computational techniques may help get beyond this obstacle by screening huge libraries of compounds and providing structural insights, which speeds up lead optimisation and identification. This study aims to investigate new avenues in "computer-aided drug design (CADD)" by identifying the most significant membrane-bound prostate cancer (PCa) indicators using structure-based approaches.

(Giladi et al., 2024) [2] There are still a lot of unanswered questions about the distinct structural and functional characteristics of TSPO ligands in health and illness, even after several classes of ligand

chemotypes have been developed and experimental structures of bacteria and non-human mammals have been clarified. Current computational approaches for simulating the natural structure and ligand-binding activity of this mysterious protein have a number of drawbacks. With this viewpoint, we provide a critical evaluation of the advancements in the use of these techniques, describing their applications, intrinsic drawbacks, and ongoing difficulties. As a means of enhancing our understanding of the TSPO, we suggest unexplored avenues for computational techniques.

(Tang et al., 2024) [8] Growing druglike "make-on-demand" libraries and an ever-increasing number of known and anticipated protein structures need novel computational approaches to structure-based computer-aided drug creation, which is notoriously laborious. By using in silico heuristics, de novo drug design expedites the search in the vast chemical space. Focussing on current developments in structure-based de novo drug design, this study covers everything from deep generative models to evolutionary algorithms, Metropolis Monte Carlo techniques, and traditional fragment-based approaches. As the production of easily accessible drug-like compounds has long been a challenge for de novo drug development, we emphasise the efforts to create synthetic access in each category as well as the benchmarking techniques used to verify the suggested framework.

(Özçelik et al., 2023) [16] Affinity prediction for unknown protein targets, the clarification of "binding mechanisms, and the rationalisation of related chemical kinetic properties" are just a few of the unresolved problems that could be addressed by structure-based drug discovery, even though ligand-based approaches have dominated deep learning efforts in this field. Developments in deep learning techniques and the availability of precise protein tertiary structure predictions support a return to structure-based methods for AI-guided drug development. In this study, the key algorithmic ideas in structure-based deep learning for drug discovery are compiled, and future prospects, uses, and difficulties are anticipated.

(Pliushcheuskaya & Künze, 2023) [10] Computational methods are a vital tool in drug discovery and may expedite lead optimisation and identification, particularly in the early phases of development. This paper covers important facts on ion channels, including their classification, structure, processes, and illness, and focusses on recent advances in computer-aided, structure-based medicine design on ion channels. We highlight research that uses modelling and chemoinformatic techniques in conjunction with structural data to identify and characterise novel compounds that target ion channels. These methods have the potential to significantly improve future ion channel medication development.

(Aplin et al., 2023) [17] prove that structural approaches have now progressed to the stage where they can investigate protein targets' dynamic information. We begin by discussing recent advances in X-ray crystallography techniques, including serial room-temperature crystallography, which allows the analysis of protein-inhibitor complexes with an unparalleled degree of shape-dynamic accuracy. Another high-resolution technique, "cryogenic electron microscopy (cryoEM)", has recently been employed to investigate proteins and protein combinations that are too intricate to crystallise. In conclusion, we introduce small-angle X-ray scattering (SAXS) as a potential high-throughput screening approach for discovering oligomerisation and protein complex inhibitors.

(Bruch et al., 2020) [6] Computer-aided and structure-based drug design methods are generally seen as having been effective in the areas of antiviral and cancer drug discovery, but not so much in the creation of antibacterial drugs. Protein kinase (Pkn) B and PknG, two serine/threonine (Ser/Thr) kinases, have long been thought to be particularly promising targets. One well-known target that has been pharmacologically verified is the DNA gyrase of Mycobacterium TB. These three case studies are the ones studied here. After highlighting some of the difficulties that logical, target-based TB drug discovery efforts continue to encounter, we concluded by talking about the new insights brought about by recent methodological advancements in structural biology and integrative approaches.

(Wang et al., 2018) [18] Computer science's progress serves as an additional incentive that facilitates the effective implementation of computational methods throughout the various phases of drug development and research. These days, researchers may estimate the affinity of ligands to target proteins with a high degree of precision and efficiency by using Structure-Based Drug Design (SBDD) techniques, which also assist forecast the location of small molecules inside a three-dimensional model of the protein structure. Additionally, they decrease the time and expense associated with drug research while speeding up the discovery of powerful drugs. We highlight the recent successes and major challenges of SBDD in drug development, providing an overview of the method's use in this context.

3 Conclusion

Despite significant advancements, structure-based drug design (SBDD) faces several challenges that hinder its full potential in novel ligand discovery. The complexity of target proteins like TSPO, limitations in current computational models, and the oversimplification of experimentally derived protein structures present significant obstacles. Existing scoring functions struggle to accurately estimate binding free energy due to protein flexibility, solvent effects, and key water molecules in target proteins. Addressing these factors remains crucial for improving protein-ligand interaction predictions. Additionally, computational approaches for drug-target interaction prediction require enhanced methodologies and better data integration. Overcoming these barriers will depend on improved data collection, curation, and more accurate homology models, particularly for human proteins where multiple structural templates remain underexplored. Despite these challenges, SBDD holds great promise for accelerating drug discovery through innovative computational techniques. Targeting unknown macromolecular structures may be facilitated by the use of "de novo ligand creation, drug-target interaction prediction, and ligand binding" site identification. The integration of deep learning into SBDD has opened new avenues, enhancing protein structure prediction, drug association mapping, and structural refinement. These developments increase the possibility of finding potent medicinal molecules by enabling a more effective search of chemical space. With continued progress in computational modeling, artificial intelligence, and data-driven methodologies, SBDD is poised to revolutionize drug discovery in the coming years.

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Review on Computational Chemistry in Drug Discovery

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Abstract

By assisting pharmaceutical scientists and medicinal chemists in the creation of new, safe therapeutic ideas via the logical design and placement of current medicines, computational techniques help reduce the necessity for animal medical research. Examine the many studies on computational approaches in drug development that have been published in this article. According to this study, computational chemistry has transformed modern drug discovery by offering strong tools and techniques for predicting and examining molecular interactions. Drug development has been greatly expedited by computer approaches, from virtual screening to lead optimisation and toxicity prediction. Molecular docking, pharmacophore modelling, MD simulations, QSAR, and virtual screening are some of the computational chemistry technologies that are used to identify drug candidates with potential bioactivities. In order to improve the drug development process, these methods should be able to describe molecules that are effective, target-selective, and absorbable. New possibilities for creativity in drug discovery are presented by recent developments in AI, ML, and high-performance computers, which further expand the potential of computational chemistry.

Keywords: Computational chemistry, Drug discovery and development, Computational technique, Computer-aided drug discovery (CADD), Molecular docking (MD), Quantitative structure–activity relationship (QSAR) techniques, etc.

1 Introduction

To guarantee the safety and efficacy of the new drugs, the time-consuming and expensive process of drug development involves clinical studies, regulatory approval, and an examination of academic

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information. Numerous applicants may not be able to finish the lengthy procedure, which might take years, and there is no assurance that it will be successful. Despite the challenges, drug development is an essential part of the healthcare industry since it produces drugs that may cure illnesses, reduce symptoms, or cure medical problems [1]. For example, antibiotics revolutionised the treatment of infectious diseases, and new developments in cancer immunotherapy have offered patients whose illnesses were previously believed to be incurable hope [2]. Validating the target, identifying the lead compounds, improving and optimising these compounds, and then proceeding to preclinical research and clinical trials are common processes in the drug development process [3].

In order to address challenging chemical issues, computational chemistry uses computer simulation. Its emphasis on comprehending tiny molecules, medications, and intricate molecular systems like DNA, proteins, and other macromolecules makes it an essential component of the molecular-level examination of biological systems [4]. Principles from chemistry, biology, and pharmacology are often combined in the intricate multidisciplinary process of drug development. Researchers can anticipate molecular characteristics and uncover possible medication candidates more effectively by using computational methods. These technologies will also save the time and money that are normally needed for exploratory testing. Close cooperation between researchers with multidisciplinary knowledge and medical scientists is necessary for this [5], [6].

A. Computational chemistry

Computational chemistry uses "computers and physics-based algorithms" to simulate chemical processes and calculate the chemical properties of atoms and molecules. Drug design and discovery use a variety of computational chemistry tools to predict and calculate events, including "the drug's binding to its target and the chemical properties" needed to create potential new drugs [7].

B. Importance of Computational Drug Discovery

"Drug design, discovery, and development" are interdisciplinary processes that take a lot of time and effort and include several study areas. Traditional medication development and research is notoriously costly and time-consuming. There are only 200 to 250 chemical compounds out of 10,000 that will get to clinical testing. Ten of these 200–250 chemicals will be examined in animal models instead of human ones. The Tufts Centre for the investigation of Therapeutic Development conducted an investigation from 1995 to 2007 that found that around 11.83 % of all therapeutic compounds that progress to Phase I of clinical trials are approved for the market. Because traditional drug discovery is expensive and has a high failure rate, researchers have turned to a new method of drug development. A novel method for quickening the drug discovery process has been made possible using CADD [8].

C. Applications of computational chemistry in drug discovery

Computational techniques facilitate the methodical investigation of chemical alterations, directing synthetic endeavours and expediting the optimisation procedure. Lead optimisation driven by computational chemistry is shown by the discovery of selective kinase inhibitors for cancer treatment. Effective treatments design requires an understanding of the molecular underpinnings of drug-target

interactions [9]. Detailed information about the binding processes is provided by computational chemistry, which also identifies important residues and interactions that influence binding affinity and specificity. To clarify the binding mechanisms of different pharmacological targets, including as ion channels, enzymes, and G protein-coupled receptors (GPCRs), MD simulations and QM calculations have been used [10]. These realisations help rationally develop medications with better binding characteristics and fewer side effects. An important part of drug development is predicting a medication candidate's toxicity. On the basis of chemical structure and established toxicological data, computational models, such as machine learning algorithms, can forecast possible toxicities [11]. In the early stages of medication development, these forecasts aid in identifying and reducing safety hazards. Several negative consequences, including hepatotoxicity, cardiotoxicity, and genotoxicity, have been predicted using computational toxicology. Scientists may make well-informed conclusions about the safety profiles of potential drugs by combining these predictions with experimental evidence [12].

D. Limitation and challenges in computational chemistry

Despite the significant advancements in computational drug discovery, there are still several problems that jeopardise the reliability and utility of these methods. Protein flexibility and solvation effects are examples of biological complexity that may not be fully replicated by the approximations used in the computer approaches. Improved sampling methods, machine learning-driven scoring systems, and ensemble docking are among recent innovations that aim to overcome these limitations [13]. Research teams without access to high-performance computers face challenges since large-scale virtual screening and high-resolution simulations need significant processing resources. The incorporation of cloud computing, GPU acceleration, and artificial intelligence-powered prediction models have all been investigated as potential solutions. Additionally, experimental validation is required for computer predictions, which may be costly and time-consuming; some anticipated medications do not exhibit the predicted in vitro and in vivo activity [14].

In order to address these issues, hybrid approaches—which combine automated high-throughput screening with computer forecasts—are being developed. AI-driven drug development is also fraught with issues, including overfitting, biassed datasets, and interpretability issues. These methods are becoming more resilient and open because to developments in federated learning, data augmentation, and explainable AI [15]. Ethical and regulatory concerns, such as data privacy, repeatability, and molecular evaluation produced by artificial intelligence, remain significant. These days, systems that emphasise transparency, reproducibility, and adherence to ethical standards are being examined by regulatory bodies [16]. These difficulties still exist, but they are gradually being overcome by continuous developments in "computer techniques, artificial intelligence, and integrated approaches". In order to define the future of computational drug development, it will be possible to expedite the discovery of novel drug candidates by improving experimental validation techniques, increasing computer efficiency, and improving prediction accuracy [3].

2 Literature Review

(Shah et al., 2024) [17] "Computer-aided drug discovery (CADD)" approaches not only reduce the time and cost of drug discovery and development, but also help to understand the molecular mechanisms of drug action and toxicity. The method known as QSAR creates mathematical connections between a group of chemicals' structural characteristics and biological activity. The current state and applications of CADD techniques are examined in this work, with a focus on "molecular docking and quantitative structure–activity relationship (QSAR) approaches". In addition to some current developments and instances of their use in drug discovery for different illnesses, this paper examines the fundamentals, benefits, drawbacks, and difficulties of these approaches. The study also discusses the potential future prospects of CADD techniques in the era of big data and artificial intelligence.

(Mahamat, 2022) [12] highlights the main computational techniques and resources utilised in drug development, such as machine learning, quantum physics, molecular docking, and molecular dynamics simulations. The article covers recent developments, examines potential future possibilities in the subject, and talks about how these approaches are used at different phases of drug development. New therapeutic candidates have been identified and optimised much more quickly thanks to the use of computational chemistry into drug development methods, which has also yielded considerable cost, time, and effectiveness gains.

(Lin et al., 2020) [18] highlighted the functions of multiscale biomolecular simulations in determining the target macromolecule's drug binding sites and clarifying the mechanics behind therapeutic activity. Virtual screening methods (such as pharmacophore modelling, QSAR, and molecular docking) were then discussed and presented, along with "structure and ligand-based classical/de novo drug design". Lastly, the evolution of machine learning techniques and their use in the previously described computational approaches to expedite the drug discovery process were examined. Additionally, a number of application scenarios involving the combination of several techniques were explored. The future of "drug screening and design" will undoubtedly involve the integration of multiple methodologies to collaboratively address the complex challenge across a variety of dimensions and sizes.

(Amrit, 2023) [19] Drug design and discovery have seen a revolution thanks to computational chemistry. Numerous benefits come with this method, such as the opportunity to explore a large chemical area and time and money savings. Examine some important uses of computational chemistry in drug design and discovery here. Thanks to the capabilities of computational chemistry, the area of drug discovery and design has seen a dramatic revolution in recent years as researchers look for safe and effective medications. Computational chemistry speeds up the drug discovery process by using sophisticated algorithms, high-performance computation, and large datasets. This ground-breaking method has made drug discovery more successful and economical, which has resulted in the creation of ground-breaking treatments that were previously thought to be unattainable.

(Schaduangrat et al., 2020) [16] provides a comprehensive analysis of the repeatability of computational drug discovery. This study covers the following topics: computer problems associated with model

building and deployment, model generation in computational drug discovery, and use case scenarios for improving the computational drug discovery procedure. To encourage partnerships and facilitate repeatability, it has become commonplace in computational fields to share data and programming codes for numerical calculations (i.e. to push the project farther by adding new ideas, extending the data, enriching the code, etc.). In the field of computational drug design, an open approach to data/code collection, curation, and sharing is thus essential.

(Xu, 2024) [15] With the Nobel Prize in Chemistry given for "protein structure prediction and design" and the Nobel Prize in Physics given for "artificial neural networks," 2024 has been a particularly interesting year for computational sciences. Given how quickly these fields are evolving, a publication summarising the current status of "computer-aided drug design (CADD) and artificial intelligence in drug discovery (AIDD)" as well as their future directions would be relevant and topical for the Journal of Medicinal Chemistry's readership. In order to contribute to current debates in the literature and on scientific blogs, this commentary attempts to highlight recent advancements, significant obstacles, and possible areas of overlap across various disciplines.

3 Conclusion

With its strong tools and methods for predicting and analysing molecular interactions, computational chemistry has completely changed the way that drugs are discovered today. Using computational techniques has greatly sped up the drug development process, from virtual screening to lead optimisation and toxicity prediction. Lately, in silico prediction techniques have shown quick results. In order to identify drug candidates with potential bioactivities, computational chemistry uses technologies such as molecular docking, pharmacophore modelling, MD simulations, QSAR, and virtual screening. By characterising molecules that are effective, target-selective, and absorbable, these methods should improve the drug development process. In order to improve effectiveness and reduce attrition in drug development, QSAR techniques are often superior for lead optimisation. "The pharmacodynamic and pharmacokinetic characteristics" of compounds may be determined using QSAR models throughout the drug research and development process. To assist optimise and prioritise drug prospects, these in silico evaluations anticipate a number of attributes (including physicochemical and ADME) and actions. Current developments in high-performance computers, artificial intelligence, and machine learning continue to expand the potential of computational chemistry and provide fresh chances for creative drug discovery. highlighted the expanding use of AI and machine learning in computational drug development, showcasing their capacity to improve molecular predictions, automate data processing, and expedite drug testing. Drug development efforts are greatly aided by hybrid techniques, which integrate machine learning and artificial intelligence with pharmacological and computational procedures.

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Natural Products in Medicinal Chemistry: Current Insights

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Abstract

Natural products have always been important to medicinal chemistry, and their importance hasn't waned. For thousands of years, plants have been used to make a variety of beneficial medications. This article reviews the various literature's study on Natural Products and Medicinal Chemistry. It concluded that natural products remain a vital source for drug discovery, offering diverse scaffolds with unique bioactivities. Advances in chemical synthesis, biosynthetic engineering, and high-throughput screening have enhanced their optimization and accessibility. Despite challenges such as sustainability and bioavailability, innovative techniques in phytochemical analysis and medicinal chemistry are addressing these limitations. The integration of genomics and modern drug discovery approaches continues to expand therapeutic potential. As research progresses, plant-derived natural products will play a crucial role in developing novel, life-saving medications, reinforcing their significance in medicinal chemistry and future drug development..

Keywords: Natural products, Medicinal chemistry, Drugs developed, Drug discovery, Plant-derived natural products, New chemical entities (NCEs), etc.

1 Introduction

Biodiversity is a paradigm shift that has the potential to transform glimpses of reductionist research from earlier years into depictions of the dynamic realm of systems biology, where organisms evolve, differentiate, and begin to diverge from the norm. In regard to potentially useful compounds, it is also a great source of originality. Nature's biodiversity has sometimes advanced to produce an astonishing array of secondary metabolites [1]. Based on empirical findings and tradition, the first and for a long time, the

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only medicines accessible to humanity were natural product extracts. The WHO reports that 80% of people worldwide, mostly in underdeveloped nations, rely on plant-derived medications for their medical needs [2]. In the West, pharmaceutical ingredients largely replace these plant-derived medicines. Natural products remained important, and during the 20th century, the pharmaceutical industry found more natural inspiration for drug development in endogenous substances including prostaglandins, steroids, and peptide hormones [3].

A. Natural Product

A natural product is a material or chemical compound that is created by a living thing and is present in the natural world. All substances created by life are considered natural products in the widest sense. The finest sources of medications and drug leads are still natural compounds, even though many pharmaceutical firms have shifted their focus over the last 20 years from natural products research to HTP screening of combinatorial libraries [4]. A crucial step in the drug development process is identifying "New Chemical Entities (NCEs)" that may have therapeutic utility. These NCEs may be generated chemically, isolated from natural sources, or a mix of the two. Despite the success stories of drug development for natural chemicals, such as paclitaxel and penicillin, there were other factors that made the sector less appealing. In the past, drug targets were exposed to crude extracts; if pharmacological activity was found, the extract was fractionated, and the active component was identified and isolated [5]. The screening procedure did not guarantee that a lead would be patentable or even chemically viable, and the approach was ineffective, labour-intensive, and lethargic. Given that natural products frequently contain molecules with more complex structures, an NCE of interest was more challenging to extract, purify, or synthesise in sufficient quantities for development and research activities [6].

B. Medicinal chemistry

The field of chemistry devoted to creating new medications and enhancing those that already exist is called medicinal chemistry, also referred to as pharmaceutical chemistry. It is an interdisciplinary discipline that blends biology, pharmacology, and chemistry [7]. Professionals strive to create and create substances that may cure illnesses, control symptoms, and enhance a patient's quality of life [8]. They optimise the structure and properties of molecules to improve interactions with target substances and molecules, in addition to "their metabolism, toxicities, and drug delivery", in order to provide targeted treatments with minimal side effects for patients. Medicinal chemistry is an art form that combines creativity and expertise to create new things, as well as a data-driven science [9].

C. Current status of Natural Products

For many years, natural goods have been essential to healthcare. Natural products have been the primary source of chemicals used in medicine research and discovery since ancient times. For thousands of years, the natural world has been a rich source of beneficial biological agents. A startling number of modern pharmaceuticals have been developed from natural sources that have been shown to be effective in traditional medicine. For thousands of years, natural products have been essential in the prevention and

treatment of human illnesses [10]. Terrestrial microorganisms and plants, marine algae and microorganisms, terrestrial invertebrates, and vertebrates are among of the sources of natural substance-based remedies. By giving humanity a wide range of tiny bioactive molecules, nature has created potential pathways for the treatment of a wide range of illnesses [11]. Among the most widely used drugs of the last century are natural products such as taxol from T. brevifolia, vincristine from Vinca rosea, and morphine from Papaver somniferum. In recent years, there has been a noticeable resurgence of interest in natural products as sources of innovative medications among both pharmaceutical corporations and the academic community. Approximately 40% of currently marketed medications were created using natural ingredients [12].

Natural items are those that come from natural sources. Examples of natural goods include the following: (1) an entire organism (e.g., a microorganism, plant, or animal) that has not been treated in any way other than a simple preservation technique (e.g., drying); (2) a portion of an organism "(e.g., an isolated animal organ, plant flowers, or leaves); (3) a portion of an organism, exudates, and an organism extract; and (4) pure substances" (e.g., terpenoids, coumarins, alkaloids, glycosides, flavonoids, steroids, sugars, lignans, etc.) that have been separated from microorganisms, animals—or plants [13]. A common term used to describe "natural products" is secondary metabolites, which are tiny molecules (mol. wt <200 amu) that organisms make but are not absolutely essential to their existence. Secondary metabolism is defined as the results of shunt metabolism during idiophase, defence mechanism regulator chemicals, overflow metabolism due to nutritional constraint, etc. Natural products may come from both terrestrial and marine sources, such as microorganisms (like Streptomyces peucetius's doxorubicin), plants (like Taxus brevifolia's paclitaxel (Taxol), or animals (such vitamin A and D from cod liver oil) [3].

2 Literature Review

(Bharate & Lindsley, 2024) [4] With the use of natural product scaffolds, this Virtual Special Issue seeks to increase knowledge and enthusiasm in drug development. A variety of potential in this field are highlighted by the articles included in this VSI, such as virtual screening of natural product libraries, lead optimisation in medicinal chemistry, and compound isolation. We genuinely hope that readers of "the Journal of Medicinal Chemistry, ACS Medicinal Chemistry Letters, ACS Bio & Med Chem Au, the Journal of Natural Products, ACS Chemical Neuroscience, and ACS Chemical Biology" will find this Virtual Special Issue of these journals both educational and entertaining as it addresses a significant topic in the field of new drug discovery.

(Chaachouay & Zidane, 2024) [14] This demand will be met in large part by natural goods via the ongoing investigation of the world's biodiversity, much of which is yet unknown. As a major source of novel therapeutic leads, drug development from medicinal plants still faces several obstacles, including the selection and application of suitable high-throughput screening bioassays, the expansion of the supply of bioactive compounds, and the procurement of plant materials. In order to explore these natural resources, multidisciplinary, national, and international cooperation in "design, synthesis, drug development, and discovery techniques" is necessary. This review article discusses the current and

upcoming advancements in the hunt for natural items, such as remedies that enhance health and wellness. Additionally, it lists ways to encourage future plant-based medication discoveries by standardising the therapeutic use of natural compounds produced from plants globally.

(Newman, 2022) [15] Angiotensin converting enzyme inhibitors and type 2 diabetes (T2DM) medications are discussed after the recent history of a number of highly significant natural products and their derivatives that are either in use or being evaluated in the fields of anti-infectives and significant cancer treatments, such as antibody drug conjugates, are covered. The agents' present structures are shown, while some peptides used in T2DM medications utilise the usual one-letter shorthand for an amino acid.

(Atanasov et al., 2021) [16] Pharmacotherapy has always benefited greatly from natural compounds and their structural mimics, particularly in the treatment of infectious and cancerous disorders. These problems are being addressed and new opportunities are being created by a variety of scientific and technological developments in recent years, such as as "improved analytical tools, genome mining and engineering methods, and developments in bioculture". Thus, there is a renewed interest in natural materials as possible therapeutic possibilities, particularly in the battle against antibiotic resistance. Here, we discuss key opportunities, highlight some key applications, and review current technological developments that are enabling drug discovery based on natural products.

(M et al., 2020) [6] A crucial step in the drug development process is identifying "New Chemical Entities (NCEs)" that may have therapeutic utility. These NCEs may be generated chemically, isolated from natural sources, or a mix of the two. Natural products made from these sources are abundant in bioactive compounds, which have been used as treatments for a variety of illnesses for many years throughout human history and evolution. This study, however, examined the origins and categories of natural items, their applications, and medications made from them. The report made many recommendations, including that the government support research in the fields of pharmacognocy, pharmaceutical chemistry, and natural goods.

(R. A. Khan, 2018) [17] It is explained how natural products chemistry has aided in the growth of the biological and physical sciences, their transdisciplinary disciplines, and the discovery of new avenues. It does this by offering new applications, constructive inputs, thrust, thorough comprehension, a wide perspective, and a fresh outlook on the future. Along with an outline of the broader developments in the field of natural products chemistry, its role, and the associated scientific and economic implications, the present goals, prospects, and impending objectives are also discussed. There is discussion on how the chemistry of natural products contributes to scientific advancement in a number of fields.

(Dar et al., 2017) [13] A key strategy for the discovery and creation of novel medications is the use of natural ingredients. There isn't a current literature review on natural goods. As a result, the current review's objectives are to update the extensive data about natural products, build a database of the most current medical and scientific studies on natural products, including foods that are medically active (nutraceuticals), and gather the sources of up-to-date natural product data for medical professionals.

(Cragg & Newman, 2013) [11] traces that are natural drug discovery, detailing significant medications derived from natural sources that transformed the way severe illnesses were treated. In addition to producing new screens, the boom of genetic data made it possible to use genome mining and combinatorial biosynthesis technologies. The identification of unknown molecules has been made possible by the acquired information. Combinatorial chemistry can optimise these novel bioactive structures, leading to new therapeutic candidates for a variety of illnesses.

3 Conclusion

Natural products (NPs) remain a vital source for drug discovery, offering diverse structural scaffolds and bioactivities that drive the development of novel therapeutics. Advances in chemical synthesis and biosynthetic engineering have enhanced the accessibility and optimization of complex NP structures, expanding their potential in medicinal chemistry. Despite challenges such as sustainable supply, accessibility, and intellectual property constraints, innovative techniques in phytochemical selection, isolation, and characterization are overcoming these barriers. The integration of genomics and high-throughput screening has further accelerated NP-based drug discovery, enabling the identification of promising bioactive compounds. Drugs produced from plants are still essential in the fight against microbial infections and serious illnesses, but the growing need for medicinal plants generates questions about how to preserve them. The combination of natural products with contemporary drug discovery techniques presents a viable avenue for the development of new therapies as medicinal chemistry advances. By addressing challenges related to bioavailability and sustainable sourcing, ongoing research will ensure the continued exploration and utilization of natural products, leading to innovative treatments for a wide range of diseases.

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Innovations in Medicinal Chemistry for Cancer Treatment

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Abstract

Millions of people die each year from cancer, an aberrant condition of cells that produces aggressive tumours and unchecked cell multiplication. The development of several novel treatment regimens and their subsequent trials are a result of our growing understanding of the illness and its molecular mechanism of progression. Many malignancies are very difficult to diagnose and identify early. High death rates are always the result of late-stage cancer discovery. The development of new, more sensitive, and more efficient diagnostic and therapeutic techniques for cancer therapy is essential. Review the many studies on advances in medicinal chemistry for the treatment of cancer in this article. The study found that by improving medication biodistribution, allowing precision medicine, and reducing adverse effects, "nanomedicine, targeted therapy, and nanotechnology" have transformed the treatment of cancer. Advances in gene therapy, immunotherapy, and AI-driven diagnostics further refine patient-specific treatments. Minimally invasive surgical techniques and thermal ablation offer effective alternatives to tumor resection. The integration of AI, nanorobots, and engineered nanomaterials enhances early detection, targeted drug delivery, and treatment efficacy. Collaborative efforts in medicinal chemistry and AI will continue to drive breakthroughs in cancer therapeutics, improving patient outcomes.

Keywords: Medicinal chemistry, Cancer treatment, Nanomedicine, Nanotechnology, Tumor, Artificial intelligence (AI), etc.

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1 Introduction

Cancer is now treated using radiation treatment, chemotherapy, immunotherapy, hormone therapy, targeted therapy, and surgery. Following the advent of targeted treatment, chemotherapy and radiation therapy—two components of conventional cancer therapy—saw a significant transformation [1]. The first innovative pharmacological method for treating cancer was the use of chemotherapeutic drugs, which were cytotoxic to the tumours. Typically, they are developed to target the dysregulated processes that occur inside cancer cells [2]. The main chemotherapeutic agents in the past were alkylating agents and antimetabolites. Alkylating agents, which are medications based on nitrogen mustard, caused cytotoxicity by adding alkyl groups to the bases of deoxyribonucleic acid (DNA) [3]. By stopping DNA replication, antimetabolites (such as gemcitabine, fluorouracil, mercaptopurine, methotrexate, and aminopterin) prevent cells from proliferating. Along with these, the chemotherapy also included anti-mitotic drugs "(Vincristine, etoposide, paclitaxel, topotecan, taxol, etc.), polyamine transport inhibitors, iron-modulating drugs (desferrioxamine, etc.)", and cytotoxic antibiotics (doxorubicin, actinomycin D, bleomycin, etc.) [4], [5].

A. Innovations and technological advancements

Technological developments and innovations have been crucial in changing the face of contemporary healthcare, especially in the field of cancer. An example of this revolutionary advancement is the use of robotic surgery in cancer [6]. Compared to laparoscopy and open operations, robotic surgery is a less invasive surgical method that has several benefits [7]. It allows surgeons to perform complex procedures more precisely and with less damage to important tissues because to its solid operating field, magnification capabilities, and three-dimensional vision. This results in advantages for patients, such as less scarring, less blood loss, faster healing, less problems from wounds, and shorter hospital stays [8], [9].

Because they provide information on tissue shape, structure, metabolism, and functioning, biomedical imaging methods are essential to the treatment of cancer. These strategies support clinical decision-making when paired with other diagnostic approaches. The accuracy of cancer staging and treatment planning is improved by hybrid imaging techniques [10]. Image-guided minimally invasive treatments may lessen side effects and enhance treatment results. Advanced imaging technologies like "computed tomography (CT) and magnetic resonance imaging (MRI)" have revolutionised surgery and medical care because of their capacity to accurately see soft tissues and bones. For many medical situations, such as cancer treatments, orthopaedic operations, reconstructive surgeries, and middle ear disorders, they improve surgical techniques [11], [12].

One revolutionary development in cancer is personalised medicine, often known as precision medicine. This technique carefully tailors therapies by taking into account a patient's medical history, lifestyle, tumour environment, and genetic composition. It enhances the overall quality of life for patients, minimises adverse effects, maintains organ function, and maximises treatment [13]. It represents a change to a more efficient and patient-centered cancer care approach. These developments are mostly

the result of translational research. The identification of prognostic and predictive molecular changes in cancer has greatly improved since a one-size-fits-all strategy was replaced with a customised one driven by molecular analysis [14]. Both localised and metastatic illness management has been significantly impacted by the detection of gene mutations, amplifications, and fusions made possible by technologies such as RNA sequencing and next-generation sequencing [15].

B. Common Cancer Treatment Options

- Blood & Bone Marrow Stem Cell Transplantation: Memorial Sloan Kettering performs hundreds of adult stem cell transplants annually, making it one of the most skilled transplantation centres in the US.
- Cancer Surgery: Not only are Memorial Sloan Kettering doctors committed to treating cancer, but they also work to ensure that patients properly recover from their treatments.
- Chemotherapy: Cancer may be cured, controlled, or its symptoms can be lessened by chemotherapy. Find out more about how we provide drug-based therapy to our patients.
- Immunotherapy Cancer Treatment: A novel approach to treating cancer is immunotherapy, which targets cancer cells by triggering the immune system.
- Interventional Radiology: For some individuals, interventional radiology offers a less intrusive option to surgery by using catheters and needles.
- Radiation Therapy for Cancer: Tumours may be destroyed by radiation treatment or may not recur. This treatment may be used alone, in conjunction with chemotherapy, surgery, or both. Find out how MSK uses radiation therapy and what kinds of treatments are available.
- Targeted Therapy & Precision Oncology: Discover precision oncology and genetic targeted treatment for cancer at MSK. In order to prevent cancer from spreading, this kind of cancer therapy targets certain gene alterations in cancer cells and tumours.

2 Literature Review

(Kuzminska et al., 2024) [16] Because of its proven ability to stop tumour development, curcumin has sparked interest in its potential to treat a number of malignancies, including those of the breast, lung, prostate, and brain. Curcumin's weak water solubility, low bioavailability, and low chemical stability, however, restrict its therapeutic use. Curcumin's pharmacological qualities, such as improved anticancer selectivity index and bioavailability, have been improved by structural alterations in response to these difficulties. This study identifies prospective curcumin chemical changes that may result in the creation of more potent anticancer treatments. Researchers hope to produce more stable, bioavailable molecules with improved therapeutic potential by functionalising the parent curcumin molecule. This makes curcumin derivatives attractive options for use in medicine.

(Liu et al., 2024) [17] Gene therapy, cell-based therapeutics, antibody-drug conjugates (ADCs), and small molecule targeted medicines are becoming highly sought-after methods. In addition to offering patients more therapeutic comfort and the possibility to slow the development of their illness, these state-

of-the-art therapy techniques also enable precise and personalised tumour targeting. We covered the many therapeutic techniques in this study, such as gene therapy, cell therapy, peptide and antibody medicines, and small molecule targeted medications. Each approach will be thoroughly explained, including its current state of development, clinical difficulties, and possible remedies. In order to provide successful therapy and more effectively progress research, the goal is to help researchers and doctors develop a greater knowledge of these many treatment alternatives.

(Kong et al., 2023) [18] Both in vitro research and in vivo applications have made the many practical applications of nanobots for cancer treatment a reality. In this study, we analyse and assess the most recent advancements in nanobots in cancer treatment, with an emphasis on their key features and applications in "drug administration, tumour sensing and diagnostics, targeted therapy, minimally invasive surgery, and other" all-encompassing therapies. At the same time, we talk about the difficulties and possible avenues for nanobot research to transform cancer therapies. Before evolving into real nanosubmarines in the bloodstream, medical nanobots are expected to become more sophisticated and capable of performing a range of medical tasks.

(Helms et al., 2023) [19] Finding novel therapy combinations to enhance outcomes for diseases like sarcomas and brain tumours requires ongoing progress in our knowledge of the biology of tumour heterogeneity. Access to new technologies that attempt to lessen or better manage therapy-related toxicities is necessary for paediatric cancer survivors. Paediatric oncology patients still need long-term, interdisciplinary subspeciality care despite improvements in survival and therapy. For paediatric cancer survivors to get the best treatment possible throughout their lives, communication between paediatric oncologists, primary paediatricians, survivorship clinics, and adult primary care must be improved. In order to emphasise recent developments and opportunities for ongoing improvement, we address five primary areas of paediatric oncology in this State-of-the-Art review: lowering toxicity, cancer biology, innovative therapeutics, detection and monitoring, and access to care.

(Shams et al., 2023) [8] highlights important developments in both medical and surgical oncology by examining the development of cancer therapies throughout time. Neoadjuvant and adjuvant therapy, as well as the importance of multidisciplinary tumour boards, are highlighted in the article, which highlights the combination of medical surgery. Additionally, it discusses developments, difficulties, and the critical function of patient-centered care. Additionally, it provides information on how the rapidly changing area of integrated oncological care is expected to develop in the future. This research provides a clear understanding of the dynamic and transformative nature of cancer treatment, reflecting the unwavering commitment of the surgical and medical communities to the ongoing fight against cancer.

(Chehelgerdi et al., 2023) [20] Cancer diagnosis and therapy might be completely transformed by the use of nanotechnology. In this study, several of the approved formulations are analysed, and the difficulties in transferring laboratory results to clinical settings are discussed. The many chemicals and nanocarriers that may be used for targeted tumours and the inherent challenges of cancer treatment are highlighted in this research. In the future, nanotechnology has promise for enhancing cancer diagnosis and therapy; however, further investigation is required to get over the present clinical translation barriers.

(Anand et al., 2022) [21] Despite its acknowledged negative effects on patients' physical and mental well-being, chemotherapy is still a commonly used treatment option for cancer, despite mounting research that suggests a more methodical and focused approach may be the way of the future. In recent decades, chemotherapeutic drugs and pharmaceuticals have been the first option for advanced-stage cancers when surgery and/or radiation treatment cannot be recommended for certain reasons. In addition to evaluating the current state of the enrolled medications and pharmaceuticals, the current report provides a concise overview of the latest developments in chemotherapy. It also thoroughly examines the growing significance of targeted and specific therapeutic approaches currently being used to improve clinical and survival rates for cancer patients.

(Pucci et al., 2019) [22] A lot of work is being done in oncological research to develop effective novel treatments that might minimise serious adverse effects from traditional treatments. Various technologies are either already in clinical use or are now being assessed in clinical studies. Bioengineering extracellular vesicles and patient cells has enabled the development of ad hoc systems and precise targeting methods, even if nanomedicine is assisting in the development of "biocompatible materials for both therapeutic and diagnostic uses". An extensive examination of the most recent developments in both fundamental and applied cancer research is given in this review.

3 Conclusion

The combination of surgical and medical advancements has resulted in a dramatic change in the field of cancer therapy in recent years. Nanomedicine, combined with targeted therapy, has significantly improved the biodistribution of chemotherapeutic agents, enhancing treatment precision while minimizing side effects. Cancer patients have fresh hope thanks to emerging techniques including "gene therapy, siRNA delivery, immunotherapy, and antioxidant compounds". Thermal ablation and magnetic hyperthermia present promising alternatives to conventional tumor resection. Additionally, radiomics and pathomics enable efficient data management, improving prognosis and treatment outcomes. In pediatric oncology, efforts are focused on breaking survival plateaus and minimizing toxicity. Medical and surgical oncology continue to evolve, with precision medicine tailoring treatments to individual patients and minimally invasive techniques prioritizing organ preservation. Advances in protein engineering and nanotechnology facilitate nanoscale targeting, improving efficacy and reducing adverse effects. AI integration in healthcare, including models like GPT-4, LLaVA-Med, and Huawei’s AI-assisted screening, is revolutionizing cancer diagnosis and early detection. To fully harness nanorobotics in cancer treatment, collaboration between material scientists, AI experts, and medical researchers is essential. Nanomaterials incorporating natural compounds enhance tumor specificity and therapeutic effectiveness, ultimately improving patient compliance. Innovations in medicinal chemistry, driven by these advancements, are reshaping cancer treatment, offering more effective, personalized, and less invasive therapeutic solutions.

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Natural Products in Drug discovery: Current Trends

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Abstract

Medical chemicals have been found in nature for thousands of years, and a staggering number of modern medicines have been shown to have natural roots. For many years, people have employed plants as herbal remedies to cure a variety of illnesses, and the numerous natural compounds they produce have served as inspiration for the creation of new medications. This demand will be met in large part by natural goods via the ongoing investigation of the world's biodiversity, much of which is yet unknown. In this article review the various literature's study on "natural products in drug discovery". In conclusion, natural products have been a fundamental component of drug discovery for an extended period, providing useful lead compounds for the development of new therapeutics. Advances in technology have enhanced the selection, identification, and optimization of plant-derived phytochemicals, improving their efficacy and safety. Despite challenges in natural product development, innovative strategies continue to drive drug discovery, addressing both communicable and non-communicable diseases. Plant-based biologics have been further emphasised as a potential vaccine development strategy during the COVID-19 pandemic. In areas such as "immunosuppression, anti-infectives, and metabolic disorders", natural products continue to be a critical source of innovative treatments, as a result of the renewed interest in them as a result of the constraints of alternative drug discovery methodologies.

Keywords: Natural products, Drug discovery, and development, Medicinal chemistry, Drug designs, Automation, Artificial intelligence (AI), etc.

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Dr. Santosh Kumar Nathsharma

1 Introduction

The majority of early medications were made from natural sources, which have also been crucial in drug development. For many serious illnesses for which there is now no effective therapy, these natural ingredients have been discovered to be a vital source of novel medications [1]. Drug prospects have long been abundant in nature, which also presents medicinal chemists and researchers with previously unheard-of chances to consistently provide the lead molecules [2]. According to the World Health Organization's study, approximately 65% of the global populace consumes natural bioactive components as the initial critical defensive measure for the treatment of numerous maladies. China, India, and many other nations have long used a wide variety of natural ingredients in their ancient medical systems [3]. Natural materials are still regarded as a useful source of medication leads in the modern period. This method was common in the pharmaceutical business. Minerals, plants, and animals are examples of natural goods that have been used to cure human illnesses [4]. Ancient knowledge, however, has served as the foundation for contemporary medicine and will continue to be a significant source of future treatments and medical knowledge. Almost as long as human civilisation has been, medicine has existed. Natural products and chemicals produced from them have traditionally provided the bulk of new pharmaceuticals (secondary metabolites) [5], [6].

A. Drug discovery

The process of finding new potential drugs is known as drug discovery in the domains of pharmacology, biotechnology, and medicine. The active component of traditional treatments was traditionally identified, or drugs were discovered by coincidence, as was the case with penicillin. In order to identify compounds with the intended therapeutic effect, classical pharmacology, a more modern method, contained screening chemical libraries of natural products, synthesised small molecules, or extracts in whole organisms or intact cells [7]. Since the human genome has been sequenced, allowing for the quick cloning and synthesis of large amounts of purified proteins, reverse pharmacology—the high-throughput screening of large compound libraries towards isolated biological targets thought to be disease-modifying—has become a standard procedure. These screens' hits are further evaluated for effectiveness in cells and subsequently in animals [5].

B. “Importance of plant-derived natural products in drug discovery”

In the treatment of infections, natural compounds and its "structural analogues" have long been important in pharmacotherapy. Apart from the physiologically active bioactive compounds derived from plants that have been shown to have direct therapeutic utility as drug substances, many additional naturally occurring bioactive chemicals have proven promise as "leads" or model molecules for drug synthesis or semi-synthesis [8]. These difficulties have recently been resolved, and a variety of technological and scientific developments, including advances in microbial culture, genome extraction, engineering methods, and enhanced analytical tools, have generated new opportunities. These developments are shown by the intricacy of bioassays employed in the creation of medicinal plants. Additionally, they provide rapid and accurate "mode of action" information at the molecular level. Consequently, there is

renewed interest in natural chemicals as possible therapeutic candidates, particularly for the treatment of antibiotic resistance [9].

C. "Multidisciplinary approach to natural products drug discovery using innovative technologies"

To package natural product molecules for use in medicine and drug research, a multidisciplinary strategy using cutting-edge technology is necessary for new drug discovery from natural products. A successful implementation of this strategy will enable the creation of next-generation medications to address the growing health issues of the present and the future [8]. Since most components of medicinal extracts work together to create their therapeutic benefits, it may not be helpful to isolate individual constituents. Researching and using these molecules, which may successfully result in novel medications, requires creative methods. Additionally, a systems biology-based approach offers an alternative perspective on natural products. Pharmacy science [10].

Utilising existing technologies like transcriptomics, proteomics, metabolomics/metabonomics, genomics, automation, and computational techniques in conjunction with a systems biology approach may open the door to novel drug design that produces superior therapeutic candidates. Molecular libraries of lead compounds derived from natural product research and development will be used to generate lead compounds and herbal tinctures for novel medications [11]. Applying cutting-edge technology in conjunction with systems biology should prioritise the synergistic effects of chemicals rather than a reductionist strategy that seeks to identify a single active ingredient. A non-reductionist approach will be necessary to comprehend the intricate molecular mechanisms of action of natural products in order to develop novel drugs [12].

D. "Computer-aided drug design from natural products"

Many global health challenges might be addressed by synthetic chemicals that are patterned after natural products. However, in numerous instances, these substances would have been denied as unsuitable for therapeutic uses. Several of the innovative designs would have failed because to the excessively strict criteria of "the rule of three and rule of five", which are often utilised when choosing drug leads [13]. In actuality, a lot of the rules utilised in medication design exhibit human bias, which limits their applicability and efficacy, particularly when it comes to natural goods. Using computer-aided designs, several medicinal synthetic chemicals, including a number of anticancer medicines, have been created. For instance, the Scaffold Hunter program was used to create virtual pieces of tiny, chemically appealing molecules by simplifying complicated natural items [14]. Such computer program must display small molecules that maintain the same biological activity as the mother substance. In fact, this technique has previously been used to find pyruvate kinase activators and inhibitors. But it's also feasible that simple molecules produced from natural products will have less activity than the original chemical [15]. A number of basic structures or chemical compounds generated from the mother material have had their biological activity predicted using the PASS software with great effectiveness. The antitumor properties of a number of marine alkaloids have been predicted using the PASS program [10].

2 Literature Review

(Chaachouay & Zidane, 2024) [9] This demand will be met in large part by natural goods via the ongoing investigation of the world's biodiversity, much of which is yet unknown. The exploration of these natural resources requires interdisciplinary, national, and international collaborations in design, synthesis, drug development, and discovery methods. The existing and upcoming methods for finding natural products, such cures for illnesses and ailments, are covered in this review article. Additionally, it lists ways to encourage future plant-based medication discoveries by standardising the therapeutic use of natural compounds produced from plants globally.

(Zeng et al., 2024) [11] Natural products (NPs) are useful resources for drug development because of their wide range of chemical structures and biological activity. The several uses of these databases in drug development, including molecular creation, knowledge graph building, and virtual screening, are next examined. Talk about the database development challenge in more detail, paying particular attention to data quality and updates. Lastly, highlight how important teamwork and toolkit innovation are to maximising the enormous potential of databases connected to NPs in order to speed up production, structural modification, and bioactivity mining. In order to support researchers in creating and managing top-notch NP databases for drug development, this paper attempts to clarify the essential characteristics and uses of NP databases.

(Sj & Shetty, 2024) [16] discusses some of the developments in the use of contemporary drug discovery technologies to create innovative treatments that are effective natural products. Along with related techniques in medicinal chemistry, nanotechnology, combinatorial chemistry, and high-throughput screening, the development prospects in natural product research are examined with the application of some of the new information technology trends, such as big data, automation, artificial intelligence (AI), computer-aided drug design, and omics strategies. The evaluation specifically focusses on the advancement of novel approaches, interdisciplinary applications, and procedures with upcoming objectives and possibilities.

(Newman, 2022) [17] Angiotensin converting enzyme inhibitors and type 2 diabetes (T2DM) medications are discussed after the recent history of a number of highly significant natural products and their derivatives that are either in use or being evaluated in the fields of anti-infectives and significant cancer treatments, such as antibody drug conjugates, are covered. The agents' present structures are shown, while some peptides used in T2DM medications utilise the usual one-letter shorthand for an amino acid.

(Nasim et al., 2022) [18] Nature provides a wealth of medications that must be found and refined for usage as necessary biologics, either alone or in combination, in the contemporary medical sector. The advancement of systems biology and computational methods for therapeutic target identification are covered in this article along with a summary of several approaches to phytopharmaceutical drug development. To make it easier for medications to reach their objectives efficiently, we examine the current drug delivery techniques. The various analytical methods for plant material fingerprinting and

authenticity are also described. Lastly, we discuss how biopharming is used to create biologics derived from plants.

(Chopra & Dhingra, 2021) [19] discusses the significance of natural products for the development and discovery of new drugs. With minor adjustments and fresh viewpoints, it explains how the natural elements may be used. An exceptional chance to create a novel molecular entity with improved pharmacological potential is presented by a number of novel structural changes. With an emphasis on finding and discovering new, effective molecules—referred to as "new entities of natural product drug discovery"—new efforts are being made in the present period to use chemicals generated from natural sources as innovative therapeutic candidates, it was found.

(Tresina et al., 2021) [20] The availability of new molecules that are easily synthesised from plant, yeast, or bacterial sources has expanded recently due to the use of molecular biological methods. Additionally, screening libraries that closely mimic drug-like molecules are being created using combinational chemistry techniques based on natural product scaffolds. By using these technologies, we have the opportunity to conduct research on screening novel compounds using a database and algorithms to identify natural products as a significant source for drug development. Finally, it leads to the discovery of the lead structure. This study covers the importance of advanced technology in the next-generation drug discovery, plant-based natural product medication development, and features from published research on plants as sources of anti-inflammatory pharmaceuticals.

3 Conclusion

Since natural products provide a wealth of bioactive chemicals for therapeutic development, they have long been a mainstay of drug discovery. The optimization of plant-derived phytochemicals has led to the creation of effective and safe drug analogs. In response to the difficulties in drug development, sophisticated methods for "the selection, identification, isolation, and characterisation" of natural components have been developed as medicinal chemists' interest in this field has grown. Despite the complexities involved, technological advancements have improved the success rate of identifying novel therapeutic agents. The ongoing need for innovative drug development strategies is evident, particularly in response to global health crises such as COVID-19. Plant-based biologics offer promising avenues for developing antiviral vaccines, highlighting the significance of natural products in combating emerging diseases. Moreover, the failure of alternative drug discovery approaches to yield sufficient lead compounds has renewed interest in natural product research, particularly in areas like immunosuppression, anti-infectives, and metabolic disorders. Reiterating their vital significance in contemporary medicine, the ongoing investigation of natural substances continues to be a crucial tactic for the creation of innovative pharmaceutical medications.

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Applications of Nanotechnology in Medicinal Chemistry Impact

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Abstract

Nanomedicine is a broad use of nanotechnology in the medical domain. Particular nanoparticles may be used in imaging and methods, biomedical implants, targeted pharmaceutical products, tissue engineering, and novel diagnostic tools. An overview of the many studies on the use of nanotechnology in medicinal chemistry may be found in this article. According to the review, nanotechnology helps to maximise therapeutic efficacy, minimise the risk of adverse effects, and address the issue of focussed therapy delivery. This method is appropriate for cancer detection, treatment, and gene therapy. The realm of nanomedicine is where nanorobotics has the most potential for application. It is used in a wide range of sectors, including the creation of vaccines, medicine delivery, wearable technologies, diagnostic and imaging equipment, and antimicrobial products. Early illness detection, more powerful drugs, and improved equipment are expected to lead to nanomedicine. Combining conventional anti-cancer medications with nanoscale technology allows them to pass through intact and circulate throughout the brain. This technique provides whole classes of existing medications, as well as vast new markets and advantages.

Keywords: Nanotechnology, Nanoparticles, Medicinal and pharmaceutical products, Medicinal chemistry, Nanomedicine, etc.

1 Introduction

Materials, devices, systems, and structures that are planned, described, produced, and used in ways that exploit nanoscale phenomena are referred to as "nanotechnology" in science and engineering. As a new

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approach to medical research, nanotechnology is now regarded as the most potential technology of the 21st century [1]. Over the last ten years, public investment for nanotechnology development and research has grown, indicating that nanotechnology will bring in a new age of productivity and wealth. Economic development may be stimulated by nanotechnology, which can also improve industrial sectors' capacity and quality. It has greatly influenced the wellbeing of society and shaped contemporary existence. It might fundamentally change human existence, economic circumstances, and cultural dynamics [2], [3].

A. Need for nanotechnology in the medical field

The field of nanotechnology and nanomedicines is so broad and diverse. Significant advancements in nanomedicine have elevated the medication to a new degree with noteworthy medical consequences. Studying nanotechnology's important potential in healthcare is necessary. Nephrology and cardiovascular disease In addition to cancer treatment and therapeutic genes, numerous medical specialities are currently conducting extensive research on the most effective methodologies and best practices [4]. The conventional therapy has made substantial progress, and the purity of nanoparticles and nanotechnology has both improved, resulting in positive outcomes. In gene therapy, nanomedicines have also been used. Many investigations on viral vectors as possible drug delivery vehicles were undertaken. Information from smart tablets and nanobots aimed at specific cancer cells are gathered by researchers to ensure that patients get the appropriate treatment [5]. By replacing current methods with more affordable and user-friendly alternatives, nanotechnology presents the possibility of in-vitro diagnostics. Nanoparticles may function as molecular imaging agents in these technologies, impacting the functional features of tumour cells and genetic alterations associated with cancer [6]. Additionally, the following nanomaterials are typically included in functional nanotechnology-based coatings, depending on their intended application: zinc oxide, iron oxide, silicon dioxide, carbon black, and silver. Tools and procedures are utilised in the field of medical device engineering to improve the safety, efficacy, and physiochemical characterisation of "nanomaterials and nanosurfaces". When developing products using new materials, sensors, and energy storage devices, scientists are essential [2].

B. Nanotechnology and cancer treatment

As the number of cancer patients worldwide rises, there is an urgent need for an inventive pharmaceutical delivery system that is more targeted, efficient, and has fewer side effects, as well as an accurate detection approach. If the therapeutic drug can reach the targeted location without causing any unfavourable side effects, anticancer therapies are often thought to be more successful [7]. To enhance this necessary targeted delivery, nanoparticle carriers' surfaces may be chemically modified. Polyethylene oxide, or PEG, is one of the best methods for altering the surface of nanoparticles. These changes improve the cancer targeting capability in addition to the medication uptake's specificity. The nanoparticles may pass through the blood until they hit the tumour because PEG stops the immune system in the body from recognising them as foreign substances [2]. Hydrogel's application in the treatment of breast cancer is a great example of this innovative technology. One kind of monoclonal antibody called Herceptin targets the human epidermal growth factor receptor 2 (HER2) on cancer cells to treat breast cancer. This has led to the development of a vitamin E-based hydrogel that can transport

Herceptin to the target spot for a few weeks with a single dosage [8]. It is a better anti-tumor agent because Herceptin is better maintained within the tumour when administered via hydrogel, which is more effective than "conventional subcutaneous and intravenous delivery techniques". Nanotechnologies may be used to modify nanoparticles in a variety of ways to improve drug localisation, boost medication effectiveness, extend circulation, and perhaps slow the development of multidrug resistance [9].

C. Nanoparticles in MRI

Cancer tumour MRI imaging is enhanced by iron oxide nanoparticles. Iron oxide nanoparticles are functionalised using aptamers, antibodies to the epthelial growth factor receptor, or short peptides such as "arginyl glycyl aspartic acid (RGD)". The “kidney, stomach, liver, breast, colon, and brain cancers” are among the cancers for which they have been suggested. Additionally, synthesised iron oxide nanoparticles may be used in research on brain inflammation and early thrombosis detection. Additionally, iron, manganese, and gadolinium nanoparticles may be used for MRI imaging. MRI research often uses these nano-objects for biological applications due to their electrical and structural band gap positions [10].

D. Nanotechnology in Diagnostic imaging.

"Computed tomography, magnetic resonance imaging, nuclear medicine, X-rays, and ultrasound" are popular imaging techniques that are often used in biochemical and medical research [11]. But only at a somewhat late stage of the disease can these methods look at changes on the surface of the tissue. They might be enhanced by using contrast and nanotechnology-based targeting agents to identify the sick region at the tissue level, improving resolution and specificity [12]. Nowadays, the majority of contrast agents used in medical imaging are small molecules with the potential for unfavourable side effects because of their rapid metabolism and non-specific distribution [13]. More stronger contrast agents for almost all imaging modalities might be made using nanoparticles as they are less harmful and have superior permeability and retention effects in tissues. This is the area in which nanotechnologies have the greatest impact on medicine. The size of the nanoparticles has a significant impact on their "biodistribution, blood circulation half-life, cellular absorption, tissue penetration, and targeting" [9], [14].

2 Literature Review

(Karahmet Sher et al., 2024) [7] investigations into nanoparticles and nano-delivery systems, focussing on their uses in virology and cancer, including both in vitro testing conducted on cell cultures and in vivo evaluations conducted on suitable animal models. This offers a fresh viewpoint by combining many elements, such as structure and formation, as well as their relationship to distinctive behaviours in organisms. Additionally, the usefulness of these systems in pharmacy and medicine was investigated, with an emphasis on cancer and viral infections. The findings suggest that the use of nanotechnological solutions to deliver medications and enhance therapeutic effects will only grow.

(Haleem et al., 2023) [2] explores the many kinds of nanoparticles that are used in medicine. explains the use of nanotechnology in the medical sector as well. The class, attributes, and features of medical nanotechnology are also provided. Collaboration across sectors will be necessary for scientists, governments, community organisations, and the general public to assess the significance of nanotechnology and guide its growth in several fields. Several potential applications of nanotechnology in the medical area are being investigated at this time. "Scientists, engineers, and researchers" will discover the study's succinct and organised summary on nanotechnology helpful for their future research.

(Sim & Wong, 2021) [9] Nanotechnology is the process of taking use of a material's unique properties at the nanoscale. In several industries, nanotechnology has gained popularity due to its ability to create smarter and better-built products. Cancer and heart disease are among the most prevalent illnesses that have been treated by nanomedicine, an application of nanotechnology in medicine. The author gives a summary of the most current developments in nanotechnology as they relate to medication delivery and imaging.

(Altammar, 2023) [5] Because of their adaptability and superior performance over their parent material, nanoparticles (NPs) are crucial for technological advancements. Hazardous reducing agents are often used to convert metal ions into uncharged nanoparticles for their manufacturing. However, a lot of efforts have been made recently to develop green technology that produces nanoparticles using natural resources rather than hazardous chemicals. Environmentally friendly, clean, safe, economical, simple, and very productive, biological approaches are used in green synthesis to synthesise nanoparticles. The green synthesis of NPs uses a wide variety of biological organisms, including plants, bacteria, actinomycetes, fungi, algae, and yeast. This study will also cover nanoparticles, including their kinds, characteristics, production techniques, uses, and future possibilities.

(Malik et al., 2023a) [15] being out in order to integrate the most recent information on pharmacological and medical applications of nanotechnology from recognised scientific sources. Nanotechnology is being effectively used in the fields of "diagnostics, diseases, regenerative medicine, gene therapy, dentistry, cancer, cosmetics, drug delivery, and therapeutics". Future developments in the area of nanomedicine will be more planned, structured, and technically programmed if doctors, clinicians, researchers, and technology work together and are thoroughly associated. Due to the pathophysiological basis of diseases, advancements are being made in overcoming barriers associated with the application of nanotechnology in the medical field. The many facets of nanomedicine are highlighted in this article, along with the ways that nanotechnology is helping the medical field. Minimising the detrimental impacts of nanotechnology on ethics, the environment, and human health is imperative.

(Abaszadeh et al., 2023) [16] Examine the applications of nanotechnology in minimally invasive “surgery, cardiac surgery, vascular surgery, ophthalmic surgery, neurosurgery, plastic surgery, orthopaedic surgery, surgical oncology, and thoracic surgery”. Among other topics, it talks about the use of nanomaterials in breast implants, bone grafting, and implant surfaces. The article also discusses the many applications of nanotechnology, such as haemostasis, nerve repair, nanorobots, stem cell-incorporated nanoscaffolds, nano-surgery, and diagnostic applications. Additionally discussed are the

safety and ethical ramifications of using nanotechnology in surgery. Nanotechnology's potential is explored, suggesting a path towards better patient outcomes. The last section of the article discusses the revolutionary impact of nanotechnology in surgical applications and its potential for further advancements.

(Anjum et al., 2021) [17] Nanomedicine, the use of nanotechnology and related nanocarriers and nanosystems in medicine, has improved disease prevention, diagnosis, and treatment in a number of ways. It has been discovered that some nanosystems are better suitable for theranostic applications than traditional techniques. The usage and limitations of medically relevant nanosystems in areas including gene therapy, targeted drug delivery, and treatment of cancer and other genetic diseases will be discussed in this review paper. Although nanotechnology has a lot of potential, it has not yet been fully utilised, and more work must be done to overcome these restrictions and utilise it to its fullest potential in order to transform the healthcare industry in the near future.

3 Conclusion

Innovative technology has often been developed with healthcare as its primary emphasis since it is a fundamental human right. The delivery of timely, acceptable, high-quality, and reasonably priced healthcare has been greatly aided by technological advancements. The development of nanoscience has led to the emergence of new types of nanostructures. The advent of nanotechnology has been a game-changer in medicinal chemistry, opening the door to focused treatment with fewer systemic adverse effects and better drug transport, solubility, and bioavailability. The use of nanoparticles in drug and gene delivery has led to significant advancements in treating cancer, rare diseases, and infections while minimizing damage to healthy tissues. Nanotechnology-based sensors and real-time monitoring devices facilitate early disease detection and personalized treatment plans. In surgical applications, nanomaterials enhance imaging, wound healing, and targeted medication delivery, reducing complications and improving precision. Nano-dentistry is emerging as a promising field, utilizing dendrimers for gene and drug delivery. Various nanomaterials, including metallic nanoparticles, quantum dots, and CNTs, have shown potential in diagnostics, particularly in cancer imaging through MRI contrast agents like iron oxide nanoparticles. Additionally, nanotechnology has improved orthopedic implants, spinal fusion efficiency, and vaccine formulations by enhancing antigen solubility and controlled release. With applications spanning drug development, diagnostics, surgery, and personalized medicine, nanotechnology continues to advance healthcare by improving treatment efficacy, reducing adverse effects, and enhancing patient outcomes.

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Role of Nanotechnology in Cancer Treatment

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Abstract

One rapidly developing cutting-edge area with several uses in novel cancer detection platforms is nanotechnology. Nanoparticles are being used to enhance the identification and treatment of a number of disorders, including cancer. Nanotechnology has enabled the use of nanoparticles in cancer therapy, which are capable of passively aggregating at tumour sites, rendering them an ideal alternative to conventional methods. This article reviews studies on the use of nanotechnology to cancer therapy from a variety of sources. From the review it concluded that nanotechnology plays a crucial role in revolutionizing cancer treatment by enhancing diagnosis, drug delivery, and therapy. Nanomedicine offers high sensitivity, specificity, and improved pharmacokinetics, enabling targeted drug delivery with reduced toxicity and enhanced therapeutic efficacy. Various nanoparticles, including polymeric, metallic, and hybrid NPs, provide platforms for combination therapy, overcoming multidrug resistance. Despite challenges in specificity, biodistribution, and clinical efficacy, ongoing research is optimizing "nanoparticle-based drug delivery". Diagnosis and therapy integration (theragnosis) exhibits significant potential for personalised cancer treatment. With continuous advancements, nanotechnology is transforming oncology, offering innovative solutions for efficient, site-specific, and cost-effective cancer management.

Keywords: Nanotechnology, Nanoparticles, Cancer diagnosis, Tumors, Cancer treatment, Chemotherapeutic, Drug delivery, Nanomedicine, etc.

1 Introduction

Cancer's high death rate and considerable incidence have made it a global problem. For patients with cancer at various stages, surgery, chemotherapy, and radiation therapy have been common first-line

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treatment choices. Most cancer patients are treated with chemotherapy either before to or after surgery [1]. Chemotherapeutic drugs target fast-dividing malignant cells, but they also impact healthy cells that replicate quickly, such those found in the gastrointestinal system, hair follicles, and bone marrow. Chemotherapy damages organs and systems via a variety of ways, including as direct toxicity, indirect toxicity caused by liver metabolites, immune system suppression, decreased oxygen delivery, and inflammation [2]. The systems and organs impacted determine the precise negative consequences and damage manifestation. Chemotherapy dosage is often restricted as a result of these adverse effects, which lowers the effectiveness of the anti-cancer treatment. Current treatments that try to reduce these side effects are insufficient since they have negative side effects of their own [3]. Therefore, in order to continue full-dose chemotherapy, the adverse effects must be reduced. Therefore, creating new, enhanced, safer, and more targeted treatments is crucial for cancer patients. A number of strategies to broaden cancer treatment beyond conventional chemotherapy have surfaced in recent decades [4]. Deciphering molecular markers and discovering new treatment targets are made possible by advanced technology, such as genomic approaches, translation advancements, and protein processing breakthroughs. Models of cancer stem cells aid in the development of methods for comprehending the behaviour, treatment resistance, and tumour heterogeneity of cancer cells [5]. Examined in both in vitro and in vivo research, precisely tailored nanotechnology drug delivery systems transform therapeutic effectiveness by demonstrating adaptability in diagnostics and targeted therapies [6].

Nanotechnology-based drug delivery has great potential for cancer diagnosis and treatment with fewer side effects, as shown by recent advancements in nanomedicine. Although nanoparticles (NPs) are far smaller than cells, they are nevertheless big enough to contain a lot of small-molecule substances. In addition, NPs' vast surface area makes them very capable of functionalising with ligands, such as peptides, small molecules, and DNA or RNA strands [7].

A. Nanoparticles

The term nanoparticles (NPs) refers to particles that have a single dimension of less than 100 nm and unique properties that are often lacking in bulk samples of an identical substance. These may be categorised as 0D, 1D, 2D, or 3D based on the general form of the nanoparticle [8]. A nanoparticle's fundamentally complex composition is made up of its "surface layer, shell layer, and core", which is essentially its central portion and frequently referred to as the NP itself. These materials are very significant in transdisciplinary fields because of their exceptional qualities, which include their "high surface-to-volume ratio, dissimilarity, sub-micron size, and enhanced targeting mechanism" [4].

According to reports, the "enhanced permeability and retention (EPR)" effects of NPs is facilitated by their deep tissue penetration. Additionally, by successfully overcoming epithelial fenestration, the surface properties affect bioavailability and half-life. For example, NPs coated with the hydrophilic polymer polyethylene glycol (PEG) reduce opsonisation and evade immune system clearance [9]. Additionally, by adjusting the properties of particle polymers, the rate of release of the medication or active moiety may be optimised. Overall, the therapeutic impact of NPs in the prevention and therapy of cancer is determined by their distinctive characteristics [10].

B. Application of NPs in cancer diagnosis

In order to successfully treat and control cancer, early diagnosis is essential. There are a number of methods for diagnosing cancer, including physical examination, laboratory testing (such as blood and urine tests), biopsy, and imaging methods (such as X-ray, CT, MRI, and PET) [11]. Cancer identification has become much more accurate and quick because to modern diagnostic techniques, which also improve patient outcomes by enabling prompt treatment commencement. Nonetheless, more precise and non-invasive diagnostic techniques are still required, as is the creation of tailored strategies that take into account the particulars of each patient's malignancy [7].

NPs, like gold NPs in home pregnancy tests, have shown a lot of promise in a variety of medical testing and screening processes. Because NPs are inexpensive and may be used to identify any kind of cancer, they have gained interest in the field of cancer detection. They can capture cancer biomarkers including DNA, circulating tumour antigens, exosomes, and different cell types, including circulating tumour cells [11]. Assays based on NPs exhibit superior selectivity and sensitivity in comparison to current cancer diagnostic methods, resulting in early cancer diagnosis and improved prognostic results. Body fluids including urine and saliva, as well as tissues and blood, contain cancer indicators. The low quantities of biomarkers in bodily fluids, timing, and heterogeneity are only a few of the obstacles that may impede the early identification of biomarkers. NPs may, however, enhance biosensors for selective diagnostics due to their great sensitivity and selectivity in specifically targeting [12].

C. Significant challenges in the clinical application of nanoparticles

Today, the amount of research and data focused on nanoparticles has increased in tandem with the growth of nanotechnology. Few of them, however, really advance to clinical testing. In vitro and in vivo stages are where the majority of them stop. Clinical translation presents unique problems for each specific nano-formulation, however the majority of NPs encounter common issues that may be categorised into biological, technical, and study-design related issues [4].

Lack of routes of administration, reducing biodistribution, NPs' ability to pass through biological barriers, their toxicity, and degradation are examples of biological obstacles. It is difficult to remain and interact with the target region when NPs are administered intravenously because the blood absorbs them. This leads to the use of a high concentration drug that could not provide the desired therapeutic effects. However, this may be avoided since 3D magnetic flies have been used in a number of "in vitro and in vivo" studies to control NP movement in opposition to blood flow. There is still a need for further research on the impact of magnetic fields on human beings, the crosstalk among magnetic fields, and a variety of other nanoparticles [13].

To regulate the biological fate of NPs is a challenging endeavour that necessitates a significant amount of attention. The potential for lung, liver, and kidney harm exists, regardless of whether nanoparticles are made from biosafety materials and are appropriately calibrated to extend their retention period and half-life. Certain variables that influence toxicity include particle shape and size, surface area, solubility, and agglomeration. "Oxidative, cytotoxic, and inflammatory consequences" have been observed in

conjunction with an increase in lung deposition caused by NPs. According to research, the healthy cells are frequently damaged by the free radicals that are generated by NPs. NPs that are derived from more biocompatible materials, including chitosan, and compounds that decompose when exposed to near-infrared light, are potential remedies [14].

2 Literature Review

(Wang et al., 2024) [15] Drugs or gene fragments may be efficiently delivered to tumour tissues by nanoparticles using active or passive targeting techniques, improving therapeutic results while causing the least amount of damage to healthy cells. The treatment effectiveness of malignant tumours may be improved by using nanoparticles in conjunction with photothermal therapy and radiation sensitisation. The use of nanotechnology in both the detection and treatment of malignant tumours is summarised in this review along with an overview of the literature. We examine the latest advancements in nanotechnology applications in relation to oncological illnesses that originate from many bodily systems and combine the pathophysiological characteristics of tumours at several locations. The promises and difficulties of nanotechnology in cancer are finally briefly covered.

(Kemp & Kwon, 2021) [16] Nanotechnology has gradually spread into the fields of imaging, diagnostics, radiation, and cancer treatment, proving its ability to enhance each and improve patient care. Nanomaterials provide a wealth of adaptability, usefulness, and uses for developing robust imaging modalities, improved radiation adjuvants, precisely targeted cancer medication, and precise early-detection tools. This study sheds light on the present preclinical and clinical nanotechnological uses for radiation treatment, imaging, diagnostics, and cancer medication therapy.

(Yu et al., 2021) [17] Nanoparticle technology offers a new way to improve on conventional therapies and diagnostics. However, there aren't many published clinical studies on nanoparticles, and the majority of research on them is being conducted in vitro and in vivo. Initially, this investigation offers a comprehensive examination of the present applications of nanoparticles in the detection and treatment of cancer. Then, using the most recent two years' worth of updated research, we suggest the problems impeding the clinical use of NPs and provide workable remedies. Our thoughts on the potential advancements of NPs in tumour detection and therapy will be presented at the conclusion.

(Alrushaid et al., 2023) [18] Numerous medications are currently available or coated with nanoparticles to ensure that they directly target tumours or damaged organs without compromising healthy tissues or cells. According to several studies, nanoparticles' antioxidant properties and ability to prevent tumour development give them inherent anticancer efficacy. Additionally, medications may be released more efficiently and with fewer adverse effects when nanoparticles are used to allow regulated release. The molecular imaging agents employed in ultrasonography are nanomaterials such as microbubbles. In this investigation, the various types of nanoparticles that are frequently employed in both the identification and treatment of cancer are examined.

(Dessale et al., 2022) [9] Nanotechnology has the potential to be a viable technology for the in vivo imaging and identification of cancer cells and biomarkers, given its extensive spectrum of applications.

The use of nanotechnology in cancer treatment may provide a rapid, secure, economical, and successful approach. Moreover, it offers concurrent cancer diagnosis and therapy via the use of nano-theragnostic particles that promote early identification and cancer cell degeneration. The best cancer diagnostic, therapy, and management alternatives must be chosen based on current and updated talks, and it is crucial to get fresh knowledge about creating efficient protocols. In addition to providing insights for the field's future, this paper discusses the utilisation of nanotechnology in cancer diagnosis, therapy, and prognosis.

(Ganesh et al., 2022) [11] Nanotechnology has enormous potential to transform the way physicians identify and treat cancer patients. Nanotechnology is already significantly influencing patient care, but it also presents significant challenges for the future, such enhancing the engineering and design of materials that target cancer. There has been a lot of work done in the last several years. committed to developing nanotechnology to reduce and enhance the dispersion and toxicity of anticancer therapies in healthy tissues, as well as the transport of anticancer drugs to tumour tissue. Many things have changed. Polymer Carbon, liposomes, dendrimers, nanoparticles, and nanoshells Novel platforms for nanotechnology include nuclei acid-based nanoparticles, superparamagnetic nanoparticles, and nanotubes.

(Zhu et al., 2022) [19] A variety of nanomaterials are used in the treatment of cancer. In order to boost medication capacity and bioavailability while overcoming cytotoxicity and limited selectivity, nanomaterials have been created for cancer therapies. Only a small number of nanodrugs have received approval for clinical use, despite the growing number of related research. Studies on targeted medication delivery using nanocarriers are required to enhance the translation of these materials. It is still necessary to address cytotoxicity, increased permeability and retention effects, and the protein corona's protective function. In this mini-review, novel nanomaterials produced in research and clinical settings are compiled, existing obstacles to their clinical adoption are examined, and the successful use of nanoparticles in cancer therapy is discussed.

(Kumar et al., 2024) [20] Nanotechnology has enabled the introduction of nanoparticles that might passively collect at tumour sites, making them a perfect alternative to conventional cancer treatment techniques. Nanoparticles have advantages such as reduced toxicity and biocompatibility, which make them suitable for targeted drug delivery. The high surface to volume ratio of nanoparticles aids in the binding, absorption, and transportation of small biomolecules, including protein molecules, ribonucleic acid drugs, and deoxyribonucleic acid, to the targeted site, enhancing the effectiveness of therapeutic agents. The aforementioned benefits make them significantly different and more successful than traditional cancer treatment methods. This paper will provide an overview of medication delivery using nanovessels and nanoparticles for cancer diagnosis.

3 Conclusion

With its great sensitivity, specificity, and multifunctionality, nanotechnology is essential to transforming cancer detection and therapy. Despite advancements in nanoparticle (NP) engineering for targeted drug delivery, challenges remain in enhancing selectivity, sensitivity, and optimal pharmacokinetics.

Multidrug resistance (MDR) may be overcome by combination therapy thanks to "NP-based drug delivery systems (DDS)", which provide enhanced biocompatibility, tumour targeting, and stability. Various NPs, including polymeric, metallic, and hybrid types, have shown promising results, yet understanding their toxicity and interaction with biological systems remains critical. Nanomedicine enables theragnosis, integrating diagnosis and treatment into a single platform, improving patient survival rates. Liposomal and protein-based nanomedicine formulations are already in clinical use, with many undergoing advanced trials. Nanocarriers offer site-specific drug delivery, reducing toxicity while enhancing therapeutic efficacy. Personalized cancer therapy benefits from nanotechnology's ability to penetrate and retain within tumors effectively. However, optimizing NP design and engineering remains essential for their full potential in clinical applications. Nanotechnology, with its ongoing developments, has the potential to revolutionise cancer treatment by improving focused therapy, reducing side effects, and increasing patient outcomes in general.

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Advancements in anticancer Drug development: Challenges and solutions

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Abstract

A local disease that may spread and affect other organs or vital functions is what cancer is, an occurrence of uncontrolled cell growth that results in the formation of an abnormally developing tumour. Cancer is one of the most deadly illnesses in modern times, taking countless lives every year. Variations in the illness throughout the world, the influence of accessible medical facilities, and other socioeconomic concerns have all affected the successful care of this disorder. In this article, review the various literature's study on the challenges and solution in anticancer drug development. From the review it concluded that development of anticancer drugs remains challenging due to high costs, long timelines, and frequent failures. While progress has been made, obstacles like toxicity and poor efficacy persist. Machine learning (ML) is transforming drug discovery, especially for natural product (NP)-derived therapies, yet more ML tools are needed. Nanocarrier advancements, combined with ML, enhance drug delivery and reduce side effects. Novel heterometallic complexes and heterocycles further improve treatment. Integrating NP-based chemotherapies with deep learning offers promising results, emphasizing the need for innovation, collaboration, and technology-driven approaches to develop more effective cancer therapies.

Keywords: Anticancer drug development, Machine learning (ML), Natural product (NP), Drug discovery and delivery, Cancer treatment, etc.

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1 Introduction

The condition known as cancer is complicated and is brought on by malignant cells that divide and spread throughout the body all the time. It is also known as a category of disorders with distinct altered dynamics and behaviours. Prostate, colon, skin, lungs, breast, and many other parts of the body may all be affected by cancer. Sustainability, societal development, and the viability of all statuses are important factors in medical research and innovation when it comes to predicting the danger of cancer in the future [1]. Anticancer medication development is a priority in order to give more effective therapy. Because cancer is a collection of illnesses that are not under the control of the cancer cells' numerical increase. Historically, anticancer medications have been an important part of the many cancer therapy approaches [2].

The disease known as cancer occurs when cells proliferate out of control, creating tumours that grow abnormally and have the potential to spread to other organs or critical systems, affecting their functionality. Cancer is considered a multifactorial illness since it is caused by genetic mutations, pollution, dietary toxins, viruses, chemicals, and ionising radiation, among other determining factors [3]. The production of two genetically identical cells is ensured by the strict regulation of cell division by a number of evolutionarily conserved cell cycle regulatory systems. Many people die from cancer every year, making it one of the deadliest diseases in modern history. This illness's global variances, the influence of accessible medical facilities, and other socioeconomic conditions have all affected how this disease should be managed [4], [5].

A. Natural products significance in Anticancer drugs

Natural products' diverse and complex chemistry, which has evolved over millions of years via natural selection, makes them important in the hunt for anticancer medications. For many years, natural materials derived from plants, microbes, and marine life have provided a plentiful supply of lead compounds for the production of pharmaceuticals, particularly anticancer drugs [6]. These compounds are well suited to target specific molecular pathways that contribute to the development of cancer since they often possess unique bioactive properties and complex molecular scaffolds. Furthermore, screening and optimising processes may access a vast chemical diversity pool present in natural products to identify novel treatment options with enhanced potency or selectivity [2].

B. Challenges in Unsustainable Sourcing

A lot of complex ethical, social, and environmental issues are brought up by non-sustainable sourcing in the development of anticancer drugs. Unsustainable sourcing methods have the potential to decrease biodiversity and cause major ecological impact [7]. Examples include over-harvesting medicinal plants and indiscriminately removing natural resources from delicate ecosystems. This habitat loss not only endangers plant and animal species, but it also puts medicinal plant populations at risk of extinction, which might make the present search for novel drugs more difficult [8]. Negative social and economic effects may also result from unethical sourcing, especially in places where populations who rely on

natural resources for their lives dwell. Overuse of medicinal plants may cause social discontent about resource allocation and access, worsen poverty, and upend traditional knowledge networks [2].

C. Economic challenges in healthcare

Significant development and research as well as financial backing are necessary when creating any form of product. However, lack of accessibility, excessive expense, and stifled innovation make the task more difficult. The cost of development is increasing daily due to the long timetable and high failure rate of newly developed techniques. Moreover, clinical studies, clearances, and other very demanding procedures must be completed by the original testaments. It continually maintains the chronology [9]. The cost of the product is also a barrier for the average person, making it more difficult for them to get these therapies. It is an economic challenge to go through the whole process of studying their medicine, producing a solution, and then making it affordable and sustainable for regular people [2].

D. Challenges in Advancing Sustainability Goals

Advancement of sustainability goals in anticancer drug research is difficult; there are several complex obstacles that need concerted efforts from stakeholders across numerous sectors. Reducing the obstacle to sustainability and profit in the pharmaceutical industry is the primary problem while producing anticancer medications. Because they fall under the green energy principles, distribution networks and local medicine manufacturing may help with this issue [10]. However, putting these ideas into practice with a viable business plan and educating healthcare professionals about the emerging technologies might be difficult. Furthermore, because it might take a lot of time and money to change and reverse anything on a large scale, the legislative environment makes it challenging to incorporate sustainable ideas into the continuing regulatory management system [11].

E. Drug Resistance in Cancer Treatment

Drug resistance is one of the most challenging issues to address when using anticancer medications to treat cancer. It happens when the cells adjust to the alterations, become less aggressive towards the cancer cells, and the rate of death falls. Genetic mutation, DNA repair processes, tumour microenvironment, drug efflux, and other factors are among the mechanisms behind medication resistance [12]. The last several decades have seen the introduction of a variety of therapeutic approaches for these processes, including immunotherapy, combination therapy, and adaptive therapy. However, despite these sophisticated therapeutic approaches, it still reduces the effectiveness of therapy. The aforementioned treatments have little effect on cancer cells that are primary resistant [13]. It may happen because of genetic variation or because the tumour cell previously included drug-resistant subpopulations. Conversely, acquired resistance occurs as a result of the selection pressure that is established during therapy. Professionals in medicine are now testing novel methods via a variety of medical trials and use biomarkers to anticipate resistance in advance [14].

F. Access to Anticancer Drugs

One crucial component of cancer treatment that presents difficulties worldwide is equitable access to anticancer medications. Access discrepancies may be caused by a number of things, such as legislative barriers, healthcare infrastructure, and economic differences. Many patients have financial obstacles due to the high cost of many anticancer medications, especially targeted treatments and immunotherapies [15]. Patients and healthcare systems are both affected financially, which often forces them to make tough decisions about how affordable treatments may be. Access issues are made worse in low-resource areas by a lack of specialised cancer facilities and a limited healthcare infrastructure [16]. Unfavourable results for patients in these areas are caused by insufficient treatment choices, delays in diagnosis, and a shortage of qualified healthcare providers. International efforts are being made to improve access to necessary anticancer drugs in order to alleviate these inequities [4]. Initiatives include assistance for low-income nations to improve their cancer care infrastructure, pricing negotiations with pharmaceutical corporations, and the creation of reasonably priced generic versions of important anticancer medications. Additionally, studies into telemedicine and cost-effective treatment methods seek to reach underprivileged groups with cancer care [17].

2 Literature Review

(Das & Agarwal, 2024) [18] To far, several phytocompounds have been used in the development of novel cancer treatments. The discovery of novel anti-cancer leads is a goal of pharmaceutical corporations and academics worldwide, and phytocompounds are a promising source in this pursuit. At the same time, because of their efficiency, reduced time-consuming nature, and cost-effectiveness, computational approaches such as virtual screening (VS), molecular dynamics (MD), pharmacophore modelling, Quantitative structure-activity relationship (QSAR), network biology, and machine learning (ML) have grown in popularity in recent years. In light of this, the current study compiles data on plant-based compounds found by in silico cancer lead acquisition strategies.

(Chunarkar-Patil et al., 2024) [19] Underlines the importance of natural products in the drug development process and explores the potential for collaboration between them and computational methods. Withaferin A and betulinic acid are two instances of in vitro and in vivo research that have shown the shift from computational to experimental validation. From preclinical research to clinical trials, the road towards medicinal uses has been shown by clinical studies of substances like silvestrol and artemisinin. Additionally, the difficulties and constraints in creating natural compounds as possible anti-cancer medications are discussed in this article. Additionally, expanding the anticancer potential of natural products may be possible via the combination of deep learning and artificial intelligence with conventional computational drug development techniques.

(Gach-Janczak et al., 2024) [20] For many years, chemists and pharmacologists have been actively searching for novel anticancer medications, either by screening hundreds of synthetic molecules or by isolating chemicals with deadly qualities from plants. Potential novel anticancer treatment candidates must be able to stop the growth of cancer cells and/or cause them to undergo apoptosis without seriously

harming healthy cells. While long-term study led to the discovery of certain anticancer chemicals, others were found by chance. A short history of the creation of the most significant classes of anticancer medications is provided in this article, emphasising the fact that each of them has a wide range of adverse effects.

(Tadesse et al., 2023) [4] Summarising previously published publications about current developments in anticancer medication discoveries was the goal of this research. Many discoveries are found via searches and categorised as plant-derived advancements, chemical compounds with in vitro or in vivo cytotoxic drug development, repurposing advances, and anticancer drug targets. In this overview, several recent developments in anticancer drug discovery are summarised based on a range of scholarly papers. Plant-derived breakthroughs in cancer therapy, certain pharmaceuticals repurposed for cancer treatment, prospective and clinically supported pharmacological targets for anticancer drug binding, and, lastly, advancements in new chemical compounds in the field of cancer therapy are discussed under this wide subject.

(Alqosaibi, 2022) [21] Heart disease is the leading cause of mortality worldwide, with cancer coming in second. To address this illness, many strategies have been devised, including as chemotherapy, radiation treatment, and surgery. Certain cancer cells may withstand apoptosis and become resistant to chemotherapy, despite the fact that its main purpose is to regulate cell division and cause cell death. Chemotherapy might have more negative consequences than positive ones, and the side effects are sometimes unbearable. Additionally, there is a great need for a dependable delivery system that guarantees prompt and precise treatment targeting since the stability and bioavailability of medications used in chemotherapy are important concerns that need to be addressed. We go over the many kinds of nanocarriers, their characteristics, and the latest developments in formulations in this overview, along with the pertinent benefits and drawbacks of each.

(Lu & Lu, 2020) [22] Developing and discovering high-quality anticancer drugs is more challenging and demanding than ever before. Overall, we need to rethink and reorganise biomedical, pharmacological, technological, and economic issues. While we have come a long way, there are still many problems and challenges from the past. This article presents interdisciplinary viewpoints on the discovery and development of anticancer drugs in an effort to address such types of biological therapeutic challenges and dilemmas.

(Singh et al., 2016) [23] Numerous signalling events are involved in the intricate process of carcinogenesis. Because of their pleiotropic properties, which allow them to target these events in a variety of ways, phytochemicals are the best candidates for the creation of anticancer drugs. The development of lead candidates from phytochemicals that may prevent or slow the spread of cancer without causing any negative side effects is underway. Numerous phytochemicals have both in vitro and in vivo anticancer properties. The action mechanisms of these lead phytomolecules on cellular and nuclear components implicated in carcinogenesis are discussed in this article. There has also been discussion of the clinical development of anticancer phytomolecules and druggability factors.

3 Conclusion

In conclusion, the development of anticancer drugs remains one of modern medicine's most significant challenges, marked by high costs, lengthy timelines, and a high failure rate. Despite considerable progress, the path from preclinical discoveries to clinical approval continues to be fraught with obstacles such as lack of clinical efficacy, toxicity, and unfavorable physicochemical properties. However, the integration of machine learning (ML)-based approaches in drug discovery, particularly for natural product (NP)-derived anticancer agents, offers promising opportunities. While existing databases like NPACT and AfroCancer are crucial, the need for more publicly available ML tools tailored to NP-based drug discovery is evident. Moreover, advancements in nanocarriers for drug delivery, combined with ML algorithms, enhance drug bioavailability and cytotoxicity while reducing side effects. Emerging compounds, such as novel heterometallic complexes and heterocyclic substances, further improve therapeutic outcomes. These developments highlight the growing potential of merging traditional natural product-based chemotherapies with cutting-edge technologies, such as deep learning, to improve cancer treatment efficacy. The future of anticancer drug development lies in continuing innovation, fostering collaboration, and embracing new technologies to create more precise, effective therapies for cancer patients.

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The Impact of Artificial Intelligence in Drug Discovery

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Abstract

The pharmaceutical industry is crucial to developing new therapies and managing complicated illnesses. However, there are many risks, costs, and hours spent on the process of finding new medications. Recent years have seen the rise of artificial intelligence (AI) as a powerful tool that has revolutionised a number of sectors, including healthcare. The many research that have been done on how artificial intelligence affects medication development are reviewed in this article. It concluded that AI technology is revolutionizing drug discovery with its predictive accuracy, enhancing productivity, patient outcomes, and personalized care. It aids in early disease prediction, personalized medicine, dose optimization, and treatment outcome prediction while reducing the reliance on in vivo bioassays. AI also accelerates drug discovery by autonomously designing and testing compounds. Its role in identifying treatments for chronic diseases and rapid drug development during pandemics underscores its transformative impact. Moving forward, interdisciplinary collaboration, robust datasets, and continued investment will be crucial for seamless AI integration in pharmaceuticals, ensuring faster, more efficient drug discovery with minimal side effects and maximum therapeutic benefits.

Keywords: Artificial intelligence (AI), Drug discovery, Pharmaceutical sector, Healthcare, Machine learning, Drug development, etc.

1 Introduction

With a collection of sophisticated computational tools geared to enhance rather than replace human skills, artificial intelligence (AI) represents a paradigm change in drug development. Fundamentally,

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artificial intelligence (AI) transforms the pharmaceutical industry by using complex algorithms to make decisions on its own based on data analysis [1]. The whole drug development process, from molecular biology and computational chemistry to lead compound optimisation and clinical trial design, might be greatly streamlined by this technique. AI applications facilitate processes such as "protein-ligand docking, molecular dynamics simulations, virtual screening, and de novo drug creation" with previously unheard-of precision, thereby expediting the discovery of potential drug candidates and generating new therapeutic opportunities [2]. Furthermore, drug development tactics are changing as a result of AI's contributions to clinical trial design, drug-target interaction prediction, and systems pharmacology. To improve trial efficiency and results, the technology helps with patient selection optimisation, real-time patient reaction tracking, and protocol adjustments. To ensure that ethical concerns, legal compliance, and scientific rigour are upheld, it is imperative to integrate AI with caution [3].

A. Artificial intelligence's function in medication development

The divide across drug discovery and development is widening as a result of the ongoing expansion of chemical space, which is making it more challenging and time-consuming to identify new medicinal compounds. In recent years, there has been a significant increase in the visibility of the potential of "artificial intelligence (AI)" to revolutionise the pharmaceutical industry through its implementation in medicinal chemistry [4]. Medicine discovery is a challenging and time-consuming process that has historically included labour-intensive techniques like high-throughput screening and trial-and-error research to uncover and create new treatments [5]. However, "machine learning (ML) and natural language processing" are two examples of artificial intelligence (AI) approaches that may speed up and enhance this process by allowing more accurate and efficient analysis of massive volumes of data [6], [7]. Consequently, AI-based methods are very beneficial throughout the drug development process, especially in the areas of target identification and validation, medication modelling, and druggable property improvement. Additionally, since patient-centered clinical trials allow for better decision-making, they are essential [8], [9].

A system that employs a network of artificially linked neurones and communicates with them to carry out different data transformations is known as "a Deep Neural Network, or DNN". The criteria for classifying drugs into their different therapeutic classes are developed using pharmacological and toxicological data. For instance, new generation AI approaches are developed using Generative Adversarial Networks (GANs) as its base. The foundation of "artificial intelligence (AI)" is machine learning. This field's base is the application of statistical characteristics [10].

B. Fundamentals of artificial intelligence

AI mimics cognitive processes in the human brain and is responsible for a number of computing technologies. Three categories of artificial intelligence devices include "machine learning, deep learning, and natural language processing". The ability of AI technologies to handle and analyse raw data varies, including "machine learning, natural language processing, and deep learning" [11]. Certain AI methods, including data analysis and predictive modelling, may analyse enormous amounts of data before devising

a suitable strategy. One person provides a definition of artificial intelligence. A computationally intelligent program or gadget that can do intricate tasks is called artificial intelligence [12]. Among the various AI technologies accessible are deep learning, machine learning, and natural language processing. In the pharmaceutical industry, ML may be responsible for managing and treating disease. Guidelines for drug development are among the many ethical and moral issues surrounding AI's uses [13]. Machine learning's potential is shown via data analysis, predictive modelling, and sophisticated algorithms. The data-driven approach, in other words, combines data from many sources to generate, repurpose, and identify therapy targets. In a variety of illnesses, the DL of AI may counteract several biological approaches. Drug target locations may be located with the use of artificial intelligence systems. Precision pharmacotherapy may be closer than previously thought thanks to AI's increasing success [14].

C. "Applications of ai in drug discovery and development"

The discovery-to-market pipeline encompasses a variety of research and development operations in which AI may be used. This section attempts to provide readers a knowledge of some possible application areas where AI might be used to help research and process inefficiencies, even if the challenges of drug development are widely established [15]. AI has the ability to greatly simplify the process of finding possible therapeutic targets. Because a protein target may be able to bind to a wide variety of chemical compounds, there are many subfields devoted to optimising virtual screening and compound creation. Particular examples of how AI engines have been effectively used in pharmaceutical research to get novel compounds to clinical trials or the market sooner than with conventional methods can already be cited [16]. Researchers can also better handle complex interactions and raw data when AI is used in drug development and discovery. Finding novel reagents, biological pathways, and indications for small compounds that are presently on the market may be greatly aided by genetic and imaging data. Nevertheless, it is difficult to manually analyse or use conventional statistical methods on datasets this huge [17]. Additionally, using AI to analyse this data may help advance predictive analytics, which enables lifestyle medications, including pain and weight-loss medications, to be tailored to the unique metabolic and genetic characteristics of potential patients. Given that most individuals react differently to the same piece of treatment depending on these variables, personalised medications will become more and more significant in the healthcare industry [18].

2 Literature Review

(Niazi & Mariam, 2025) [12] In order to treat both common and uncommon illnesses, generative AI is speeding up the creation and reengineering of pharmaceutical compounds. New compounds for idiopathic pulmonary fibrosis and HLX-0201 for fragile X syndrome have entered clinical trials, despite the fact that no AI-generated medication has received FDA approval as of yet. However, because of algorithmic bias and a lack of model transparency, AI models are often seen as "black boxes," which limits their potential and makes it difficult to grasp their results. The process and financial risks of bringing new medications to market have been accelerated by AI-driven drug discovery, which has significantly lowered development timeframes and prices despite these challenges. It is anticipated that

AI will continue to have a favourable influence on pharmaceutical innovation in the future, accelerating, improving, and expanding the development of life-saving drugs.

(Yadav et al., 2024) [8] This brief provides an overview of how AI is revolutionising the pharmaceutical industry, speeding up the development of new pharmaceuticals, and assisting in drug discovery. Various phases of the drug development process are changing as a result of AI approaches including "machine learning and deep learning". This article shows how AI helps with drug development via "target identification, lead compound optimisation, medication design, drug repurposing, and clinical trial improvement". Integration of AI may speed up the development of new therapies, reduce expenses, and enhance patient outcomes. Laws, algorithm interpretability, and data accessibility concerns must be addressed if artificial intelligence is to reach its full potential in pharmaceutical research and development.

(Rehman et al., 2024) [19] Examine the finding of "leads, diagnostics, target identification, screening, and disease" identification as part of the drug development process. In these phases, artificial intelligence's capacity to examine large datasets and identify trends is crucial, improving forecasts and efficiency in the management of clinical trials, drug development, and illness detection. It is emphasised that AI can examine vast volumes of data and expedite the creation of new medications, reducing the time and cost associated with introducing new medications to the market. This article discusses the significance of data quality, algorithm training, and ethical issues, particularly when managing patient data during clinical trials. AI promises to revolutionise medication creation by taking these aspects into account, with major advantages for both patients and society.

(F., 2024) [14] By increasing productivity, cutting costs, and shortening turnaround times, the pharmaceutical industry is undergoing a revolution thanks to the use of artificial intelligence (AI) into drug research and development. Artificial intelligence (AI) can evaluate enormous volumes of biological and chemical data, forecasting molecular interactions and improving compound design by using machine learning, deep learning, and natural language processing. The present and prospective uses of AI in drug research are reviewed, along with the difficulties in implementing it and the revolutionary potential of AI to improve personalised treatments and precision medicine. Notwithstanding developments, technological, moral, and legal obstacles have prevented AI from reaching its full potential in drug discovery.

(Visan & Negut, 2024) [20] Examine the utilisation of a variety of AI methodologies, such as deep learning and machine learning, in the areas of drug development, virtual screening, and target identification. It highlights AI's potential to completely transform medicine delivery systems by discussing its role in repositioning current medications and identifying pharmacological combinations. The paper highlights the technological advancements and possible future directions in the area of drug discovery while providing a comprehensive review of the AI platforms and algorithms now in use. In addition to outlining the existing status of AI in drug development, this paper projects its future course, emphasising the benefits and difficulties that may arise.

(Blanco-González et al., 2023) [3] demonstrates the potential of artificial intelligence (AI) in drug development and offers information on the obstacles and possibilities for achieving this promise. The purpose of this paper was to evaluate ChatGPT's (a chatbot built on the GPT-3.5 language model) capacity to help human writers write review articles. The AI's capacity to produce material autonomously was assessed using the text that was produced by it after we gave it instructions (see Supporting Information). The human writers essentially updated the document after completing a comprehensive review, making an effort to strike a compromise between the initial concept and the scientific standards. The last part discusses the benefits and drawbacks of employing AI for this purpose.

(Narayanan et al., 2022) [21] The introduction of artificial intelligence caused a change in the way that different phases of drug development were conceptualised. Artificial intelligence may assist shorten the time required for each step of the drug development process. Numerous pharmaceutical firms are using AI-based drug discovery techniques to treat a range of illnesses, including diabetes, Alzheimer's, Parkinson's disease, obsessive compulsive disorder, and more. AI is additionally employed in the development of products for the production of nanorobots and nanomedicines. The fact that so few AI-based medications are now undergoing clinical trials suggests that AI-driven drug development is expanding. We have emphasised the use of AI in pharmaceutical product development and drug discovery in this study.

3 Conclusion

By increasing predicted accuracy and efficiency, the pharmaceutical industry has undergone a revolution thanks to the use of "artificial intelligence (AI) in drug research". AI enables early disease prediction, personalized medicine development, dose optimization, and treatment outcome forecasting. Additionally, it forecasts off-target effects and drug-like qualities, which minimises the necessity for in-vivo bioassays and demands less thorough experimental validation, thereby lowering animal deaths. Applications of AI go beyond drug development to include nutrigenomics, mRNA vaccination, healthcare administration, and surgery. For AI to be adopted smoothly, cooperation between biologists, regulatory agencies, and AI specialists is essential. Drug development will be accelerated by automation-driven decision-making, which will allow AI to create and test molecules on its own. AI-driven medication development is only possible with strong datasets and continuous investment in AI technologies. In order to find treatments for debilitating diseases like diabetes, Alzheimer's, and Parkinson's, prominent pharmaceutical companies are using artificial intelligence. The shift towards AI-based drug discovery has proven especially beneficial during the COVID-19 pandemic, accelerating the identification of potential therapies with optimal efficacy and minimal side effects. AI continues to redefine pharmaceutical research, offering transformative solutions for faster, more precise, and cost-effective drug development.

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Emerging Contaminants in Water: A Review of Detection and Remediation Techniques

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Abstract

The enduring nature and possible health hazards posed by emerging contaminants (ECs) in water sources have sparked worldwide alarm. The development of enhanced remediation techniques is imperative, as conventional water treatment procedures may not always be sufficient to eliminate these contaminants. This study discusses many ways of detection and treatment, with a focus on nanotechnology, membrane filtration, and photocatalysis. Photocatalytic breakdown using semiconductor materials like titanium dioxide and metal-organic frameworks has been shown to work very well under UV and visible light. Moreover, micropollutants may be efficiently removed by membrane filtration techniques like as reverse osmosis and ultrafiltration. The study emphasises sustainable and ecologically friendly synthesis methodologies as a mechanism for nanomaterials to enhance pollutant degradation. Despite promising advancements, further optimisation is required for practical applications in the areas of increasing catalyst stability, cutting costs, and widespread implementation. Multidisciplinary research may help to solve these problems and provide sustainable water treatment solutions. To reduce the impact of ECs on aquatic ecosystems and human health, it is critical to incorporate hybrid technologies and examine their environmental and economic feasibility.

Keywords: Emerging contaminants, photocatalysis, membrane filtration, nanotechnology, water treatment

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1. Introduction

Research on emerging contaminants has recently become popular. Regulatory authorities are faced with a significant issue due to the high number of emerging contaminants. In order to address emerging contaminants, how should we prioritise research? Since we know so little about the environmental behaviour of these novel compounds and their potential harmful impacts on humans and ecosystems, how can we prioritise the establishment of quality standards for them? Academics' demands for more funding and attention for their studies likely contribute to the current fascination in emerging contaminants. Keeping up with the latest developments is crucial for researchers who are trying to get funding. (Finčur et al., 2021)

Because of her 1962 book "Silent Spring," Rachel Carson is likely to be credited with the "emergence" of knowledge on emerging contaminants (Kokkinos et al., 2020). As the title suggests, she provided compelling evidence that the extensive use of DDT to eradicate mosquitoes and other pests had resulted in the extinction of several bird species (Morin-crini et al., 2022). Carson faced significant backlash for her audacity in questioning the many societal advantages associated with pesticide use, particularly DDT. Here we see how an environmentalist sounded the alarm, and how academic research subsequently backed up the alarm with factual data and uncovered the truth and dangers associated with DDT—which had been synthesised approximately a century prior to Carson's book and had been liberally distributed during the second world war—proving her right and leading to its eventual ban (Lin et al., 2023). The message that pesticides and chemicals in general may be dangerous was brought to our attention by her, and we are grateful to her.

The first step in addressing "emerging contaminants" is to clarify our objectives. Something that was considered a significant concern with environmental contamination a decade or two ago may no longer be considered an emerging contaminant, since the definition of "emerging" is subjective (Mergenbayeva et al., 2021). Expanding the scope to include contaminants of emerging concerns, which have been present for some time but have just now come to light as a source of worry, and emerging contaminants, which have only recently emerged, would be a good place to start.

Concerns about the potential effects of contaminants of emerging concern (CECs) on aquatic life have led to an uptick in the detection of PPCPs and pharmaceuticals at low concentrations in surface water. The EPA must have a system in place to assess the possible effects of CECs and PPCPs on aquatic life and a method to establish safe limits for these creatures. (Kumar et al., 2022)

A. Categories of Emerging Contaminants

There are several sources from which emerging contaminants might develop, including pharmaceutical waste and agricultural runoff. The chemical composition, durability, and toxicity of these chemicals dictate their effects (Blasco & Tovar-Sánchez, 2022). The table below summarises the main categories of emerging contaminants and their most common locations.

Table 1 Categories of Emerging Contaminants and Their Sources

Category	Examples	Primary Sources	Potential Impact
Pharmaceuticals & PPCPs	Antibiotics, painkillers, cosmetics	Hospitals, households, wastewater plants	Antibiotic resistance, endocrine disruption
Endocrine-Disrupting Chemicals	BPA, phthalates, synthetic hormones	Plastic waste, industrial discharge	Hormonal imbalance, reproductive issues
Per- and Polyfluoroalkyl Substances (PFAS)	Fire retardants, non-stick coatings	Industrial effluents, consumer products	Carcinogenic potential, bioaccumulation
Pesticides & Herbicides	Glyphosate, DDT, organophosphates	Agriculture, runoff into water bodies	Aquatic toxicity, soil degradation
Microplastics & Nanoparticles	Synthetic fibers, plastic fragments	Textile industries, wastewater discharge	Marine pollution, ingestion by organisms

B. Detection Techniques for Emerging Contaminants

Due to their low quantities and complicated chemical structures, emerging contaminants in water must be detected using very sensitive analytical methods. Biosensors and real-time monitoring systems have gained popularity due to their efficiency and reduced operating costs, despite the fact that traditional techniques such as chromatography and spectroscopy are still frequently employed. (Coronado-Apodaca et al., 2023)

a. Chromatographic and Spectroscopic Techniques

Chromatography-based methods, including High-Performance Liquid Chromatography (HPLC) and Gas Chromatography-Mass Spectrometry (GC-MS), are highly effective in the identification and quantification of contaminants (Pontius, 2021). These methods give accurate results, but they need expensive equipment and a lot of work to get the samples ready.

Although spectroscopic techniques like ultraviolet-visible spectroscopy and fluorescence spectroscopy provide rapid analysis, they may lack specificity when analysing complex mixtures. Improved detection sensitivity for trace-level contaminants has been achieved with recent improvements in Surface-Enhanced Raman Spectroscopy (SERS).

Table 2 Advantages and Limitations of Detection Techniques

Technique	Advantages	Limitations
HPLC & GC-MS	High accuracy, precise quantification	Expensive, requires skilled operators
UV-Vis Spectroscopy	Fast, cost-effective	Limited sensitivity for complex samples
Biosensors	Real-time monitoring, eco-friendly	May suffer from interference effects
SERS (Surface-Enhanced Raman Spectroscopy)	Ultra-sensitive, detects low concentrations	High equipment cost, complex calibration

C. Remediation Techniques for Emerging Contaminants

Traditional treatment procedures, including filtration and coagulation, are often inadequate because many emerging contaminants are resilient (Wells, 2013). Three sophisticated remediation techniques—adsorption, oxidation, and biological degradation—have gained attention recently.

a. Advanced Oxidation Processes (AOPs)

In order to degrade contaminants into less dangerous byproducts, AOPs produce very reactive hydroxyl radicals (•OH). Among these methods are Fenton reactions, ozonation, and photocatalysis, which employs materials such as titanium dioxide (TiO_2).

b. Biological Treatment Methods

To eliminate contaminants in a more organic way, biological methods include phytoremediation and microbial decomposition. Constructed wetlands are being used for cost-effective remediation due to the ability of aquatic plants to absorb contaminants. (Mathew & Kanmani, 2020)

Table 3 Comparison of Remediation Techniques

Method	Principle	Effectiveness	Challenges
Activated Carbon Adsorption	Adsorbs contaminants on porous surfaces	High removal efficiency for organic pollutants	Requires frequent regeneration
Ozonation	Generates ozone to break down pollutants	Effective for persistent contaminants	High operational costs
Photocatalysis	Uses light-activated catalysts	Sustainable, energy-efficient	Limited efficiency in turbid water
Bioremediation	Microorganisms degrade pollutants	Eco-friendly, cost-effective	Slower process, requires optimal conditions

2. Literature Review

(Bratovčić, 2023) Compared to traditional treatment procedures, organic contaminants (drugs, agrochemicals, and colours) need new, more sophisticated approaches to water purification due to their chemical complexity. Photocatalytic degradation is one approach. Scientists clearly elucidated the process by which toxic organic compounds are degraded by using semiconductor materials with photocatalytically active characteristics in conjunction with ultraviolet or visible light. We will go over the procedures and components that go into making the most recent photocatalysts, how stable they are, and what percentage of organic contaminants they remove. To activate them using visible light and reduce electron and hole recombination, as well as to achieve a stronger photocatalytic impact in degradation, we provide a diverse selection of components for the development of distinct composite photocatalysts. Real wastewater samples, rather than the typical synthetic solutions of specific organic contaminants that have been extensively examined thus far, should be used in future trials.

(Arman et al., 2021) Several relevant topics regarding EPs in aquatic environments, including strategies for eliminating EPs, were examined in the review. While there are pros and cons to each method, EPs treatment procedures include physico-chemical, biological, and advanced oxidation procedures, among others. However, ultrafiltration, a membrane-based filtration approach, is seen to be one of the technologies that offers the most potential for micropollutant removal in water. This treatment strategy is more popular than traditional ones due to its fascinating qualities, such as a modest working way and remarkable selectivity. This paper provides a thorough overview of EP, including its environmental presence, health effects, and possible remediation and removal methods.

(Datta & Roy, 2023) The review covered photocatalysis, which has shown great promise in the degradation of organic contaminants and the disinfection of water in wastewater treatment. Photocatalytic applications for wastewater treatment have recently seen advancements such as: Inorganic photocatalysts: Titanium dioxide (TiO2) and other conventional photocatalysts work best in the very narrow range of ultraviolet (UV) light, which is only a fraction of the total solar energy. Photocatalysts that respond to visible light, such carbon nitride, perovskites, and metal sulphides, have recently been the focus of research and development. Energy efficiency and cost-effectiveness are enhanced by these materials' ability to use a wider range of the solar spectrum.

(Heydari et al., 2019) The study looked at the passive form of solar photocatalysis and how effective it was. A common photocatalyst in a passive system was buoyant anatase TiO2-coated hollow glass microspheres. The chosen model contaminants were Killex®, CPA, and sulfolane. While 2, 4-D was degraded to a maximum of 99.8% in the Killex® solution, sulfolane was degraded to 97.4% and CPA to 100% in aqueous solutions, respectively. Dicamba and MCPP were totally destroyed in the solution. With catalyst loadings of 4.78 mg/cm2 and 11.95 mg/cm2, respectively, the total organic carbon (TOC) of Killex® samples was decreased by 53% and 88%. At catalyst loadings of 4.78 mg/cm2 and 11.95 mg/cm2, respectively, sulfolane samples showed a 28% and 64% reduction in TOC, following the same pattern. Both catalyst loadings resulted in a 77% reduction in total organic carbon in CPA solutions. The

findings demonstrated that the passive photocatalysis, when conducted in the late summer and autumn employing buoyant photospheres and exposed to natural sunshine in a northern environment (51, 4' N, 114, 8' W; altitude: 1114 m), was successful.

(Gholami et al., 2019) In a controlled laboratory setting, the degradation of the antibiotic Clindamycin hydrochloride was examined using a heterogeneous UV/TiO2 procedure. According to the findings, photocatalysis was unaffected by direct adsorption and photolysis. At pH=5, with a Clindamycin concentration of 2 g/L and a catalyst quantity of 0.5 g/L, the sweet spot was seen after 90 minutes. The pseudo-first-order degradation kinetics Findings from this research demonstrate that the UV/TiO2 procedure is a powerful tool for eliminating clindamycin hydrochloride from water.

(Ramrakhiani et al., 2022) A number of innovative separation techniques have had their performance efficiency tested for the removal of various emerging contaminants. Some of these methods show promise, including electrochemical processes, ozonation, adsorption, and UV/H2O2/Fe3+ aided photocatalysis. The clean and green approach has great promise for membrane-based technologies such as size-exclusive separation in ultra-filtration, nanofiltration, and reverse osmosis, as well as membrane bioreactor processes. Considering the processes' potential industrial use, however, thorough techno-economic examination is necessary. To ensure environmental sustainability, it is crucial to do a life cycle analysis (LCA) on ECs. The broad variety of emerging contaminants necessitates extensive study to identify the best methods of treatment that combine established and cutting-edge technologies for maximum removal efficiency while minimising negative impacts on the environment and the bottom line.

(Gomes et al., 2020) Given the widespread reliance on these compounds, it is hard to implement a source-based strategy to reduce ECs. In order to reduce potential dangers to public health, it is crucial to find effective ways to eliminate ECs. There are a number of options available to DWTPs that might lower the concentration of ECs in the water that is treated. More comprehensive data on the impact of ECs on the DW microbiota is urgently needed. In order to enhance the tactics utilised for ECs treatments and to correctly prioritise their removal in DWTPs, this knowledge is vital. The pharmaceutical ECs often researched for their impacts on water microbiomes—including antibiotics (ciprofloxacin, erythromycin, and sulfamethoxazole), carbamazepine, and diclofenac—are not the only ones with a substantial impact on microbial behaviour, as this work shows. The importance of antibiotics and other antimicrobial agents in the development of antibiotic resistance is undeniable. When it comes to the impact of ECs on biofilm behaviour and formation, nevertheless, the existing research is not very definitive. The current findings are contentious since they call for the creation of standardised tests in order to accurately analyse the effects of ECs. Keep in mind that ECs' effects could be conditional on a variety of variables, such as concentration, nutrient availability, hydrodynamics, exposure duration, etc. The primary obstacles to a "One Health" ECs prioritisation are the unknown effects of non-pharmaceutical ECs, the existence of combinations of ECs, and the unpredictability of experimental settings.

(Rojas et al., 2022) One novel class of photoactive materials for water remediation is metal-organic frameworks (MOFs), which have arisen in the ongoing quest for novel heterogeneous photocatalysts.

Among the many subclasses of metal-organic frameworks (MOFs), titanium-based MOFs (Ti-MOFs) stand out for their exceptional structural characteristics, great chemical stability, and potential optoelectronic and photocatalytic applications. Nevertheless, it is challenging to ascertain if Ti-MOF photocatalysts are feasible for use in real-world water treatment due to the lack of data from the published experiments. In this research, we first highlighted the potential of a Ti-MOF in the photodegradation of a combination of pertinent Emerging Organic Contaminants (EOCs) in actual water after screening it with numerous MOFs. At first, four photoactive Ti-MOF structures and two difficult medicines, namely the β-blocker atenolol (At) and the veterinary antibiotic sulfamethazine (SMT), were chosen in a sensible manner. The most promising photocatalyst was selected from this first screening as the mesoporous Ti-trimesate MIL-100(Ti). It exhibited greater individual photodegradation of At or SMT (100% of At photodegradation in 2 hours and 4 hours, respectively).

(Hassaan et al., 2023) Nanotechnology has the capacity to store solar energy and eliminate organic contaminants from the environment because of the distinctive properties of nanomaterials. The possibilities of artificial photosynthesis systems are vast. Methods for producing these NPs that are environmentally friendly, easily available, and safe are necessary to address present-day environmental issues. Green or biosynthetic solutions based on biomass feedstock often have a short response time, a low temperature, and a lack of chemical intervention. By mimicking the properties of naturally occurring photoactive green nanomaterials, we may build light-harvesting assemblies, develop novel approaches to fuel synthesis, and design tools to produce novel functional materials for use in solar cells, water-splitting units, pollution control devices, and many other applications. An eco-friendly and practicable method has to be developed to produce metallic NPs without the use of harmful chemicals. Researchers from all around the globe are now engaged in developing novel methods to produce metallic NPs, as mentioned in this article. Consequently, compared to other synthesis techniques, the production of metallic NPs that is less harmful to the environment is becoming more competitive. Using a wide range of organisms, including plants, bacteria, fungus, and algae, this article also discusses the environmentally benign production of metallic NPs that operate as photocatalysts.

(Krakowiak et al., 2021) The quest for novel approaches to surface and groundwater cleansing is a major focus of current scientific research. The area of heterogeneous catalysis may discover several uses for anatase TiO2. Titania, in its many forms (bare TiO2, dopant, or composite systems), has found usage in the breakdown of substrates derived from an extraordinarily diverse range of chemical compounds. The following substances can be classified as emerging contaminants: analgesics, antibiotics, anticonvulsants, β-blockers, lipid regulators, NSAIDs, organic dyes, psychiatric drugs, sex steroids; when permitted to freely disperse in the surrounding ground and water reservoirs, they pose a danger to the environment. We must take the necessary measures to decrease their rate of environmental deposition in order to avoid harm to ecosystems, human health, and the quality of life overall. Researchers are devoting a lot of time and energy to finding the best way to deal with emerging contaminants, which has led to a plethora of new ideas.

(Espinosa Jiménez et al., 2021) A basic wet approach was used to generate two Ce-doped ZnO photocatalysts with distinct surface, morphological, and structural features, at pH 4 and 8. They reduce the rate of zinc photodissolving in water compared to the undoped catalyst under the specified experimental conditions 5. After three hours of visible light irradiation, the Ce-doped ZnO catalyst, which was synthesised at pH 8, had excellent photocatalytic activity in degrading carbamazepine and phenol, with a degradation rate of over 45%.

Table 4 Summary of the literature review

Study	Key Focus	Detection/Degradation Method	Findings
Bratovčić (2023)	Photocatalytic degradation of organic contaminants	Semiconductor-based photocatalysts with UV/visible light	Enhanced photocatalytic efficiency with composite materials, but real wastewater studies needed
Arman et al. (2021)	Removal of emerging pollutants (EPs) in water	Physico-chemical, biological, and membrane-based filtration	Ultrafiltration is a promising method due to efficiency and selectivity
Datta & Roy (2023)	Photocatalysis for wastewater treatment	TiO_2 and visible light-responsive photocatalysts	Advanced photocatalysts expand usability beyond UV range
Heydari et al. (2019)	Passive solar-based photocatalysis	TiO_2-coated hollow glass microspheres	Effective in degrading herbicides and industrial solvents under natural sunlight
Gholami et al. (2019)	Removal of antibiotics from water	UV/TiO_2 photocatalysis	Effective degradation of Clindamycin hydrochloride with pseudo-first-order kinetics
Ramrakhiani et al. (2022)	Advanced separation techniques	UV/H_2O_2/Fe^{3+}, ozonation, adsorption, electrochemical, membrane filtration	Combination of conventional and novel methods needed for optimal removal
Gomes et al. (2020)	Effects of ECs on water microbiome	Monitoring pharmaceutical and non-pharmaceutical ECs	ECs impact microbial behavior, requiring standardized testing for prioritization

Rojas et al. (2022)	MOFs for ECs degradation	Titanium-based MOFs (Ti-MOFs)	Promising potential for real-world water treatment but further studies needed
Hassaan et al. (2023)	Nanotechnology for ECs removal	Green synthesis of metallic nanoparticles	Sustainable nanomaterials hold promise for pollution control
Krakowiak et al. (2021)	Water purification using TiO_2	TiO_2 in composite and doped systems	Effective against a wide range of pharmaceutical and chemical pollutants
Espinosa Jiménez et al. (2021)	Ce-doped ZnO photocatalysis	Visible-light-driven degradation of pharmaceuticals	Effective degradation (>45%) of carbamazepine and phenol

3. Conclusion

Pharmaceuticals, agrochemicals, and dyes are just a source of the emerging contaminants that are making water filtration systems work harder. When standard treatment processes fail to properly remove these contaminants, more complex technologies must often be used. One such method is photocatalysis, which may decompose numerous chemical compounds when subjected to ultraviolet and visible light. Recent research has led to the development of novel photocatalysts exhibiting enhanced stability, efficiency, and broader spectral activity. These consist of metal-organic frameworks, perovskites, and metal sulphides.

Although there is much evidence of the efficacy of photocatalysis based on semiconductors, there is still room for improvement in terms of its practical use. Research highlights the need of doing pilot-scale experiments using genuine wastewater samples. This is because laboratory settings often use artificial solutions that fail to reflect all of the complexities of the environment. Hybrid treatment systems, nanotechnology-based technologies, and membrane filtration may all work together to remove contaminants more efficiently.

The future of water remediation lies in methods that are long-lasting, low-cost, and easy to expand. For photocatalytic solutions to be widely used, issues like catalyst stability, energy use, and the production of byproducts need to be fixed. Furthermore, to ensure environmental and economic sustainability, these technologies must be deployed according to life cycle assessments and techno-economic analyses. Long-term success with emerging contaminants in water resources requires a multidisciplinary approach including specialists in environmental engineering, material science, and policymaking.

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