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# Review of Application of Artificial Intelligence in natural products research

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## Abstract

**Background**: The use of artificial intelligence (AI) in natural product research is an emerging field that has the potential to revolutionize the discovery of new drugs Given the potential of AI in the research and exploration of natural products, this study will aim to explore the application of AI in the research and development of natural products.

**Methods**: The study involved a comprehensive review of the application of AI in the research and development of natural products. The review includes sections around the potential application of AI in the research, development, and evaluation of AI in natural products followed by the challenges in this area.

**Results**: AI has had a major impact on the field of natural product discovery and development. By automating the analysis of large amounts of data, AI algorithms can identify potential new natural products much faster and more accurately than traditional methods. Another important application of AI in natural product research is the analysis of high-throughput screening data, a technique used to screen large numbers of compounds for specific biological activities. AI used for computer-aided drug design for the creation of novel biologically active chemicals can be improved, and the time and money required to create a new drug are reduced. By analyzing the vast amounts of data on natural products, AI has the potential to uncover meaningful relationships and logical connections between the chemical structures of these products and their functions against a specific disease.

**Conclusion**: Despite these limitations, the application of AI in natural product research holds significant promise in the development of natural products. By leveraging the latest developments in AI and machine learning, researchers can continue to push the boundaries of what is possible in the discovery of new natural products with therapeutic activities.

**Keywords:** artificial intelligence; Application; Review; Natural products.

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## 1. Introduction

The global health problem brought on by both communicable and non-communicable diseases poses a significant public health challenge. Despite the progress achieved in the creation of medications to treat conditions including HIV/AIDS, malaria, hypertension, diabetes, and cancer, these illnesses continue to wreak havoc on communities worldwide and have high mortality rates (Newman et al., 2003). The traditional pharmaceutical R&D approaches, which concentrate on developing "blockbuster" medications, are insufficient to address this issue and warrant innovative approaches to drug discovery, and critical to address the burden of global disease (Hotwani et al., 2014).

One such approach is the return to nature, as it has proven to be successful in the past. For instance, anticancer drugs like Taxol (from Taxus brevifolia) and Vinblastine (from Catharanthus roseus), as well as antimalarial drugs like quinine (from Cinchona spp.) and Artemisinin (from Artemisia annua) were all discovered from natural products and have proven to be effective treatments for these diseases (Ernst et al., 2015). Therefore, natural products R&D has the potential to play a crucial role in finding new and innovative drugs to address the global public health crisis (Gozubuyuk et al., 2014).

The use of artificial intelligence (AI) in natural product research is an emerging field that has the potential to revolutionize the discovery of new drugs (Thomford et al., 2018). AI algorithms can be trained to analyze large amounts of data, identify patterns, and make predictions, which can speed up the discovery of new compounds with potential therapeutic activities (Liu et al., 2011). One of the ways AI can be used in natural products research is through virtual screening, where large databases of compounds are screened using computer algorithms to identify those that are most likely to have a specific biological activity (Tang et al., 2021). This approach can significantly reduce the time and cost involved in screening large numbers of compounds and increase the chances of finding new drugs.

Another application of AI in natural products research is the use of machine learning algorithms to predict the properties of new compounds, such as their toxicity, solubility, and pharmacokinetics (Verma et al., 2022). This information can guide the development of new drugs and help identify compounds with the highest potential for success. AI has the potential to transform natural product research and accelerate the discovery of new drugs (Hotwani et al., 2014). Given the increasing number of people suffering from diseases, new and effective treatments must be developed. By revisiting nature, we have the opportunity to tap into the vast wealth of knowledge and resources that have been available for millions of years (De Luca et al., 2012). This approach involves screening natural sources such as plants, microbes, and marine organisms for active compounds that can be developed into new drugs (Flachenecker, 2016).

One of the advantages of this approach is that natural products are often structurally and chemically diverse, making them a rich source of novel compounds that can be used to treat diseases (Rodrigues et al., 2016). Additionally, many natural products have already undergone millions of years of evolution, selection, and survival in their respective environments, which makes them robust and stable. This is particularly important for the discovery of new drugs, as compounds that are unstable or toxic are unlikely to be suitable candidates. Therefore, natural product research and development have the potential to play a major role in the discovery of new and innovative drugs to treat and manage diseases (Gozubuyuk et al., 2014).

The use of natural products in drug discovery has a long and successful history, with many foods and drug administration (FDA)-approved drugs based on plants, microbes, or marine organisms (Mitchell-Olds, 2014). Approximately 25% of all FDA and EMA-approved drugs are plant-based, and notable examples include Paclitaxel and Morphine. In fact, over the past 20 years, about a third of FDA-approved drugs have been derived from natural products or their derivatives (De Luca et al., 2012). By leveraging this approach, we can improve people's health and well-being worldwide and address the global public health crisis.

The discovery of penicillin from a fungus in the 1940s marked the beginning of a new era in drug discovery, as it paved the way for the screening of microorganisms for potential antibiotics (Weng et al., 2012). This approach has resulted in the discovery of many new drugs that have revolutionized medicine and transformed the way diseases are treated. The use of natural products as a source of new drugs offers several advantages (Wei Chang, 2013). For one, they are structurally and chemically diverse, making them a rich source of novel compounds with potential therapeutic activities (Rodrigues et al., 2016). Additionally, they have undergone millions of years of evolution, selection, and survival in their respective environments, which makes them robust and stable. This stability is crucial for the discovery of new drugs, as compounds that are unstable or toxic are unlikely to be suitable candidates (Gordaliza, 2007).

By leveraging this technology, we can identify new compounds with therapeutic activities more quickly and efficiently, and help to address the global public health crisis. Given the potential of AI in the research and exploration of natural products, this study will aim to explore the application of AI in the research and development of natural products.

## 2. Subjects and Methods

The study involved a comprehensive review of the application of AI in the research and development of natural products. The review includes sections around the potential application of AI in

the research, development, and evaluation of AI in natural products followed by the challenges in this area

## 3. Results

### 3.1. AI in data analysis for natural products discovery and development

AI has had a major impact on the field of natural product discovery and development (W. Cassidy, 2020). AI algorithms have been used to analyze large amounts of chemical data to identify patterns and relationships that would otherwise be difficult to detect (Bohr, 2020). One of the key applications of AI in this field has been in the analysis of chemical structures to identify potential new natural products. One study that exemplifies this application of AI is the work of Patra et., in 2018 who used machine learning algorithms to analyze a large database of known natural products to identify new structures with potential biological activity (Patra et al., 2018).

By automating the analysis of large amounts of data, AI algorithms can identify potential new natural products much faster and more accurately than traditional methods (Saldívar-González et al., 2022). In addition, AI algorithms can also identify novel structures that might not have been detected using traditional methods, allowing for the discovery of new natural products with potential therapeutic activity (Lopes et al., 2017). AI has had a major impact on the field of natural product discovery and development, particularly in the analysis of chemical structures to identify potential new natural products. By automating the analysis of large amounts of data, AI algorithms have the potential to greatly speed up the process of natural product discovery and development and to identify novel compounds with potential therapeutic activity (Méndez et al., 2003).

### 3.2. AI in high-throughput screening

Another important application of AI in natural product research is the analysis of high-throughput screening data, a technique used to screen large numbers of compounds for specific biological activities (Zhavoronkov et al., 2020). However, analyzing the vast amounts of data generated from these screens can be a challenging and time-consuming task, AI algorithms can be used to analyze data, identify promising compounds, and prioritize them for further study (Ferrero et al., 2017).

For instance, to create a Bayesian cytotoxicity forecasting model, Pfizer gathered information from several assays conducted in their facilities and from the literature for around 100,000 chemicals (Ekins & Freundlich, 2011). Due to the volume of biological data generated as a result of high-throughput screening, storage databases, and databases are required to produce a wealth of data for the development of computational models (Paulose et al., 2018). The use of AI in the analysis of chemical structures has the potential to greatly speed up the process of natural product discovery and development (Moshawih et al., 2022).

### 3.3. AI for computer-aided drug design

In the past, the development of novel medications was accomplished through empirical observations of the effects of natural materials for known disorders and random drug screening (Maia et al., 2020). Even though it was ineffective, this random screening method helped to identify several significant substances up until the 1980s. High-throughput screening (HTS), which is appropriate for automating the screening procedure of many thousands of compounds against a molecular target or cellular assay extremely fast, has improved this approach as of late. This procedure is generally time-consuming, exhausting, and expensive.

Typically, a new drug's development costs between $1 and USD 2 billion and takes 10 to 17 years (Leelananda and Lindert, 2016). The creation of novel biologically active chemicals can be improved, and the time and money required to create a new drug are reduced, thanks to the usage of CADD. Thus, the development of structural-based virtual screening has advanced the process of discovering new drugs and has been recognized as one of the most promising in silico methods for developing new natural drugs (Meng et al., 2011).

### 3.4. AI for assessing the effectiveness of natural

The advancements in artificial intelligence, particularly in the realm of deep learning, can make informed predictions based on a thorough understanding of knowledge and patterns (Arabfard et al., 2019). The abundance of data available on the functions of natural products presents a unique opportunity to utilize the latest developments in deep learning to tackle the significant challenge of predicting biological activity from the chemical structure of these products (Annang et al., 2015). By analyzing the vast amounts of data on natural products, AI has the potential to uncover meaningful relationships and logical connections between the chemical structures of these products and their functions against a specific disease (Ma et al., 2021).

AI has the potential to make predictions based on patterns and knowledge that may not be immediately obvious to researchers. By utilizing these predictions, scientists can guide their research and focus on compounds that are most likely to have therapeutic activities, leading to a more efficient discovery process (Baba et al., 2015). The use of AI in natural product research can transform our understanding of these compounds and help identify new compounds with therapeutic activities (Merk et al., 2018). By leveraging the latest developments in deep learning, we can unlock the full potential of natural products and address the global public health crisis.

## 4. Discussion

AI has been widely applied in the pharmaceutical and biological sectors in recent years. Numerous

AI-based technologies with more effective, automated processes that incorporate predictive and data-driven judgments are widely used in these areas (Chen & Kirchmair, 2020). By revisiting nature, we can find new compounds with potential therapeutic activities and develop drugs that can improve the health and well-being of people worldwide (Merk et al., 2018). By leveraging this approach, we can help to address the global public health crisis and improve the lives of millions of people (Gordaliza, 2007), it offers a substantial amount of data that is used to train subsequent models. AI can help in the identification of new natural products by using computational methods to search for compounds with specific properties (Baldo, 2019). By using machine learning algorithms, AI can predict the properties of new compounds, such as toxicity, solubility, and bioactivity, based on the structural and chemical characteristics of known compounds (Balakin et al., 2004). This information can translate to prioritizing new compounds for further study and help to accelerate the discovery process (Newman et al., 2003).

Drug discovery now mostly disproportionately relies on the basic idea of computer-aided drug discovery, including ML and DNN methods. ML tools are anticipated to play a crucial role in reducing the time and costs for finding new lead compounds, discovering off-targets, and dereplicating new drugs from natural products (Eldridge et al., 2002). This includes revealing new areas in the chemical space, utilizing natural and naturally-inspired products in the pharmaceutical industry, all the way to structure- and ligand-based high-throughput virtual screening (Liu, 2015).

Researchers are increasingly and constantly creating new techniques and algorithms to find acceptable natural items quickly and affordably. An important change in the success rate of drug development has been the introduction of AI and computational chemistry. These approaches can be used individually or in combination to create new tactics that involve a variety of effective algorithms that improve predictions made using natural products.

However, despite the potential benefits of AI in natural product research, there are still some challenges to be overcome. One of the main challenges is the lack of large and diverse datasets for training AI algorithms for the development of drugs including natural products (Thakur et al., 2020). To overcome this, researchers are working to digitize natural product data and develop new data-driven approaches that can be used to train AI algorithms. However, it's important to note that AI is still in the early stages of development in natural product research and there are limitations to its application. Another limitation is the quality and reliability of the data used to train the AI algorithms (Esmaeilzadeh, 2020). To overcome this, researchers must ensure that the data they use is high-quality, well-curated, and representative of the diversity of natural products.

In addition, the interpretability of AI models also presents a significant challenge in the research

of AI applications in natural products. AI models often generate predictions based on complex algorithms, making it difficult for researchers to understand the logic behind the predictions (Sakkiah et al., 2017). This makes it challenging to validate the results and apply the findings in a meaningful way. To overcome these limitations, researchers are working to develop new AI algorithms that are more interpretable and better able to handle complex natural product data. This includes the development of new deep learning algorithms that can learn from large and diverse datasets, as well as the use of explainable AI (XAI) algorithms that can provide insight into the reasoning behind predictions (Jeon et al., 2014).

## 5. Conclusion

Despite these limitations, the application of AI in natural product research holds significant promise in the development of natural products. By leveraging the latest developments in AI and machine learning, researchers can continue to push the boundaries of what is possible in the discovery of new natural products with therapeutic activities. With the growing global need for innovative solutions to public health challenges, the use of AI in natural product research is an important and exciting area of study that has the potential to make a significant impact in the years to come.

## 6. Declarations

### 6.1 Conflict of Interest Statement

The authors have no conflict of interests to declare.


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