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ARTIFICIAL INTELLIGENCE AND MULTI-OMICS IN ETHNOPHARMACOLOGY: ADVANCING PRECISION DRUG DISCOVERY FROM TRADITIONAL MEDICINE

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ABSTRACT

Ethnopharmacology has played a pivotal role in drug discovery by documenting traditional knowledge of medicinal plants and their therapeutic applications. Numerous clinically important drugs, including aspirin, artemisinin, quinine, and paclitaxel, originated from ethnopharmacological investigations. However, conventional approaches are often constrained by time-intensive phytochemical analyses, limited mechanistic understanding, poor standardization, and complex validation processes. Recent advances in artificial intelligence (AI) and multi-omics technologies offer transformative opportunities to overcome these limitations and accelerate evidence-based natural product research. This review examines the integration of AI with genomics, transcriptomics, proteomics, metabolomics, and microbiomics to improve the identification, characterization, and validation of bioactive phytochemicals. Machine learning, deep learning, natural language processing, and computer-aided drug design facilitate the prediction of biological activity, molecular targets, pharmacokinetic properties, and toxicity profiles, thereby streamlining the drug discovery pipeline. Complementary approaches such as network pharmacology, molecular docking, molecular dynamics simulations, and systems biology enable comprehensive analysis of the multi-component, multi-target mechanisms of herbal medicines. The convergence of AI and multi-omics bridges traditional medicinal knowledge with modern precision medicine by enabling the discovery of novel therapeutic candidates and personalized treatment strategies. Furthermore, this review highlights current challenges, including data standardization, experimental validation of computational predictions, ethical considerations, explainable AI, and regulatory compliance. Addressing these challenges through interdisciplinary collaboration and robust analytical frameworks will enhance the reliability, reproducibility, and clinical translation of ethnopharmacological research. Overall, the integration of AI and multi-omics represents a promising paradigm for advancing precision phytomedicine and accelerating the development of safe and effective plant-derived therapeutics.

KEYWORDS: Ethnopharmacology; Artificial Intelligence (AI); Multi-Omics; Precision Medicine; Medicinal Plants; Natural Products; Machine Learning; Network Pharmacology; Drug Discovery; Systems Biology; Molecular Docking; Phytochemicals.

1. INTRODUCTION

Ethnopharmacology is an interdisciplinary scientific field that explores traditional medicinal knowledge and the therapeutic applications of natural resources, including medicinal plants, animals, fungi, and minerals. It integrates concepts from pharmacology, ethnobotany, anthropology, pharmacognosy, chemistry, toxicology, and molecular biology to investigate the efficacy, safety, mechanisms of action, and quality of traditional medicines. By combining indigenous knowledge with modern scientific research, ethnopharmacology plays a vital role in the discovery of novel bioactive compounds and the development of evidence-based therapeutics.[1-3]

Traditional medicine encompasses a wide range of healthcare systems, cultural practices, and therapeutic approaches that have evolved over generations. Ethnopharmacological studies focus on documenting traditional medicinal knowledge while evaluating the taxonomy, phytochemistry, pharmacological activities, toxicity, dosage, and clinical efficacy of natural products. Increasing emphasis on evidence-based validation has improved the scientific credibility and global acceptance of herbal medicines in modern healthcare.[4–6]

Recent advances in computational biology, artificial intelligence (AI), machine learning, bioinformatics, and network pharmacology have revolutionized ethnopharmacological research. These technologies enable the integration and analysis of large-scale biological and phytochemical datasets, facilitating the prediction of bioactive compounds, molecular targets, pharmacokinetic properties, and toxicity profiles. Furthermore, network pharmacology, molecular docking, and systems biology provide valuable insights into the complex multi-component and multi-target mechanisms of herbal medicines. The convergence of AI with multi-omics technologies has accelerated natural product-based drug discovery and supports the advancement of precision medicine by bridging traditional knowledge with modern biomedical science.[7–12]

Table 1: Historical Evolution of Ethnopharmacology from Traditional Knowledge to Precision Medicine.

Period	Timeline	Major Developments	Significance
Prehistoric Era	Before 3000 BCE	Early humans used plants, minerals, and animal products based on observation and experience.	Laid the foundation of traditional medicine.
Ancient Civilizations	3000 BCE–500 CE	Development of organized medical systems such as Ayurveda, Traditional Chinese Medicine, Egyptian, and Greek medicine.	Initiated systematic documentation of medicinal knowledge.
Medieval Period	500–1500 CE	Herbal medicine expanded through trade, cultural exchange, and translation of medical texts.	Promoted the spread of traditional medicinal knowledge across civilizations.
Renaissance and Early Modern Era	1500–1800 CE	Advances in botanical classification and scientific observation of medicinal plants.	Connected herbal medicine with scientific research.
Modern Pharmacognosy Era	1800–1950	Isolation of bioactive compounds such as morphine, quinine, and salicin from medicinal plants.	Marked the shift from crude herbal remedies to purified pharmaceutical agents.

Contemporary Ethnopharmacology	1950–2000	Integration of pharmacology, phytochemistry, toxicology, and clinical research.	Enabled scientific validation of traditional medicines.
Digital and Precision Medicine Era	2000–Present	Application of genomics, proteomics, metabolomics, artificial intelligence, machine learning, network pharmacology, and molecular modelling.	Transformed ethnopharmacology into a data-driven discipline supporting precision medicine and natural product-based drug discovery.

1.1 Importance in Healthcare

Ethnopharmacology plays a vital role in modern healthcare by serving as a valuable source for the discovery and development of novel therapeutic agents derived from natural products. Traditional medicinal knowledge has contributed significantly to the identification of bioactive compounds with therapeutic potential against infectious, metabolic, inflammatory, neurological, cardiovascular, and cancer-related diseases. Additionally, ethnopharmacological research supports the scientific validation, quality control, safety assessment, and rational use of herbal medicines, thereby improving their integration into evidence-based healthcare. The discipline also promotes biodiversity conservation, sustainable utilization of medicinal plants, and the preservation of indigenous knowledge. Furthermore, the integration of artificial intelligence (AI), systems biology, network pharmacology, and multi-omics technologies has accelerated natural product research by enabling efficient identification of bioactive compounds, prediction of molecular targets, and development of precision therapeutics, thereby strengthening the role of ethnopharmacology in future drug discovery and personalized medicine.[13–20]

1.2 Traditional Knowledge Systems

Traditional knowledge systems encompass centuries of accumulated empirical observations, cultural practices, and healthcare traditions related to disease prevention, diagnosis, and treatment. Although these medical systems differ in their philosophical foundations and therapeutic approaches, they share a common emphasis on the use of natural resources, holistic patient care, and restoration of physiological balance. These systems have significantly contributed to the discovery of bioactive compounds, the development of herbal medicines, and the advancement of modern pharmacotherapy. In recent years, scientific validation through pharmacological, phytochemical, and molecular studies has strengthened their relevance in evidence-based medicine and natural product drug discovery.[21–30]

Table 2: Comparison of Major Traditional Knowledge Systems in Ethnopharmacology

Traditional Medical System	Origin	Fundamental Principles	Common Therapeutic Resources	Representative Medicinal Plants	Contribution to Modern Drug Discovery
Ayurveda	India (≈3000–5000 years)	Balance of Vata, Pitta, and Kapha	Herbal medicines, diet, yoga, Panchakarma	*Curcuma longa*, *Withania somnifera*, *Tinospora cordifolia*, *Azadirachta indica*	Source of anti-inflammatory, antioxidant, immunomodulatory, and antidiabetic agents
Traditional Chinese Medicine (TCM)	China (>2500 years)	Balance of Yin-Yang and Qi	Herbal prescriptions, acupuncture, moxibustion, Tai Chi	*Artemisia annua*, *Panax ginseng*, *Glycyrrhiza uralensis*, *Ephedra sinica*	Led to the discovery of artemisinin and supports multi-target therapies
Unani	Greece;	Balance of four	Herbal	*Nigella sativa*,	Provides antioxidant,

Medicine	developed in the Arab-Persian world	humors	medicines, diet therapy, regimental therapy	*Glycyrrhiza glabra*, *Foeniculum vulgare*, *Cassia angustifolia*	antimicrobial, hepatoprotective, and immunomodulatory compounds
African Traditional Medicine	Indigenous African communities	Holistic care integrating physical, social, environmental, and spiritual health	Medicinal plants, animal products, traditional rituals	*Prunus africana*, *Vernonia amygdalina*, *Hypoxis hemerocallidea*, *Sutherlandia frutescens*	Source of lead compounds for cancer, malaria, infectious, and metabolic diseases
Siddha	Southern India (Tamil Nadu)	Balance of Vatham, Pitham, and Kabam	Herbal medicines, processed minerals, yoga, diet	*Phyllanthus amarus*, *Aloe vera*, *Piper longum*, *Adhatoda vasica*	Potential therapies for liver, respiratory, metabolic, and inflammatory disorders
Indigenous Medicine	Americas, Australia, Asia, and Oceania	Healing based on ecosystem knowledge and cultural traditions	Wild medicinal plants, fungi, animal products, healing ceremonies	*Echinacea purpurea*, *Salix* spp., *Uncaria tomentosa*, *Tabebuia impetiginosa*	Preserves ethnobotanical knowledge and provides novel bioactive compounds for drug discovery

1.3 Contribution of Natural Products to Modern Medicine

Natural products have played a fundamental role in the discovery and development of modern medicines. Traditional medicinal plants have provided numerous bioactive compounds that serve either as therapeutic agents or as lead molecules for the development of new drugs. These compounds have significantly improved the treatment of infectious diseases, inflammatory disorders, cardiovascular diseases, neurological conditions, and cancer. The integration of traditional knowledge with modern pharmacological research continues to facilitate the identification of safe and effective plant-derived medicines.[31–33]

Several clinically important drugs have originated from natural sources. Aspirin was developed from salicin isolated from the bark of *Salix alba* and remains one of the most widely used analgesic, antipyretic, anti-inflammatory, and antiplatelet agents. Quinine, isolated from the bark of *Cinchona* species, revolutionized the treatment of malaria and laid the foundation for the development of modern antimalarial drugs. Artemisinin, derived from *Artemisia annua*, represents one of the greatest achievements in ethnopharmacology and is currently the cornerstone of artemisinin-based combination therapies for malaria.[34-36]

Natural products have also made remarkable contributions to cancer therapy. Paclitaxel, isolated from *Taxus brevifolia*, inhibits cancer cell division by stabilizing microtubules and is widely used in the treatment of breast, ovarian, and lung cancers. Similarly, morphine, isolated from *Papaver somniferum*, remains one of the most effective opioid analgesics for the management of severe acute and chronic pain. These examples demonstrate that natural products continue to provide valuable chemical scaffolds for drug discovery and remain indispensable resources for the development of innovative therapeutics. Advances in phytochemistry, biotechnology, artificial intelligence, and multi-omics technologies are expected to further accelerate the identification of novel bioactive compounds from natural sources.[37-40]

1.4 Need for Artificial Intelligence and Multi-Omics in Ethnopharmacology

Although ethnopharmacology has contributed significantly to the discovery of therapeutic agents from natural products, conventional research approaches remain labour-intensive, time-consuming, and expensive. The identification of bioactive compounds typically requires extensive phytochemical screening, biological evaluation, isolation, structural characterization, and experimental validation. In addition, herbal medicines are composed of multiple bioactive constituents that interact with numerous molecular targets, making it challenging to elucidate their mechanisms of action using traditional experimental methods alone.[41–43]

Artificial intelligence (AI) has emerged as a powerful tool to overcome these challenges by accelerating various stages of natural product-based drug discovery. Machine learning, deep learning, and natural language processing enable rapid virtual screening of phytochemicals, prediction of biological activities, identification of molecular targets, optimization of lead compounds, and assessment of pharmacokinetic and toxicity profiles. These computational approaches reduce the time and cost associated with conventional drug discovery while improving the accuracy of candidate selection.[44–46]

Simultaneously, advances in multi-omics technologies, including genomics, transcriptomics, proteomics, metabolomics, and microbiomics, have transformed the understanding of medicinal plants at the molecular level. These technologies provide comprehensive insights into gene expression, protein interactions, metabolic pathways, and host responses, thereby facilitating the identification of biomarkers and therapeutic mechanisms underlying herbal medicines.[47–49]

The integration of AI with multi-omics, network pharmacology, molecular docking, and systems biology represents a new paradigm in ethnopharmacological research. By combining computational prediction with high-throughput biological data, researchers can better understand the multi-component and multi-target nature of herbal medicines, identify novel drug candidates, and support precision medicine. Consequently, these interdisciplinary approaches are expected to accelerate evidence-based validation of traditional medicines and promote the development of safer, more effective natural product-derived therapeutics.[50–53]

2. Evolution of Ethnopharmacology

Ethnopharmacology has evolved from the documentation of traditional medicinal knowledge to a multidisciplinary scientific field integrating pharmacology, phytochemistry, biotechnology, computational biology, and precision medicine. While early research primarily focused on identifying medicinal plants based on traditional use, recent technological advances have enabled a deeper understanding of the molecular mechanisms underlying herbal medicines. The incorporation of artificial intelligence (AI), bioinformatics, network pharmacology, and multi-omics technologies has significantly improved the efficiency and accuracy of natural product research.[54–56]

2.1 Traditional Drug Discovery

Traditional drug discovery in ethnopharmacology relied on ethnobotanical knowledge and the empirical use of medicinal plants by indigenous communities. Plants with therapeutic potential were selected based on traditional practices, followed by extraction, phytochemical isolation, pharmacological evaluation, and clinical validation. Although this approach has led to the discovery of important drugs such as aspirin, quinine, artemisinin, and morphine, the process is often slow, labour-intensive, and expensive. In addition, the presence of multiple bioactive constituents in

herbal medicines makes it difficult to identify the compounds responsible for therapeutic activity using conventional experimental methods.[57–59]

2.2 Modern Drug Discovery

Modern ethnopharmacology combines advanced analytical techniques with computational approaches to accelerate natural product research. Technologies such as high-performance liquid chromatography (HPLC), gas chromatography-mass spectrometry (GC-MS), liquid chromatography-mass spectrometry (LC-MS), and nuclear magnetic resonance (NMR) spectroscopy enable rapid identification and characterization of phytochemicals. Computational tools, including molecular docking, molecular dynamics simulations, quantitative structure–activity relationship (QSAR) analysis, and network pharmacology, facilitate prediction of molecular targets and biological activities. AI-based models further improve lead identification, pharmacokinetic prediction, and toxicity assessment, thereby reducing the time and cost required for drug development.[60–63]

2.3 Reverse Ethnopharmacology

Reverse ethnopharmacology represents a target-oriented strategy for natural product discovery. Instead of beginning with medicinal plants, this approach starts with a validated molecular target associated with a specific disease. Computational methods are then used to identify potential bioactive compounds, which are subsequently linked to medicinal plants through ethnobotanical knowledge and phytochemical databases. The identified candidates are validated through experimental and clinical studies. This strategy has shown considerable promise in identifying therapeutic agents for infectious diseases, cancer, diabetes, inflammatory disorders, and neurological diseases.[64–66]

2.4 Current Trends in Ethnopharmacology

Recent advances in ethnopharmacology emphasize the integration of AI, multi-omics technologies, systems biology, and network pharmacology to improve the scientific understanding of herbal medicines. Machine learning algorithms are increasingly used to analyse ethnobotanical databases, predict pharmacological activities, and prioritize promising natural compounds for further investigation. At the same time, genomics, transcriptomics, proteomics, and metabolomics provide comprehensive insights into the molecular mechanisms of herbal medicines and facilitate biomarker discovery. These interdisciplinary approaches support precision medicine by enabling personalized herbal therapies and accelerating the development of evidence-based natural product therapeutics.[67–70]

3. Artificial Intelligence in Ethnopharmacology

Artificial intelligence (AI) has become an important tool in ethnopharmacology by improving the efficiency of natural product research and drug discovery. Traditional ethnopharmacological studies often require extensive phytochemical isolation, biological screening, and experimental validation, making the process time-consuming and resource-intensive. AI enables rapid analysis of large ethnobotanical, phytochemical, and pharmacological datasets, facilitating the identification of bioactive compounds, prediction of molecular targets, toxicity assessment, and lead optimization. The integration of AI with traditional medicinal knowledge has significantly accelerated the discovery of plant-derived therapeutics.[71–73]

3.1 Artificial Intelligence: Concepts and Types

Artificial intelligence refers to computational systems capable of performing tasks that normally require human intelligence, including learning, prediction, pattern recognition, and decision-making. In ethnopharmacology, AI

analyzes complex biological and chemical datasets to support natural product research. Major AI approaches include machine learning (ML), deep learning (DL), natural language processing (NLP), computer vision, and expert systems, each contributing to different stages of drug discovery and development.[74–76]

3.2 Machine Learning and Deep Learning

Machine learning uses algorithms that learn from existing data to predict biological activity, classify medicinal plants, and identify promising lead compounds. Commonly used algorithms include Random Forest, Support Vector Machine, Decision Tree, and Gradient Boosting. Deep learning, a subset of machine learning based on artificial neural networks, enables the analysis of complex molecular structures, prediction of protein–ligand interactions, virtual screening, and biomarker discovery. These technologies have substantially improved the efficiency and accuracy of natural product-based drug discovery.[77–79]

3.3 AI-Assisted Natural Product Discovery

AI-assisted drug discovery integrates phytochemical databases, ethnobotanical knowledge, and computational models to identify compounds with high therapeutic potential. Machine learning algorithms predict pharmacological activities, pharmacokinetic properties, and toxicity, thereby reducing the number of compounds requiring experimental evaluation. AI also supports molecular docking, network pharmacology, and natural language processing for mining scientific literature and traditional medicinal records, enabling faster identification of candidate molecules for diseases such as cancer, diabetes, and infectious disorders.[80–82]

3.4 AI for Target Prediction and Lead Optimization

Target identification and lead optimization are essential steps in modern drug discovery. AI models predict interactions between phytochemicals and disease-associated proteins, helping researchers understand molecular mechanisms and identify potential therapeutic targets. Furthermore, AI-guided molecular modelling improves lead compounds by enhancing efficacy, selectivity, and safety while reducing experimental costs and development time. Combined with molecular docking and molecular dynamics simulations, AI has become an indispensable tool in ethnopharmacological research.[83–84]

4. Multi-Omics Technologies

Multi-omics technologies have transformed ethnopharmacology by providing a comprehensive understanding of the molecular mechanisms of medicinal plants. Unlike conventional pharmacological studies that focus on single compounds, multi-omics integrates genomics, transcriptomics, proteomics, and metabolomics to investigate the complex interactions between phytochemicals and biological systems. Combined with artificial intelligence (AI) and bioinformatics, these technologies facilitate biomarker discovery, identification of therapeutic targets, elucidation of molecular pathways, and development of precision medicine. Consequently, multi-omics has become an essential tool for validating traditional medicines and accelerating natural product-based drug discovery.[85–88]

4.1 Genomics

Genomics is the study of the complete genetic material of an organism. In ethnopharmacology, genomic tools are used to authenticate medicinal plant species, identify genes involved in the biosynthesis of bioactive compounds, and evaluate genetic diversity. Techniques such as DNA sequencing and DNA barcoding improve the quality, authenticity, and conservation of medicinal plants while supporting the sustainable production of valuable phytochemicals.[89–91]

4.2 Transcriptomics

Transcriptomics examines gene expression by analysing RNA transcripts. It helps identify differentially expressed genes involved in phytochemical biosynthesis, stress responses, and therapeutic activities. RNA sequencing (RNA-Seq) has become an important approach for understanding the molecular mechanisms of herbal medicines and discovering regulatory pathways associated with disease treatment.[92–94]

4.3 Proteomics

Proteomics focuses on the large-scale study of proteins and their biological functions. Since proteins regulate most cellular processes, proteomic analysis helps identify molecular targets, signaling pathways, enzyme activities, and biomarkers influenced by herbal medicines. Advanced analytical techniques such as liquid chromatography–mass spectrometry (LC-MS/MS) have significantly improved protein identification and functional analysis in ethnopharmacological research.[95–97]

4.4 Metabolomics

Metabolomics is the comprehensive analysis of small-molecule metabolites produced during cellular metabolism. It provides valuable information on the chemical composition, quality, safety, and pharmacological effects of medicinal plants. Analytical platforms including nuclear magnetic resonance (NMR), gas chromatography–mass spectrometry (GC-MS), and liquid chromatography–mass spectrometry (LC-MS) are widely used to characterize phytochemicals and identify biomarkers associated with therapeutic responses.[98–100]

4.5 Integrated Multi-Omics

Integrated multi-omics combines genomics, transcriptomics, proteomics, and metabolomics to provide a systems-level understanding of medicinal plants and herbal formulations. When integrated with AI, machine learning, and bioinformatics, multi-omics enables comprehensive analysis of biological pathways, molecular interactions, and disease mechanisms. This approach supports biomarker discovery, target identification, precision herbal medicine, and evidence-based validation of traditional therapies. The integration of AI with multi-omics is expected to play a central role in future ethnopharmacological research and natural product-based drug discovery.[101–104]

5. Computational Approaches in Ethnopharmacology

Computational approaches have become essential tools in modern ethnopharmacology by accelerating the discovery of bioactive compounds from medicinal plants. These in silico methods reduce the time, cost, and experimental effort required for drug discovery. They also support the identification of molecular targets, prediction of biological activities, and optimization of lead compounds. The major computational approaches used in ethnopharmacology include molecular docking, molecular dynamics simulation, network pharmacology, and virtual screening.[105–107]

5.1 Molecular Docking

Molecular docking predicts how a phytochemical binds to a target protein and estimates the strength of this interaction. It is widely used to identify potential drug candidates and understand the molecular mechanisms of herbal compounds.[108-109]

5.2 Molecular Dynamics Simulation

Molecular dynamics (MD) simulation evaluates the stability and behaviour of protein–ligand complexes under physiological conditions. It complements molecular docking by providing detailed information about binding stability and molecular interactions over time.[110-111]

5.3 Network Pharmacology

Network pharmacology uses a systems biology approach to investigate interactions among phytochemicals, genes, proteins, signalling pathways, and diseases. Unlike the conventional "one drug–one target" concept, network pharmacology explains the multi-component and multi-target nature of herbal medicines.[112-113]

5.4 Virtual Screening

Virtual screening is a computational technique used to rapidly identify compounds with potential biological activity from large phytochemical libraries. It helps prioritize promising candidates before experimental testing, thereby improving the efficiency of natural product drug discovery.[114-115]

Overall, these computational approaches, when integrated with artificial intelligence and multi-omics technologies, significantly enhance target identification, lead optimization, and evidence-based validation of medicinal plants.[116]

6. AI and Multi-Omics for Precision Drug Discovery

The integration of artificial intelligence with multi-omics technologies has opened new opportunities for precision drug discovery from medicinal plants. AI enables the analysis of large biological datasets generated through genomics, transcriptomics, proteomics, and metabolomics, helping researchers understand the complex mechanisms of herbal medicines and identify novel therapeutic targets.[117–119]

6.1 Multi-Target Drug Discovery

Many chronic diseases involve multiple molecular pathways. AI combined with network pharmacology can identify phytochemicals capable of acting on several targets simultaneously, leading to more effective therapies with reduced risk of drug resistance.[120]

6.2 Biomarker Discovery

AI-assisted analysis of multi-omics data facilitates the identification of biomarkers associated with disease progression, diagnosis, prognosis, and treatment response. These biomarkers are valuable for developing precision medicine strategies.

6.3 Personalized Herbal Medicine

The integration of AI with genomic and clinical information supports personalized herbal medicine by predicting the most appropriate herbal therapies for individual patients. This approach has the potential to improve therapeutic efficacy while minimizing adverse drug reactions.

6.4 Lead Optimization

AI-based computational models assist in optimizing lead compounds by predicting structural modifications that improve biological activity, selectivity, pharmacokinetic properties, and safety. This significantly shortens the drug development process.[121]

7. Challenges and Limitations

Despite significant progress, several challenges remain in applying AI and multi-omics to ethnopharmacology. One major limitation is the availability of high-quality, standardized, and well-annotated datasets. Variability in ethnobotanical records, phytochemical composition, and experimental protocols can affect the accuracy of AI predictions.

Experimental validation remains another important challenge. Although computational approaches effectively prioritize potential drug candidates, laboratory experiments and well-designed preclinical and clinical studies are essential to confirm their efficacy and safety.

Ethical and regulatory issues also require attention. Protection of indigenous knowledge, equitable benefit-sharing, biodiversity conservation, data privacy, and harmonized regulatory frameworks are necessary to ensure the responsible development and commercialization of AI-assisted natural product research.

Overall, overcoming these scientific, technical, ethical, and regulatory challenges will facilitate the successful integration of AI and multi-omics into ethnopharmacology and accelerate the development of safe, effective, and evidence-based herbal medicines.[122]

8. Future Perspectives

The future of ethnopharmacology will be driven by the integration of artificial intelligence (AI), multi-omics technologies, and precision medicine. AI is expected to accelerate the discovery of bioactive compounds, improve prediction of drug targets, and support the development of safer and more effective plant-derived medicines. The use of machine learning and advanced computational tools will further reduce the time and cost involved in natural product drug discovery.

Another important direction is the digitalization of traditional medicinal knowledge. The development of digital ethnopharmacology databases, electronic herbariums, and standardized ethnobotanical repositories will help preserve indigenous knowledge and make it more accessible for scientific research worldwide. These resources will also facilitate data sharing and improve the reproducibility of ethnopharmacological studies.

Precision medicine is expected to play an important role in future herbal drug development. Integrating genomic information, clinical data, and AI-based predictive models may enable personalized herbal therapies according to an individual's genetic profile and disease characteristics. In addition, explainable AI (XAI) will improve the transparency and reliability of AI-based predictions, increasing confidence among researchers, clinicians, and regulatory agencies.
Overall, the combination of AI, multi-omics, computational biology, and traditional medicinal knowledge is expected to accelerate evidence-based herbal medicine research and support the discovery of novel therapeutics for complex diseases.[123]

9. CONCLUSION

Ethnopharmacology has evolved into a multidisciplinary field that combines traditional medicinal knowledge with modern technologies, including artificial intelligence, computational biology, and multi-omics. These advances have significantly improved the identification of bioactive compounds, molecular targets, and mechanisms of action of medicinal plants, thereby accelerating natural product-based drug discovery.

The integration of genomics, transcriptomics, proteomics, metabolomics, molecular docking, molecular dynamics simulation, virtual screening, and network pharmacology has enhanced the understanding of the multi-component and multi-target nature of herbal medicines. These technologies support evidence-based validation of traditional medicines and contribute to the development of precision therapeutics.

Despite these advances, challenges such as data standardization, experimental validation, explainable AI, ethical issues, and regulatory frameworks remain important for the successful clinical translation of AI-assisted ethnopharmacological research. Addressing these challenges through interdisciplinary collaboration will improve the reliability and acceptance of herbal medicines in modern healthcare.

In conclusion, the convergence of traditional knowledge with AI and multi-omics represents a promising strategy for future drug discovery. Continued collaboration among ethnopharmacologists, pharmacologists, computational scientists, and clinicians will facilitate the development of safe, effective, and personalized plant-based therapeutics for global healthcare.[124]

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