Natural Resources for Human Health
eISSN: 2583-1194

Original Research

Received 18 March 2026
Revised 20 April 2026
Accepted 14 May 2026

Natural Resources for Human Health 2026, Vol. 6 (3): 210–217

KEYWORDS:
Artificial intelligence; Natural products; Drug discovery; Machine learning; Deep learning; Generative AI; Explainable AI; Precision medicine; Virtual screening; Molecular docking; ADMET prediction; Pharmacogenomics.

Artificial Intelligence in Natural Product Research: Transforming Drug Discovery and Precision Medicine

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ABSTRACT: Natural products remain important for the discovery of bioactive compounds for drug development; traditional screening and development are tedious, time-consuming, and expensive. Artificial Intelligence (AI) has transformed natural product research, enabling scientists to rapidly identify phytochemicals, predict molecular targets, perform virtual screening, perform molecular docking, perform ADMET property evaluation, and optimize leads. The processing of billions of chemical and biological data points is improved by machine learning, deep learning, generative AI, and explainable AI, which all help to improve the accuracy and efficiency of medication development. In addition, AI-powered multi-omics integration, pharmacogenomics, and clinical data are crucial for precision medicine, facilitating biomarker identification, personalized treatment strategies, and data-driven clinical decision-making. Progress has been made; however, there are challenges related to data quality, model interpretability, ethical concerns, and regulatory acceptance. Advancements in explainable and generative AI will accelerate the advancement of autonomous drug discovery and enhance the conversion of natural product therapeutics to the clinic. This review highlights recent progress, current challenges, and future perspectives of precision medicine from an AI perspective regarding natural products.

1. INTRODUCTION

The ability of natural products to provide an inexhaustible supply of structurally diverse, bioreactive, and evolutionarily optimized therapeutic agents is a fact that cannot be overlooked when considering their importance in modern drug discovery. Many clinically useful drugs, such as anti-inflammatory agents, anticancer agents, antimicrobial agents, antiviral agents, immunosuppressive agents, and cardiovascular agents, have been found or synthesized from natural products. The plants, microorganisms, marine organisms, fungi, and other biological resources produce a vast array of secondary metabolites, many of which have very complex molecular structures and are valuable in the discovery of new pharmacological targets, as nature's molecules are often more complex than synthetic molecules (1). Despite these advantages, there is still a low percentage of success in traditional natural product research (long lead times to develop a product), and the methods are still time-consuming, expensive, and labor-intensive. But in the age of artificial intelligence (AI), the definition is evolving, and computational techniques are becoming capable of processing huge amounts of biological, chemical, and clinical data within close to real-time and achieving high accuracy. The use of machine learning, deep learning, graph neural networks, generative AI, explainable AI and more is helping to discover phytochemicals, perform metabolomic profiling, predict biosynthetic pathways, perform molecular docking, virtual screening, quantitative structure–activity relationship modelling, perform ADMET prediction, de novo molecular design and identify biomarkers. Also, AI can enable the integration of multi-omics data, EHR, and pharmacogenomic information to help advance precision medicine, which can lead to the discovery of more effective, personalized, and safer therapeutic interventions based on patient-specific characteristics (2). Natural product science and AI are therefore a game-changing solution to enhance every stage of the drug discovery process from target identification to clinical decision support. This review aims to provide a comprehensive overview of the advancements in Natural Product research driven by AI technology, encompassing the newest developments in computational techniques, significant applications in drug discovery and precision medicine, current challenges and issues in data quality, interpretability, and regulatory approval, and the future outlook for intelligent, sustainable, and patient-centric pharmaceutical innovation (3).

2. NATURAL PRODUCTS IN MODERN DRUG DISCOVERY

Today natural products are one of the most abundant sources of therapeutics in the discovery process thanks to their unparalleled chemical diversity and biological specificity and evolution. They are isolated from plants, microorganisms, fungi, marine organisms and animals, and have a complex molecular structure and stereochemistry, which is very difficult to synthetic. The bioactive natural compounds include alkaloids, flavonoids, terpenoids, phenolics, glycosides, peptides and polyketides that have anti-cancer, antimicrobial, antiviral, anti-inflammatory, antioxidant, neuroprotective and cardioprotective properties (4). The continued importance of natural products to the development of clinically useful drugs, including paclitaxel, artemisinin, vincristine, penicillin and cyclosporine, is clearly seen. The advent of new analytical techniques and computational technologies has also enabled the exploration and characterisation of natural compounds, the prediction of biological activity and lead optimization in a timely fashion. Over the last few years, many natural product databases emerged that proved to be valuable resources for storing natural product structures, bioactivities, pharmacologies, and natural targets, such as COCONUT, NPASS, SuperNatural, ChEMBL, PubChem and Dictionary of Natural Products (5). These databases can also be utilized in virtual screening, molecular docking, prediction models built using artificial intelligence (AI) and in quantitative structure–activity relationship (QSAR) analysis, enhancing the speed and efficiency of lead identification.

Figure 1 illustrates that biological materials from diverse sources provide structurally diverse bioactive compounds and, when combined with AI computational methods, can speed up and streamline the target prediction, compound prioritization, and drug discovery process. With all these developments, however, some constraints hinder the extensive use of natural products. There is also diversity in phytochemical composition, and some metabolites are not available; isolation and structural elucidation of some metabolites are difficult; biological annotation of metabolites and data heterogeneity exist; and there is a lack of satisfactory standardization, which also hinders reproducibility and large-scale computational analysis. Furthermore, the data integration, the data quality, and the availability of limited datasets with experimental validation can affect the validity and applicability of AI models (6). By tackling these challenges by standardising the generation of data, the creation of integrated databases, high-throughput omics technologies, and powerful AI algorithms, the translation of natural products into innovative treatments and applications in precision medicine will be further improved.

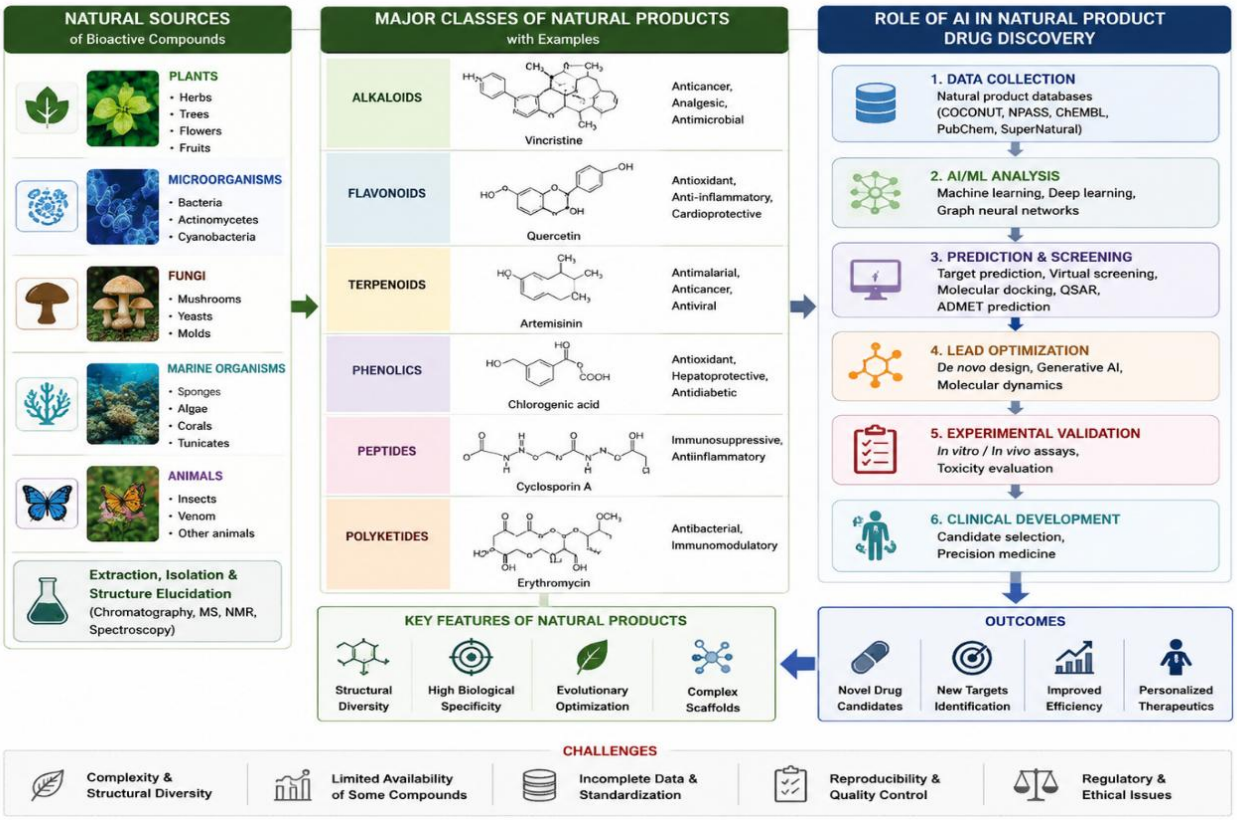

Figure 1. Classification of Natural Products and Their Role in AI-Assisted Drug Discovery

3. ARTIFICIAL INTELLIGENCE TECHNOLOGIES IN BIOMEDICAL RESEARCH

In the field of biomedical research, artificial intelligence (AI) has emerged as a game-changer, especially when it comes to processing and analysing vast amounts of intricate data like biological, chemical, and clinical information. Machine learning (ML), which leverages the application of statistical algorithms that can be trained to predict the biological activity of a compound, classify a compound, identify a therapeutic target, or optimize a lead molecule, is one of its main approaches, which is supported by structured data. Supervised learning, unsupervised learning, and reinforcement learning are well-known techniques, and many applications are known, such as quantitative structure–activity relationship (QSAR) modeling, virtual screening, ADMET prediction, and identification of biomarkers (7). Deep learning (DL) is a specific type of machine learning that is based on multilayer artificial neural networks that can be applied to automatic feature extraction from massive amounts of data without the need for any manual feature engineering. Transformers, graph neural networks (GNNs), recurrent neural networks (RNNs), and convolutional neural networks (CNNs) have been used with great success in molecular property prediction, protein–ligand binding site prediction, metabolomics, genomics, and protein structure prediction (8). Generative AI (Generative Artificial Intelligence), which involves creating new chemical scaffolds with desired pharmacological properties using tools such as variational autoencoders (VAEs), generative adversarial networks (GANs), diffusion models, and large language models (LLMs), has swept the molecular design world by storm in the past several years. The technologies can be used in de novo drug design, lead optimization, creation of molecular scaffolds/scaffolds deconstruction, and compounds repurposing, drastically reducing time and costs of conventional drug discovery processes. With the increasing complexity of AI models, however, comes a rise in concerns regarding transparency and reliability, which is why Explainable Artificial Intelligence (XAI) was brought into existence. XAI's ability to explain model features and molecular characteristics that are relevant to AI predictions helps with model validation, model reproducibility, regulatory acceptance, and model trust, resulting in more interpretable and transparent decision-making (9). The AI technologies vary in the areas they are applied to, as listed in Table 1, such as predictive analytics, molecular modelling, customised therapeutics, and precision medicine. Together, the

complementary AI strategies offer an efficient, precise and data-driven route to the discovery of new bioactive natural products, optimization of therapeutic candidates and the development of next-generation precision healthcare.

Table 1. Comparison of Artificial Intelligence Techniques Used in Natural Product Research

AI Technique	Principle	Common Algorithms/Models	Major Applications in Natural Product Research	Advantages	Limitations
Machine Learning (ML)	Learns patterns from structured datasets for prediction and classification	Random Forest, Support Vector Machine (SVM), XGBoost, Decision Tree	QSAR modeling, virtual screening, ADMET prediction, target identification	High predictive accuracy, efficient with moderate datasets	Requires feature engineering and high-quality labeled data
Deep Learning (DL)	Multi-layer neural networks automatically learn complex features	CNN, RNN, Graph Neural Network (GNN), Transformer	Molecular property prediction, protein–ligand interaction, metabolomics, genomics	Handles large and complex datasets with superior accuracy	Computationally intensive and less interpretable
Generative AI	Generates novel molecular structures and chemical scaffolds	Variational Autoencoder (VAE), GAN, Diffusion Models, Large Language Models (LLMs)	De novo drug design, lead optimization, compound generation, drug repurposing	Rapid generation of novel drug candidates and scaffold diversity	Requires extensive training data and experimental validation
Explainable AI (XAI)	Provides interpretable and transparent AI predictions	SHAP, LIME, Attention Mechanisms, Feature Attribution Methods	Model interpretation, biomarker discovery, regulatory compliance, clinical decision support	Improves transparency, reliability, and user trust	May reduce model simplicity and increase computational complexity

4. AI-DRIVEN NATURAL PRODUCT DISCOVERY

The application of artificial intelligence (AI) in the natural product drug discovery has revolutionized the field by utilizing complex computational algorithms, chemical, biological, and pharmacological data to accelerate drug discovery and development from natural sources. One of the first applications of AI is in phytochemical identification, which involves inputting mass spectrometry (MS), nuclear magnetic resonance (NMR), and liquid chromatography–mass spectrometry (LC–MS) spectroscopic and chromatographic data into machine learning and deep learning algorithms for quick identification, classification, and annotation of bioactive compounds in complex natural extracts (10). After the identification of compounds, AI can be applied to predict targets, such as analysing the molecular structure of a compound, pathways in living systems, protein–ligand interactions, and omics data, to discover deeper insights into possible therapeutic targets and the mechanism by which a compound acts than traditional computational techniques. The application of AI-powered virtual screening can screen millions of natural compounds against the disease-associated targets, saving time and cost of the experimental high-throughput screening, and increasing the chances of finding potential lead compounds (11). Molecular docking, in addition to virtual

screening, uses AI-driven scoring functions and deep learning models to generate predictions of protein–ligand binding affinity, binding conformation and binding stability, which can enhance the selection of high-affinity compounds to proceed to further testing. An important use is ADMET prediction, where an ML model is used to predict the absorption, distribution, metabolism, excretion, and toxicity at the early stages of drug development. The identification of adverse pharmacokinetic (PK) or toxicological (PT) characteristics at the early stages of the drug discovery process will help to minimise late-stage clinical failures and improve the overall efficiency of the drug discovery process (12). Moreover, AI is a key enabler in the process of lead optimization, offering insights into structure–activity relationships, recommended chemical adjustments, creation of new molecular analogs via generative AI models, and optimization of efficacy, selectivity, pharmacokinetic behavior, and safety. There is a marked reduction in experimental effort, and speed up of development time, and improved chances of clinical success using these AI-powered techniques. The synergy of machine learning, deep learning, generative AI and explainable AI with contemporary computational chemistry, structural biology and multi-omics technologies has thus created a highly efficient, data-driven framework to accelerate the execution of natural product research and create a new drug discovery process for tackling complex human diseases, which is faster, more accurate and precision-oriented (13).

5. ARTIFICIAL INTELLIGENCE IN PRECISION MEDICINE

AI's integration of diverse biological and clinical information allows it to develop individualized therapeutic routes tailored to each patient, thus playing a crucial role in enabling precision medicine. A great application of AI is in the discovery of biomarkers, and machine learning algorithms and deep learning algorithms, which can analyze genomic, transcriptomic, proteomic, metabolomic, and clinical data, to look for reliable biomarkers that can be used in the diagnosis, prognosis, therapeutic response, and patient stratification of disease. These markers can be used to identify the disease early and to help make the best treatment decisions. AI also integrates various omics layers, such as genomics, transcriptomics, proteomics, metabolomics, microbiomics, and epigenomics, to provide a comprehensive understanding of disease mechanisms and biological pathways (14). A systems-level view can help identify complex molecular interactions and reveal novel therapeutic targets. AI is also used in pharmacogenomics to understand the genetic differences that affect how drugs are metabolized, their effectiveness, and their side effects, helping healthcare providers to optimize treatment for each patient and prevent negative drug interactions. Such predictive models can also be useful to optimize the use of drugs derived from natural sources, which may be patient-specific and have genetic importance in treatment success. Beyond this, AI can support personalized therapeutics by linking molecular information with lifestyle habits, environmental triggers and EHRs to recommend tailored treatment plans, fine-tune treatment doses, and even monitor real-time therapeutic outcomes (15).

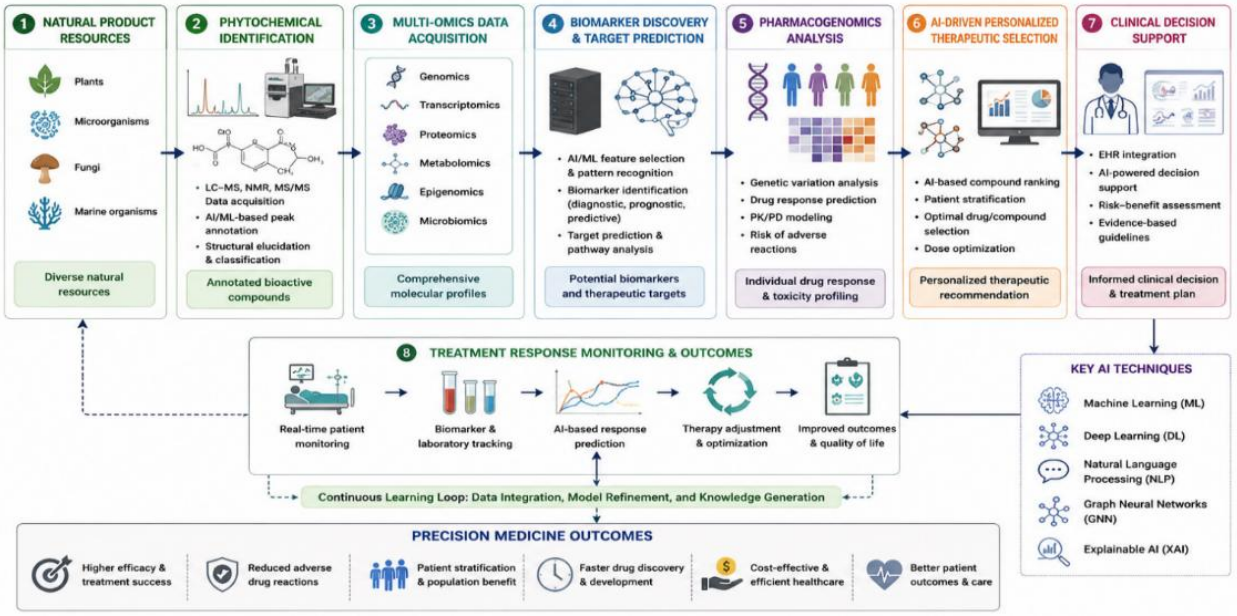

Figure 2. AI-Based Precision Medicine Workflow from Natural Products to Personalized Therapy

As AI becomes part of natural product research, it can help identify compounds with the greatest potential for therapeutic benefits in certain patient groups, improving treatment efficacy and minimizing potential side effects. Moreover, AI-driven clinical decision support systems can help healthcare practitioners by sifting through vast amounts of clinical literature, imaging data, lab reports, and patient histories to provide rapid, comprehensive, and evidence-based diagnostic and therapeutic recommendations. As illustrated in Figure 2, the precision medicine journey with AI begins with natural product resources and concludes with monitoring patient outcomes, with each step involving various stages of phytochemical characterization, multi-omics analysis, biomarker identification, target prediction, pharmacogenomic evaluation, personalized therapeutic selection, and clinical decision support. The system provides a comprehensive solution that boosts clinical management, diagnostic accuracy, therapeutic efficiency, and patient care, resulting in improved, more efficient, and less one-size-fits-all interventions (16).

6. CHALLENGES, LIMITATIONS, AND ETHICAL CONSIDERATIONS

Although there has been significant progress, there are still some hurdles to using AI in natural product research. AI algorithms used to build models are heavily dependent on the availability of well-annotated, good-quality datasets that are standardized and, if possible, not fragmented or heterogeneous to ensure the reliability of the results. In the same way, many of the more advanced AI models are also "black boxes" and lack interpretability, which can be an obstacle to clinical trust and acceptance, as well as regulatory approval. Ethical implications, including privacy, bias, transparency, and accountability, need to be taken into account in the implementation of AI in healthcare (17). Moreover, there are still no harmonised regulations and standardised validation procedures to constrain safe, reliable, broadly clinically-discovered natural product discoveries powered by AI.

7. FUTURE PERSPECTIVES

The potential applications of AI in Natural Product research are promising and will require the synergy of Explainable AI (XAI), generative AI, and foundation models. These sophisticated technologies aim to accelerate the autonomous drug discovery cycle, enabling the automatic design of compounds, the prediction of targets, the optimization of leads, and experimental design with little to no human intervention. AI will also play a central role in providing personalised healthcare, where multi-omics data, pharmacogenomics data and real-world clinical data will be used to develop a personalised therapeutic approach. These new advances in AI will revolutionize natural product drug discovery, as outlined in Table 2, into a more rapid and accurate precision medicine system that delivers clinical impact.

Table 2. Future Opportunities and Emerging Trends of AI in Natural Product Drug Discovery and Precision Medicine

Future Trend	Application	Expected Impact
Explainable AI (XAI)	Transparent AI predictions	Improved reliability and regulatory acceptance
Generative AI	Novel molecule and lead generation	Faster drug discovery
Foundation Models	Multi-omics data integration	Enhanced target and biomarker identification
Autonomous Drug Discovery	Automated screening and optimization	Reduced time and cost
Precision Medicine	Personalized treatment strategies	Improved therapeutic outcomes
Clinical Decision Support	AI-assisted diagnosis and treatment	Better clinical decision-making
Digital Health	Real-time patient monitoring	Personalized healthcare management
Drug Repurposing	Identification of new therapeutic uses	Accelerated and cost-effective drug development

8. CONCLUSION

AI is also a transformative technology that is redefining and changing the natural product research landscape by speeding up the identification of phytochemicals, the prediction of targets, virtual screening, molecular docking, ADMET evaluation, and lead optimization. The combination of AI with multi-omics technologies, pharmacogenomics, and precision medicine can be

used to create more personalized, safer, and effective therapeutics. Despite the ongoing challenges of data accessibility, model explanation and regulatory approval, the prospect of AI in drug discovery is bright with ongoing progress in explainable AI, generative AI and autonomous discovery poised to triumph over these obstacles. In conclusion, AI-assisted natural product research holds great potential for driving innovation in drug discovery and precision healthcare.

DECLARATIONS

Funding: The authors received no specific financial support for the research, authorship, and/or publication of this article.

Conflict of Interest: The authors declare that there are no conflicts of interest regarding the publication of this manuscript.

Author Contributions: All authors contributed substantially to the conception, literature review, manuscript preparation, critical revision, and approval of the final version of the manuscript.

Ethical Approval: Ethical approval was not required because this study is a review article based exclusively on published literature.

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