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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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