Vamshi S. Zool. Allied Sci. Lett., Vol.1, Iss.1, January-June, 2026: 1-10

Zoology and Allied Sciences Letters
Content Available at www.lapinpress.com ISSN (O): XXXX-XXXX
(An online peer reviewed Referred Journal)

Review Article

OPEN ACCESS

AI-ASSISTED PHARMACOGNOSY: INTEGRATING ARTIFICIAL INTELLIGENCE WITH NATURAL PRODUCT DRUG DISCOVERY

VAMSHI SHARATHNATHKAVETI

Associate Professor, Department of Pharmacognosy, Nalla Narasimha Reddy Education Society's Group of Institutions, School of Pharmacy, Chowdariguda, Ghatkesar, Medchal, Hyderabad, Telangana, India – 500 088.

***Corresponding Author**
Dr. Vamshi Sharathnathkaveti

Article History: Received: 14 Jan 2026, Revised: 04 Feb 2026, Accepted: 26 Feb 2026

Abstract: Artificial Intelligence (AI) is rapidly transforming pharmacognosy by enabling data-driven discovery of bioactive natural compounds from plants, microorganisms, and marine organisms. Traditional pharmacognosy relies on ethnomedicinal knowledge, phytochemical isolation, and biological screening; however, these approaches are time-consuming, costly, and often inefficient due to structural redundancy and chemical complexity inherent in natural products. The integration of AI methodologies such as machine learning (ML), deep learning (DL), natural language processing (NLP), and generative models has significantly enhanced the speed and precision of natural product drug discovery. AI-assisted pharmacognosy facilitates predictive modeling of phytochemical bioactivity, virtual screening of compound libraries, dereplication of known molecules, and multi-omics data integration for target identification. Furthermore, AI enables the interpretation of complex metabolomic and spectral datasets, improving compound annotation and accelerating lead identification. The convergence of computational intelligence with pharmacognosy is also reshaping ethnopharmacology by mining large-scale textual databases to uncover hidden therapeutic knowledge from traditional medicine systems. Despite these advances, challenges such as limited curated datasets, poor standardization of phytochemical information, model interpretability issues, and lack of experimental validation frameworks remain significant barriers. Future directions include integration of explainable AI (XAI), digital twins of medicinal plants, federated learning systems, and generative chemistry models for de novo drug design. Overall, AI-assisted pharmacognosy represents a paradigm shift from empirical discovery to predictive, computationally driven natural product research, significantly improving efficiency, scalability, and translational success in drug development pipelines.

Keywords: *Artificial Intelligence; Pharmacognosy; Natural Products; Machine Learning; Drug Discovery; Metabolomics.*

1. INTRODUCTION

Natural products have historically served as one of the richest sources of therapeutic agents. More than 60% of currently approved drugs are either derived from or inspired by natural compounds. Classical pharmacognosy integrates botany, phytochemistry, microbiology, and pharmacology to identify bioactive molecules from natural sources.

However, the traditional workflow suffers from:

- Redundant isolation of known compounds
- Low throughput screening techniques
- Fragmented ethnopharmacological knowledge
- Lack of predictive prioritization tools
- Inefficient structure–activity exploration

With increasing chemical space complexity-estimated at $>10^{60}$ possible drug-like molecules-traditional experimental approaches alone are insufficient[1].

1.1 Emergence of Artificial Intelligence in Pharmacognosy

Artificial Intelligence has emerged as a transformative computational paradigm capable of learning patterns from large-scale chemical and biological datasets. In pharmacognosy, AI is applied to:

- Predict biological activity of phytochemicals
- Identify novel bioactive scaffolds
- Automate literature mining

- Integrate multi-omics datasets
- Optimize lead compounds

AI enables transition from **"trial-and-error discovery" to "predictive discovery"**.

2. HISTORICAL EVOLUTION OF COMPUTATIONAL PHARMACOGNOSY

The development of AI in pharmacognosy can be divided into five phases:

2.1 Phase I: Empirical Ethnopharmacology

Drug discovery based on traditional knowledge systems such as Ayurveda, Traditional Chinese Medicine, and Unani.

2.2 Phase II: Phytochemical Isolation Era

Bioactivity-guided fractionation and chromatographic techniques dominated.

2.3 Phase III: Chemoinformatics Era

Introduction of QSAR models and molecular docking.

2.4 Phase IV: Machine Learning Era

Supervised and unsupervised ML applied for prediction of biological activity.

2.5 Phase V: Deep Learning and Generative AI Era

Neural networks, transformers, and generative models for de novo drug design [2].

3. DIGITAL TRANSFORMATION OF PHARMACOGNOSY

AI has enabled digitization of pharmacognostic data including:

- Chemical structure databases
- Herbarium records
- Spectral libraries (NMR, LC-MS, GC-MS)
- Genomic sequences of medicinal plants
- Ethnobotanical literature archives

This transformation allows integration of heterogeneous datasets into unified predictive systems.

4. DATA ECOSYSTEM IN AI-ASSISTED PHARMACOGNOSY

AI models rely on multi-source datasets.

4.1 Chemical Databases

Examples:

- PubChem
- ChEMBL
- NPASS (Natural Product Activity and Species Source Database)
- SuperNatural II

4.2 Biological Databases

- UniProt (protein targets)
- KEGG (pathways)
- DrugBank

4.3 Ethnopharmacological Databases

- Dr. Duke's Database
- TCMID (Traditional Chinese Medicine Integrated Database)

4.4 Omics Data

- Genomics
- Transcriptomics
- Proteomics
- Metabolomics

Table 01: Data Sources in AI-Assisted Pharmacognosy

Data Type	Source	Role in AI Modeling	Example Use
Chemical data	PubChem, ChEMBL	Feature extraction	QSAR modeling
Natural product data	NPASS	Bioactivity mapping	Lead identification
Spectral data	NMR/LC-MS libraries	Compound identification	Dereplication
Genomic data	NCBI, UniProt	Target identification	Pathway mapping
Ethnobotanical data	Literature mining	Knowledge extraction	Drug repositioning

5. ARTIFICIAL INTELLIGENCE TECHNIQUES IN PHARMACOGNOSY (DEEP EXPANSION) [3]

5.1 Machine Learning Algorithms

Machine learning models used include:

- Support Vector Machines (SVM)
- Random Forest (RF)
- k-Nearest Neighbors (k-NN)
- Gradient Boosting Machines (GBM)

These models are widely used for:

- Activity prediction
- Toxicity classification
- Compound clustering

5.2 Deep Learning Approaches

Deep learning architectures include:

- Convolutional Neural Networks (CNN)
- Recurrent Neural Networks (RNN)
- Graph Neural Networks (GNN)
- Transformers

Applications:

- Molecular fingerprint learning
- Protein–ligand interaction prediction
- Spectral image recognition
- De novo molecule generation

5.3 Natural Language Processing (NLP)

NLP enables:

- Extraction of medicinal plant uses from literature
- Mining historical texts
- Identifying disease–plant relationships

Example:

- Extraction of anti-inflammatory plants from Ayurveda texts

5.4 Generative AI in Drug Discovery

Generative models include:

- Variational Autoencoders (VAE)
- Generative Adversarial Networks (GANs)
- Transformer-based molecular generators

These models can design novel compounds with desired properties.

6. WORKFLOW OF AI-ASSISTED PHARMACOGNOSY [4]

The integrated pipeline includes:

1. Data collection from natural sources
2. Data cleaning and normalization
3. Feature engineering (molecular descriptors)
4. Model training (ML/DL)
5. Virtual screening
6. Biological validation
7. Lead optimization

7. INTEGRATION WITH TRADITIONAL PHARMACOGNOSY

AI does not replace classical pharmacognosy but enhances it by:

- Prioritizing plant species for screening
- Reducing experimental redundancy
- Identifying hidden bioactive compounds
- Predicting synergistic effects in herbal formulations

Table 02: AI Integration Points in Pharmacognosy

Pharmacognosy Stage	Traditional Method	AI Enhancement	Outcome
Plant selection	Ethnobotanical survey	NLP-based mining	Faster prioritization
Extraction	Solvent	Predictive	Higher yield

	extraction	optimization	efficiency
Screening	In vitro assays	Virtual screening	Reduced cost
Compound identification	Chromatography	Spectral AI matching	Faster dereplication
Lead optimization	Medicinal chemistry	Deep learning models	Improved potency

8. ROLE OF SPECTROSCOPY AND AI INTEGRATION

AI significantly enhances interpretation of:

- NMR spectra
- Mass spectrometry data
- Infrared spectroscopy

Deep learning models classify spectral patterns to identify unknown compounds with high accuracy [4].

9. AI-DRIVEN APPLICATIONS IN NATURAL PRODUCT DRUG DISCOVERY

AI has shifted pharmacognosy from a descriptive discipline to a predictive and precision-oriented science. This section discusses major application domains where AI significantly enhances natural product-based drug discovery.

9.1 AI in Anticancer Drug Discovery from Natural Products

Cancer remains one of the most complex diseases, characterized by heterogeneous molecular pathways. Natural products have historically provided key anticancer agents such as paclitaxel and vincristine. AI now accelerates identification of similar compounds [5].

AI Contributions:

- Prediction of cytotoxic phytochemicals using ML classifiers
- Virtual screening of plant metabolite libraries
- Identification of apoptosis-inducing compounds
- Multi-target pathway prediction

AI models integrate molecular docking scores with deep learning-based activity prediction to shortlist candidate compounds with higher specificity toward cancer-related targets such as:

- EGFR
- BCL-2
- PI3K/AKT pathway proteins

Key Insight:

AI reduces screening time from years to weeks in anticancer natural product discovery.

9.2 Antimicrobial Drug Discovery Using AI

The rise of antimicrobial resistance (AMR) has intensified the need for novel antibiotics.

AI Applications:

- Classification of antibacterial phytochemicals
- Prediction of MIC (Minimum Inhibitory Concentration)
- Identification of membrane-disrupting compounds
- Screening of microbial secondary metabolites

AI models trained on microbial metabolite datasets can identify novel antibiotic scaffolds from:

- Actinomycetes
- Fungi
- Marine bacteria

Graph neural networks (GNNs) are particularly effective in predicting antimicrobial activity by analyzing molecular structure connectivity [6].

9.3 Neuropharmacological Applications

Natural products play a critical role in neurodegenerative diseases such as Alzheimer's and Parkinson's disease.

AI Contributions:

- Identification of acetylcholinesterase inhibitors
- Blood-brain barrier permeability prediction
- Neuroprotective compound screening
- Pathway-level modeling of neuroinflammation

AI systems integrate:

- Protein–ligand docking
- QSAR models
- Transcriptomic data

This enables identification of plant-derived flavonoids, alkaloids, and terpenoids with neuroprotective potential.

9.4 Anti-inflammatory Drug Discovery [7]

Inflammation is a major pathological component of chronic diseases.

AI Applications:

- Prediction of COX-1 and COX-2 inhibition
- NF-κB pathway modulation screening
- Cytokine suppression modeling

Machine learning models prioritize phytochemicals such as:

- Curcuminoids
- Flavonoids
- Saponins

These compounds are evaluated for binding affinity and pharmacokinetic stability using AI pipelines.

9.5 Metabolic Disease Applications

AI-assisted pharmacognosy plays a crucial role in:

- Diabetes mellitus
- Obesity
- Dyslipidemia

Mechanisms:

- α-glucosidase inhibition prediction
- Insulin receptor pathway modeling
- Lipid metabolism modulation

Natural compounds such as berberine-like alkaloids and polyphenols are identified using predictive ML systems.

10. AI-DRIVEN MOLECULAR DOCKING AND HYBRID APPROACHES

10.1 Classical Docking vs AI-Augmented Docking

Traditional docking methods are often limited by:

- Rigid receptor assumptions
- Limited conformational sampling
- High computational cost

AI enhances docking through:

- Flexible binding prediction
- Faster scoring functions
- Deep learning-based pose prediction [8].

10.2 Hybrid AI–Docking Pipelines

A typical hybrid workflow includes:

1. ML-based compound filtering
2. Docking simulation
3. Deep learning rescoring
4. ADMET prediction
5. Final compound ranking

This integration improves prediction accuracy significantly.

10.3 Deep Learning Scoring Functions

Neural networks are trained to predict:

- Binding affinity
- Interaction energy
- Ligand orientation

This reduces dependence on physics-based scoring alone.

11. Network Pharmacology and AI Integration

Natural products often act on multiple targets simultaneously.

11.1 Multi-Target Mechanism Prediction

AI enables:

- Construction of compound–target networks
- Identification of synergistic interactions
- Mapping of disease pathways

11.2 Systems Pharmacology Approach [8].

AI integrates:

- Genomic data
- Proteomic interactions and Metabolic networks to build holistic models of drug action.

Table 03: AI Applications in Therapeutic Domains

Therapeutic Area	AI Technique	Natural Product Source	Outcome
Cancer	Deep learning + docking	Plant alkaloids	Target-specific inhibitors
Infectious diseases	ML classification	Microbial metabolites	Antibiotic discovery
Neurology	Network pharmacology	Flavonoids	Neuroprotection
Inflammation	QSAR + ML	Polyphenols	Anti-inflammatory leads
Metabolic disorders	Predictive modeling	Herbal extracts	Enzyme inhibition

12. AI IN METABOLOMICS AND SPECTRAL DATA ANALYSIS [9].
Metabolomics generates high-dimensional datasets requiring advanced computational tools.
12.1 Mass Spectrometry Interpretation
AI algorithms:
- Identify unknown metabolites
- Match spectral fingerprints
- Classify compound families

12.2 NMR-Based Compound Identification
Deep learning models interpret:
- Chemical shifts
- Peak intensities
- Structural correlations

This significantly accelerates structural elucidation.
12.3 Multi-Omics Integration
AI integrates:
- Metabolomics
- Transcriptomics
- Proteomics

To identify:
- Biosynthetic pathways
- Bioactive metabolite clusters [10].

13. ETHNOPHARMACOLOGY AND AI-BASED KNOWLEDGE MINING
Traditional medicinal systems contain vast unstructured knowledge.
13.1 NLP-Based Text Mining
AI extracts:
- Plant–disease relationships
- Traditional formulations
- Therapeutic indications

13.2 Knowledge Graph Construction
AI builds:
- Herb–compound–target–disease networks
- Semantic relationships among medicinal plants

13.3 Drug Repositioning from Traditional Knowledge [11].
AI identifies modern therapeutic uses for:
- Previously known medicinal plants
- Underutilized herbal species

14. CASE STUDIES IN AI-ASSISTED PHARMACOGNOSY
14.1 Curcumin Derivatives Optimization
AI models optimized curcumin analogs for:
- Improved bioavailability
- Enhanced anti-inflammatory activity

14.2 Artemisinin Derivative Prediction
Machine learning models identified:
- New antimalarial scaffolds
- Resistance-modifying compounds [12].

14.3 Marine Natural Products Screening
AI helped identify:
- Anticancer peptides from marine sponges
- Antiviral compounds from algae

15. LIMITATIONS IN CURRENT AI APPLICATIONS [14].
Despite progress, several limitations persist:
- Data imbalance in natural product datasets
- Lack of high-quality labeled training data
- Limited interpretability of deep learning models
- Experimental validation bottlenecks
- Computational resource constraints

16. ADVANCED AI TECHNOLOGIES TRANSFORMING PHARMACOGNOSY
Recent advances in Artificial Intelligence are reshaping pharmacognosy from predictive modeling to fully generative and autonomous drug discovery systems [15].
16.1 Generative AI for Natural Product Drug Design
Generative models enable the creation of entirely new chemical structures inspired by natural products.
Key Architectures:
- Variational Autoencoders (VAE)
- Generative Adversarial Networks (GANs)
- Transformer-based molecular generators

Applications:
- De novo phytochemical design
- Optimization of natural scaffolds
- Bioactivity-directed molecule generation

AI can generate analogs of plant-derived compounds with:
- Improved solubility
- Reduced toxicity
- Enhanced receptor binding

This represents a shift from **discovery → design → optimization [16]**.
16.2 Transformer Models in Pharmacognosy
Transformer-based architectures (originally developed for NLP) are now widely used in chemistry.
Applications:
- SMILES-based molecule generation
- Protein–ligand interaction prediction
- Literature mining of ethnopharmacology

These models capture long-range dependencies in molecular structures more effectively than classical ML.
16.3 Graph Neural Networks (GNNs)
Natural products are inherently graph-structured molecules [17].
GNN Advantages:
- Captures atomic connectivity
- Models bond interactions
- Predicts bioactivity with high accuracy

Applications:
- Target prediction
- ADMET profiling
- Toxicity assessment

16.4 Federated Learning in Pharmacognosy
Federated learning allows AI training without sharing raw data.
Benefits:
- Data privacy preservation
- Multi-institution collaboration
- Secure pharmacological model development

This is particularly useful for proprietary herbal drug datasets.
17. AI IN PRECISION AND PERSONALIZED NATURAL PRODUCT MEDICINE [18].
AI enables transition from generalized herbal therapy to precision phytomedicine.

17.1 Patient-Specific Herb Response Prediction

AI models integrate:

- Genomic variability
- Metabolic profiles
- Drug–herb interaction networks

to predict patient-specific responses.

17.2 Herb–Drug Interaction Prediction

Machine learning systems identify:

- Cytochrome P450 interactions
- Transporter inhibition
- Synergistic or antagonistic effects

This improves safety of herbal formulations.

18. CHALLENGES IN AI-ASSISTED PHARMACOGNOSY (EXPANDED ANALYSIS)

Despite rapid advancements, several structural challenges remain.

18.1 Data Quality and Standardization Issues

Natural product data suffers from:

- Inconsistent nomenclature
- Missing structural annotations
- Poor experimental reproducibility

This directly affects AI model performance.

18.2 Limited Annotated Datasets

Deep learning requires large labeled datasets, but:

- Many phytochemicals lack biological activity data
- Ethnobotanical records are unstructured [19].

This creates a data bottleneck.

18.3 Black-Box Nature of AI Models

Many deep learning models lack interpretability.

Consequences:

- Difficult scientific validation
- Limited regulatory acceptance
- Reduced clinical trust

18.4 Computational and Infrastructure Limitations

High-performance AI models require:

- GPU clusters
- Large memory systems
- Cloud-based computing pipelines

These are not always accessible in developing research environments.

18.5 Regulatory Challenges

AI-generated drug leads face uncertainties in:

- Intellectual property ownership
- Regulatory approval pathways
- Validation standards

Global agencies are still developing AI-specific frameworks [20].

Table 04: Key Challenges and Emerging Solutions

Challenge	Impact	Proposed Solution
Data inconsistency	Reduced model accuracy	Standardized databases
Small datasets	Overfitting risk	Data augmentation
Black-box AI	Low interpretability	Explainable AI (XAI)
Validation gap	Clinical uncertainty	Hybrid experimental workflows
Regulatory uncertainty	Approval delays	AI regulatory guidelines

19. FUTURE PERSPECTIVES OF AI-ASSISTED PHARMACOGNOSY

The future of pharmacognosy will be deeply integrated with autonomous AI systems.

19.1 Autonomous Drug Discovery Pipelines
Future systems will perform:
- Data mining
- Hypothesis generation
- Compound design
- Virtual screening
- Optimization with minimal human intervention [21].

19.2 Digital Twins of Medicinal Plants
Digital twin technology will simulate:
- Plant metabolism
- Secondary metabolite production
- Environmental response

This will revolutionize plant-based drug production.

19.3 Integration of Multi-Omics AI
Future AI systems will integrate:
- Genomics
- Proteomics
- Metabolomics
- Transcriptomics

to create holistic biological models.

19.4 Blockchain-Enabled Pharmacognosy Databases
Blockchain can ensure:
- Data integrity
- Traceability of plant sources
- Secure sharing of pharmacological data

19.5 AI-Guided Sustainable Drug Discovery
AI will help identify:
- Endangered medicinal plant alternatives
- Synthetic substitutes of natural compounds
- Sustainable harvesting strategies [221].

20. ETHICAL CONSIDERATIONS
AI-assisted pharmacognosy raises ethical concerns:
- Biopiracy of traditional knowledge
- Ownership of AI-generated compounds
- Environmental impact of large-scale data systems
- Fair access to AI technologies

Ethical frameworks are required to ensure equitable benefit sharing.

21. CONCLUSION
AI-assisted pharmacognosy represents a revolutionary convergence of traditional natural product science and modern computational intelligence. By integrating machine learning, deep learning, generative models, and multi-omics data analytics, pharmacognosy is transitioning into a predictive and highly efficient discipline. AI significantly enhances every stage of natural product drug discovery, including compound identification, dereplication, bioactivity prediction, molecular optimization, and toxicity assessment. Furthermore, AI enables the integration of ethnopharmacological knowledge with modern pharmacological databases, uncovering hidden therapeutic potential in traditional medicine systems. However, challenges such as limited data availability, lack of interpretability, and regulatory uncertainty must be addressed before full-scale clinical translation can occur. The future of pharmacognosy lies in autonomous AI-driven discovery systems, digital twin modeling, and multi-omics integration frameworks. Overall, AI is not replacing pharmacognosy but redefining it into a data-driven, predictive, and precision-oriented scientific discipline capable of accelerating the discovery of next-generation therapeutics from natural sources.

22. FUNDING
Nil

23. ACKNOWLEDGEMENT

Not Declared.

24. CONFLICT OF INTEREST

Nil

25. INFORMED CONSENT

Not applicable

26. ETHICAL STATEMENT

Not Applicable.

27. REFERENCES

1. Newman DJ, Cragg GM. Natural products as sources of new drugs over the nearly four decades from 01/1981 to 09/2019. Journal of natural products. 2020 Mar 12;83(3):770-803.
2. Vamathevan J, Clark D, Czodrowski P, Dunham I, Ferran E, Lee G, Li B, Madabhushi A, Shah P, Spitzer M, Zhao S. Applications of machine learning in drug discovery and development. Nature reviews Drug discovery. 2019 Jun;18(6):463-77.
3. Chen H, Engkvist O, Wang Y, Olivecrona M, Blaschke T. The rise of deep learning in drug discovery. Drug discovery today. 2018 Jun 1;23(6):1241-50.
4. Schneider G. Automating drug discovery. Nature reviews drug discovery. 2018 Feb;17(2):97-113.
5. Segler MH, Waller MP. Neural-symbolic machine learning for retrosynthesis and reaction prediction. Chemistry–A European Journal. 2017 May 2;23(25):5966-71.
6. Terfloth L, Spycher S, Gasteiger J. Drug discovery: An overview. Applied Chemoinformatics: Achievements and Future Opportunities. 2018 Jun 5:165-94.
7. Atanasov AG, Zotchev SB, Dirsch VM, Supuran CT. Natural products in drug discovery: advances and opportunities. Nature reviews Drug discovery. 2021 Mar;20(3):200-16.
8. Wolfender JL, Litaudon M, Touboul D, Queiroz EF. Innovative omics-based approaches for prioritisation and targeted isolation of natural products–new strategies for drug discovery. Natural product reports. 2019;36(6):855-68.
9. Wishart DS, Jewison T. Guo, a. Oler, E., Wang, F., n um,., Peters, H.,… Gautam.;2021.
10. Blanco-Gonzalez A, Cabezon A, Seco-Gonzalez A, Conde-Torres D, Antelo-Riveiro P, Pineiro A, Garcia-Fandino R. The role of AI in drug discovery: challenges, opportunities, and strategies. Pharmaceuticals. 2023 Jun 18;16(6):891.
11. Gilmer J, Schoenholz SS, Riley PF, Vinyals O, Dahl GE. Neural message passing for quantum chemistry. InInternational conference on machine learning 2017 Jul 17 (pp. 1263-1272). Pmlr.
12. Liu Z, Zhou J. Introduction to graph neural networks. Springer Nature; 2022 May 31.
13. Mater AC, Coote ML. Deep learning in chemistry. Journal of chemical information and modeling. 2019 Jun 13;59(6):2545-59.
14. Jiménez-Luna J, Grisoni F, Weskamp N, Schneider G. Artificial intelligence in drug discovery: recent advances and future perspectives. Expert opinion on drug discovery. 2021 Sep 2;16(9):949-59.
15. Li Y, Fan Z, Rao J, Chen Z, Chu Q, Zheng M, Li X. An overview of recent advances and challenges in predicting compound-protein interaction (CPI). Medical Review. 2023 Dec 15;3(6):465-86.
16. Lee M, Shin H, Park M, Kim A, Cha S, Lee H. Systems pharmacology approaches in herbal medicine research: a brief review. BMB reports. 2022 Sep 30;55(9):417..
17. Ren X, Yan CX, Zhai RX, Xu K, Li H, Fu XJ. Comprehensive survey of target prediction web servers for Traditional Chinese Medicine. Heliyon. 2023 Aug 1;9(8).
18. Wang X, Li J, Chen R, Li T, Chen M. Active ingredients from Chinese medicine for combination cancer therapy. International journal of biological sciences. 2023 Jul 9;19(11):3499.
19. Stokes JM, Yang K, Swanson K, Jin W, Cubillos-Ruiz A, Donghia NM, MacNair CR, French S, Carfrae LA, Bloom-Ackermann Z, Tran VM. A deep learning approach to antibiotic discovery. Cell. 2020 Feb 20;180(4):688-702.
20. Cho MH, Jin H, Ha J, Chu S, An S. An Integrated Systems Pharmacology Approach Combining Bioinformatics, Untargeted Metabolomics and Molecular Dynamics to Unveil the Anti-Aging Mechanisms of Tephroseris flammea. Biomolecules. 2025 Dec 15;15(12):1740.
21. Ahmad L, Fan M, Zemede J, Chen G, Hu GW. Medicinal Plants for Asthma in Pakistan: A Systematic Review of Traditional Use, Pharmacological Validation, and Therapeutic Prospects. Pharmacological Validation, and Therapeutic Prospects.
22. Coley CW. Defining and exploring chemical spaces. Trends in Chemistry. 2021 Feb 1;3(2):133-45.