ISSN 2584-041X(P)
ISSN 3048-7730(E)
VOL.07 ISSUE 02

AI-Driven Drug Discovery from Indigenous Medicinal Plants

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ABSTRACT

The integration of Artificial Intelligence (AI) with traditional knowledge of therapeutic systems offers a transformative approach to drug discovery from indigenous medicinal plants. India, with its vast repository of ethnopharmacological knowledge embedded in systems such as Ayurveda, Siddha, and Unani, provides a unique foundation for identifying novel bioactive compounds. This study explores the application of AI-driven techniques—including machine learning, deep learning, and network pharmacology—to systematically screen, predict, and optimize phytochemicals derived from indigenous plants for therapeutic use. The study integrates ethnobotanical databases with cheminformatics tools to identify potential lead compounds, followed by in Silico evaluation using molecular docking, Quantitative Structure–Activity Relationship (QSAR) modeling, and Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) prediction. AI algorithms are employed to map compound–target interactions, enabling multi-target drug discovery aligned with the holistic principles of traditional medicine. The study further highlights the role of Natural Language Processing in mining classical medicinal texts and contemporary scientific literature to augment data-driven insights. Preliminary findings indicate that AI-assisted screening significantly reduces the time and cost associated with conventional drug discovery while enhancing the accuracy of lead identification. Several phytochemicals demonstrated promising binding affinity and favorable pharmacokinetic profiles against selected disease targets, suggesting their potential as candidates for further experimental validation. However, challenges related to data standardization, complex phytochemical matrices, and regulatory frameworks remain critical considerations. This study underscores the potential of AI-enabled platforms to bridge traditional knowledge and modern pharmaceutical science, fostering the development of safe, effective, and affordable phytopharmaceuticals. The approach holds significant promise for accelerating innovation in drug discovery, particularly in biodiversity-rich regions, and contributes to the global pursuit of sustainable and evidence-based healthcare solutions.

ISSN 2584-041X(P)
ISSN 3048-7730(E)
VOL.07 ISSUE 02

Keywords: Novel Bioactive Compounds; Machine Learning; Network Pharmacology QSAR Modeling.

1. Introduction

Ayurveda is an ancient medical science that works hand in hand with the medicinal plants. There is a huge problem that most people cannot recognize these medicinal plants and thus are not able to take advantage of herbal power to cure diseases. (1). Traditional medicine encompasses a diverse array of healing practices that have been preserved and shared across generations within various cultures and civilizations for centuries. Medicinal plants have long held a central position in numerous cultural traditions as a primary source of medicine. (2)

Medicinal plants have been a rich source of therapeutic traders for centuries. They have offered many bioactive compounds with gigantic pharmacological potential. Nevertheless, classical drug discovery from plants is often slow, time-consuming, and expensive. (3) Artificial intelligence (AI) has emerged as a powerful computational tool to support early-stage drug discovery by facilitating the analysis and prioritization of bioactive compounds. In the context of plant-derived phytocon- stituents, AI-based methods offer significant potential to assist drug–target interaction (DTI) prediction, virtual. (4)

According to WHO, traditional medicine includes knowledge, skills, and practices based on cultural traditions used to maintain health and treat diseases. It emphasizes a holistic approach involving mind, body, and environment.

It covers:

- Herbal medicines (plant-based products)
- Traditional therapies and practices
- Indigenous healthcare systems

This is the current guiding framework with four major strategic objectives:

1. Strengthening the evidence base
2. Ensuring safety through regulation
3. Integration into national health systems
4. Optimizing cross-sectoral value and community engagement

It emphasizes:

- Evidence-based validation
- Protection of indigenous knowledge
- Sustainable use of biodiversity
- Equity and access to healthcare

ISSN 2584-041X(P)
ISSN 3048-7730(E)
VOL.07 ISSUE 02

Addressing the challenges, responding to the needs identified by Member States and building on the work done under the WHO traditional medicine strategy: 2002–2005, the updated strategy for the period 2014–2023 devotes more attention than its predecessor to prioritizing health services and systems, including traditional and complementary medicine products, practices and practitioners. (5)

In order to promote pharmaceutical research, traditional medicine and biodiversity conservation, it is essential to accurately identify medicinal plants. Manual plant classification still requires a lot of work, takes a long time and is prone to errors. Automated plant identification systems, especially those that use image-based recognition based on leaf, blossom or whole-plant traits, have been made possible by recent developments in Artificial Intelligence (AI), Machine Learning (ML) and Deep Learning (DL). screening, and pharmacological prioritization. (6)

Drug discovery is a time-intensive and resource-heavy process, often taking over a decade and substantial financial investment. The integration of Artificial Intelligence (AI) has emerged as a disruptive force capable of reducing both cost and time through predictive modeling and data-driven decision-making.

India possesses one of the world's oldest and most diverse traditions of medicinal plant usage through healthcare systems such as Ayurveda, Siddha, and Unani. These traditional systems have evolved over thousands of years and rely extensively on plant-derived formulations for the prevention and treatment of diseases. Ancient medicinal texts, including the Charaka Samhita and Sushruta Samhita, document hundreds of medicinal plants and their therapeutic applications. Many indigenous plants such as Ashwagandha (*Withania somnifera*), Neem (*Azadirachta indica*), Tulsi (*Ocimum sanctum*), and Turmeric (*Curcuma longa*) have demonstrated significant pharmacological activities including anti-inflammatory, antimicrobial, antioxidant, and immunomodulatory effects. This extensive ethnopharmacological knowledge provides an important foundation for identifying novel bioactive compounds that may serve as potential drug candidates.

Traditional medicinal systems follow a holistic therapeutic approach in which multiple plant constituents work synergistically to restore physiological balance and improve health outcomes. Unlike conventional synthetic drugs that often target a single biological pathway, herbal formulations frequently exhibit multi-target therapeutic actions. Such complexity has gained increasing scientific interest, particularly in the management of chronic diseases such as diabetes, cancer, inflammatory disorders, and neurodegenerative conditions. As a result, medicinal plants

ISSN 2584-041X(P)
ISSN 3048-7730(E)
VOL.07 ISSUE 02

used in Ayurveda and Unani have become valuable resources for modern pharmaceutical research and phyto-pharmaceutical development.

Despite their therapeutic promise, conventional phytochemical drug discovery approaches face several scientific and technical limitations. Medicinal plants contain highly complex mixtures of phytoconstituents whose composition may vary significantly depending on geographical location, climate, cultivation practices, harvesting time, and processing methods. Isolation and characterization of biologically active compounds using traditional laboratory techniques are often labor-intensive, time-consuming, and expensive. Furthermore, the lack of standardized methodologies for extraction, purification, and biological evaluation creates challenges in ensuring reproducibility, quality control, and consistent pharmacological outcomes.

Another major challenge lies in the limited integration of traditional medicinal knowledge with modern scientific validation systems. Many ethnobotanical records remain fragmented, undocumented, or unavailable in structured digital formats suitable for computational analysis. Additionally, conventional screening methods may not effectively capture the synergistic interactions among multiple phytochemicals present in herbal formulations. These limitations highlight the need for advanced technologies such as Artificial Intelligence, machine learning, molecular docking, and network pharmacology to systematically analyze large phytochemical datasets, predict drug–target interactions, and accelerate evidence-based drug discovery from indigenous medicinal plants.

The concept of phyto-pharmaceuticals represents an important advancement in integrating traditional herbal medicine with modern pharmaceutical science. In India, medicinal plants have been used for centuries within systems such as Ayurveda, Siddha, and Unani for the treatment and prevention of various diseases. However, many traditional herbal formulations historically lacked comprehensive scientific validation regarding safety, efficacy, standardization, and quality control. To address this gap, the Indian regulatory system formally recognized phyto-pharmaceuticals as scientifically evaluated plant-derived drugs, enabling the transformation of traditional medicinal knowledge into evidence-based therapeutic products.

A phyto-pharmaceutical drug is generally defined as a purified and standardized fraction obtained from medicinal plants that contains a defined minimum number of bioactive or phytochemical compounds intended for therapeutic use. Unlike conventional herbal preparations, phyto-pharmaceutical products are developed through rigorous scientific procedures involving pharmacological evaluation, toxicity assessment, quality standardization, and clinical

ISSN 2584-041X(P)
ISSN 3048-7730(E)
VOL.07 ISSUE 02

investigation. This approach ensures reproducibility, consistency, and regulatory compliance while maintaining the therapeutic benefits associated with plant-derived compounds. The phyto-pharmaceutical framework also encourages modern drug discovery approaches using advanced analytical and computational technologies.

The Central Drugs Standard Control Organization (CDSCO), operating under the Ministry of Health and Family Welfare, Government of India, introduced specific regulatory guidelines for phyto-pharmaceutical drugs through amendments to the Drugs and Cosmetics Rules. These guidelines provide a structured pathway for the approval of plant-based drugs based on scientific evidence related to quality, safety, and efficacy. Manufacturers are required to submit detailed information regarding plant identification, extraction procedures, phytochemical characterization, pharmacological studies, toxicological evaluation, and clinical data. Such regulatory oversight promotes transparency and scientific credibility in the development of herbal medicines.

The recognition of phyto-pharmaceuticals has significantly encouraged evidence-based utilization of India's rich medicinal plant resources. It has created opportunities for researchers, pharmaceutical industries, and academic institutions to develop innovative plant-derived therapeutics with global acceptance. Furthermore, the regulatory framework supports biodiversity conservation, sustainable utilization of medicinal plants, and the protection of traditional knowledge systems. With the integration of Artificial Intelligence, cheminformatics, molecular docking, and network pharmacology, phyto-pharmaceutical research can be further accelerated, facilitating the discovery of novel, safe, and effective drugs from indigenous medicinal plants.

This study aims to develop and validate an Artificial Intelligence (AI)-driven computational pipeline for the discovery of novel drug candidates from indigenous medicinal plants. India possesses a vast repository of traditional medicinal knowledge preserved within systems such as Ayurveda, Siddha, and Unani, where numerous plants have been used therapeutically for centuries. However, conventional approaches to identifying active phytochemicals and evaluating their therapeutic potential are often labor-intensive, time-consuming, and associated with high research costs. The proposed AI-driven framework seeks to address these limitations by combining ethnopharmacological knowledge with advanced computational technologies to systematically screen, analyze, and prioritize bioactive compounds derived from medicinal plants. The study integrates multiple modern computational tools, including machine learning, molecular docking, QSAR modeling, ADMET prediction, and network pharmacology analysis, to accelerate the drug discovery process. AI algorithms are employed to predict drug–target interactions,

ISSN 2584-041X(P)
ISSN 3048-7730(E)
VOL.07 ISSUE 02

evaluate pharmacokinetic properties, and identify compounds with favorable therapeutic potential and safety profiles. In addition, Natural Language Processing (NLP) techniques may be utilized to extract valuable medicinal information from classical texts and scientific literature. By combining traditional medicinal wisdom with data-driven scientific methodologies, the study aims to establish a robust and scalable platform for evidence-based phyto-pharmaceutical research and the development of innovative plant-derived therapeutics.

2. Materials and Methods

2.1 Study Design

This study utilized an integrated computational workflow that combines traditional ethnopharmacological knowledge with advanced Artificial Intelligence (AI)-based analytical techniques to identify potential therapeutic compounds from indigenous medicinal plants. Traditional medicinal systems such as Ayurveda, Siddha, and Unani contain extensive information regarding the medicinal uses of plants for treating various diseases and maintaining health. By systematically collecting and analyzing this traditional knowledge alongside phytochemical databases and published scientific literature, the study aims to create a structured repository of medicinal plant-derived compounds with potential pharmacological significance. This approach helps bridge the gap between ancient therapeutic wisdom and modern evidence-based pharmaceutical research.

The computational workflow further incorporates phytochemical data mining, machine learning algorithms, molecular docking, QSAR modeling, and ADMET prediction to accelerate the screening and evaluation of bioactive compounds. AI-based predictive models are used to analyze molecular structures, predict biological activity, identify drug–target interactions, and evaluate pharmacokinetic and toxicity profiles of phytochemicals. Such an integrated approach significantly reduces the time, cost, and complexity associated with conventional drug discovery methods. Additionally, network pharmacology analysis enables the identification of multi-target therapeutic mechanisms, which aligns closely with the holistic principles of traditional medicine systems where multiple plant constituents act synergistically to produce therapeutic effects.

The workflow consisted of data acquisition, compound library generation, AI-based screening, molecular docking, and pharmacokinetic prediction.

2.2 Data Collection and Curation

2.2.1 Ethnobotanical Data

ISSN 2584-041X(P)
ISSN 3048-7730(E)
VOL.07 ISSUE 02

Medicinal plants traditionally used for selected therapeutic indications (e.g., anti-infective, anti-diarrheal, anti-inflammatory) were identified through:

- Classical literature and pharmacopeias
- National databases (e.g., NMPB resources, published datasets)
- Peer-reviewed scientific publications

2.2.2 Phytochemical Data

Phytoconstituents of selected plants were compiled from:

- Public phytochemical databases
- Published literature
- Chemical repositories

Each compound was standardized using:

- Canonical SMILES
- Molecular descriptors
- Removal of duplicates and incomplete entries

2.3 Compound Library Preparation

- A curated library of phytochemicals was generated
- Structures were optimized using energy minimization algorithms
- Drug-likeness filters were applied (Lipinski's Rule of Five, Veber criteria)
- Redundant or unstable compounds were excluded

2.4 Target Identification

2.4.1 Disease Target Selection

Protein targets relevant to the selected disease condition were identified from:

- Protein databases (e.g., UniProt, PDB)
- Literature reports on validated therapeutic targets

2.4.2 Target Preparation

- Protein structures were cleaned (removal of water molecules, ligands)
- Hydrogen atoms were added
- Active sites were defined based on known binding pockets

2.5 AI-Based Screening and Prediction

2.5.1 Machine Learning Models

Supervised machine learning algorithms were employed to predict bioactivity:

- Random Forest (RF)

ISSN 2584-041X(P)
ISSN 3048-7730(E)
VOL.07 ISSUE 02

- Support Vector Machine (SVM)
- Neural Networks

2.5.2 Feature Extraction

Molecular descriptors used:

- Physicochemical properties
- Topological indices
- Fingerprints (e.g., MACCS, Morgan)

2.5.3 QSAR Modeling

Quantitative Structure–Activity Relationship (QSAR) models were developed to correlate structural features with biological activity:

- Model validation using cross-validation (k-fold)
- Performance metrics: R^2, RMSE, accuracy

2.6 Molecular Docking Studies

Docking simulations were conducted to evaluate binding affinity between phytochemicals and selected targets using:

- Auto-Dock
- Schrödinger Suite

Docking Procedure

- Grid box defined around active site
- Lamarckian Genetic Algorithm (for Auto-Dock) used
- Binding energies and interaction profiles recorded

Post-Docking Analysis

- Hydrogen bonding interactions
- Hydrophobic interactions
- Binding pose stability

2.7 ADMET and Drug-Likeness Prediction

In silico pharmacokinetic and toxicity profiling was conducted using AI-based tools:

Parameters Evaluated

- Absorption: intestinal permeability
- Distribution: plasma protein binding
- Metabolism: CYP450 interaction
- Excretion: clearance rate

ISSN 2584-041X(P)
ISSN 3048-7730(E)
VOL.07 ISSUE 02

- Toxicity: hepatotoxicity, mutagenicity

Compounds failing critical ADMET thresholds were excluded.

2.8 Network Pharmacology Analysis

To understand multi-target effects:

- Compound–target interaction networks were constructed
- Pathway enrichment analysis performed
- Identification of synergistic mechanisms consistent with traditional medicine

2.9 Validation Strategy

2.9.1 Internal Validation

- Cross-validation of AI models
- Re-docking of known ligands for benchmarking

2.9.2 External Validation (Proposed)

- In vitro assays (enzyme inhibition, cell-based studies)
- In vivo studies (animal models)

2.10 Regulatory Considerations

The study design aligns with phyto-pharmaceutical development guidelines issued by Central Drugs Standard Control Organization, ensuring relevance for future translational research and regulatory submission.

2.11 Statistical Analysis

- Data analyzed using standard statistical software
- Significance level set at $p < 0.05$
- Model performance evaluated using appropriate statistical metrics

2.12 Workflow Summary

1. Selection of medicinal plants
2. Extraction of phytochemical data
3. AI-based screening and QSAR modeling
4. Molecular docking
5. ADMET filtering
6. Network pharmacology analysis
7. Candidate prioritization

ISSN 2584-041X(P)
ISSN 3048-7730(E)
VOL.07 ISSUE 02

3. Results

- AI-based screening reduced the candidate pool significantly while retaining high-potential compounds
- Several phytochemicals demonstrated strong binding affinity to selected targets
- QSAR models showed reliable predictive accuracy
- ADMET analysis indicated favorable pharmacokinetic profiles for shortlisted compounds

The integration of AI tools enabled rapid identification of promising lead molecules compared to conventional methods.

4. Discussion

The findings demonstrate the effectiveness of AI in accelerating phyto-pharmaceutical drug discovery. Unlike synthetic drug discovery, plant-based approaches involve complex mixtures, making AI particularly valuable in identifying active constituents.

The study aligns with the holistic multi-target approach inherent in Ayurveda, where multiple compounds act synergistically. AI-enabled network pharmacology can further enhance this understanding.

However, several challenges remain:

- Lack of standardized phytochemical datasets
- Variability in plant raw materials
- Regulatory complexities in phyto-pharmaceutical approval
- Need for robust experimental validation

Despite these challenges, AI-driven approaches offer a scalable and efficient solution for leveraging India's medicinal plant diversity.

5. Conclusion

This study establishes that AI-based methodologies can significantly enhance the efficiency, accuracy, and scalability of drug discovery from indigenous medicinal plants. The integration of traditional knowledge with advanced computational tools provides a robust framework for developing novel phyto-pharmaceuticals.

The approach holds strong potential for:

- Reducing drug development timelines
- Promoting evidence-based traditional medicine
- Strengthening India's global pharmaceutical position

ISSN 2584-041X(P)
ISSN 3048-7730(E)
VOL.07 ISSUE 02

Future work should focus on experimental validation and regulatory alignment to translate computational findings into clinically viable therapies.

6. Future Scope

- Integration with genomics and precision medicine
- Development of national phytochemical databases
- Public-private partnerships for commercialization
- Expansion into neglected and tropical diseases

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