

AI in Traditional and Herbal Medicine

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ABSTRACT

This review surveys the convergence of artificial intelligence (AI), machine learning (ML), natural language processing (NLP), and data science (DS) with traditional and herbal medicine on a global scale. We synthesize data landscapes, methodological advances, and translational pathways that enable rigorous, reproducible, and ethically responsible integration of AI-driven insights with traditional knowledge. Core topics include data sources spanning herbal constituent databases, ethnobotanical records, pharmacology and omics datasets, and analytical chemistry repositories; AI/ML/NLP/DS methodologies such as graph neural networks, multi-omics integration, QSAR, feature selection, NLP for literature-based knowledge discovery, computer vision for species identification and quality assessment, and spectroscopy-driven learning for quality control and adulteration detection; and application domains including diagnosis support, formula optimization, herb–drug interaction prediction, safety pharmacovigilance, and quality assurance. We emphasize interpretability, reproducibility, and data provenance, and we devote substantial attention to regulatory, ethical, and socio-economic dimensions, including benefit-sharing, traditional knowledge protection, and post-market surveillance of herbal products. Challenges such as data heterogeneity, standardization, and cross-cultural validation are analyzed, and a practical research roadmap is proposed to accelerate safe, evidence-based AI-enabled integration of traditional and herbal medicines into modern healthcare. The review identifies critical gaps and outlines concrete paths for future work, including standardized benchmarks, open datasets, and robust pipelines that can be adopted by researchers pursuing doctoral-level contributions.

Keywords- Artificial intelligence, machine learning, natural language processing, data science

I.INTRODUCTION

Traditional and herbal medicines have served as foundational health systems across civilizations, delivering a wealth of empirical knowledge about plant-based therapies, multi-component formulations, and holistic care. However, the modern evidence paradigm—characterized by standardized study designs, reproducibility requirements, pharmacovigilance, and regulatory scrutiny—presents both challenges and opportunities for these systems. Artificial intelligence (AI) and related data-science approaches offer unprecedented means to organize, analyze, and translate traditional knowledge into testable hypotheses, actionable insights, and clinically relevant recommendations. The objective of this review is to present a rigorous, global synthesis of AI-enabled research in traditional and herbal medicine, with particular emphasis on data landscapes, methodological breadth, translational pathways, and regulatory/ethical considerations that shape responsible innovation.

Over the past decade, AI methods have been employed to (i) map complex multi-target interactions among phytochemicals and disease pathways, (ii) infer mechanisms from multi-omics and pharmacokinetic data, (iii) extract and synthesize knowledge from historical and contemporary literature, (iv) identify and authenticate botanical materials through image analysis and spectroscopic data, and (v) monitor safety signals through pharmacovigilance data and real-world evidence. These approaches span global traditions, including traditional Chinese medicine (TCM), Ayurveda, Unani, and diverse indigenous systems from Africa, Latin America, and other regions. A unifying theme is the construction of integrative pipelines that link high-dimensional data (chemical, genomic, clinical, and textual) to interpretable models capable of guiding discovery, formulation optimization, quality control, and clinical translation, all while respecting the cultural and intellectual property dimensions of traditional knowledge.

Despite substantial methodological progress, several recurring challenges impede translational impact. Data fragmentation and heterogeneity—across identifiers for herbs and formulations, metabolite annotations, disease ontologies, and clinical endpoints—limit cross-study comparability. Standardization of data formats, provenance

tracking, and reproducible workflows remains inconsistent across domains. The interpretability and trustworthiness of AI models are critical, especially in contexts where patient safety and cultural considerations intersect. Regulatory frameworks governing quality control, pharmacovigilance, and claim substantiation for herbal products vary by region and are continually evolving. Finally, ethical considerations such as benefit-sharing, protection of traditional knowledge, and equitable access to AI-enabled healthcare must accompany technical advances.

This review is organized to reflect a global, cross-cultural perspective while maintaining an explicit emphasis on methodological rigor. We begin with a comprehensive overview of data landscapes and data quality considerations. We then present a taxonomy of AI/ML/NLP/DS methods relevant to traditional/herbal medicine, followed by sections on core application areas, network pharmacology, and case studies illustrating concrete AI-driven advances. A dedicated discussion on regulatory, ethical, and translational aspects accompanies an in-depth treatment of reproducibility and open science. We conclude with a forward-looking roadmap that identifies high-priority research questions, recommended benchmarks, and pathways to practical impact in clinical, regulatory, and public-health contexts.

II. DATA LANDSCAPE AND DATA QUALITY

2.1 Herbal Constituent Databases A set of curated resources provides structured information on herbs, constituents, and predicted interactions. Prominent examples include comprehensive herbal databases and cheminformatics repositories that catalog phytochemicals, their physicochemical properties, and reported biological activities. These resources underpin many AI-driven pipelines for feature extraction, target prediction, and network analyses. However, there is substantial heterogeneity in coverage, taxonomic resolution, and standardization of identifiers. To maximize cross-database interoperability, harmonization protocols should align herb IDs (scientific names, synonyms, vernacular names), constituent identifiers (IUPAC, PubChem, InChI), and activity annotations (assay types, endpoints, units). Data quality assurance—covering completeness, accuracy, and currency—remains essential as new constituents are discovered and reannotated.

2.2 Ethnobotanical Databases and Textual Resources Ethnobotanical databases capture traditional usage patterns, preparation methods, regional indications, and cultural context. NLP-enabled extraction from ethnobotanical literature and historical pharmacopoeias supports knowledge discovery and hypothesis generation. Challenges include inconsistent taxonomic mapping across eras, varying quality of primary sources, and potential biases in recorded use. Standardized vocabularies, ontologies for traditional concepts, and rigorous provenance metadata are needed to enable reliable AI-driven synthesis across texts and time.

2.3 Phytochemical/Pharmacology Data Publicly available pharmacology databases collate bioactivity data, including target proteins, signaling pathways, and phenotypic readouts. Integrating these data with herb–constituent information requires careful alignment of assay conditions, units, and target nomenclature. When data are sparse or noisy, ML models must incorporate uncertainty quantification and robust validation strategies. Cross-referencing with *in silico* predictions (e.g., docking scores or QSAR estimates) can augment limited experimental data but should be approached with transparent caveats.

2.4 Omics and Systems Biology Data Multi-omics datasets (transcriptomics, proteomics, metabolomics) illuminate mechanistic links between phytochemicals and biological systems. Network-based approaches can integrate omics layers with herb–target–disease networks to uncover indirect or synergistic mechanisms. However, experimental designs in traditional medicine contexts often lack standardized controls, and sample heterogeneity can confound integrative analyses. Harmonization of experimental metadata, sample provenance, and normalization pipelines is critical to enable reproducible cross-study synthesis.

2.5 Analytical Chemistry and Spectroscopy Datasets Quantitative and qualitative analysis of herbal constituents frequently relies on chromatographic and spectroscopic modalities (HPLC-DAD-MS, NMR, NIR, Raman). AI/ML models applied to these data support quality control, adulteration detection, and metabolite profiling. Open data sharing in spectroscopy and chromatographic datasets offers opportunities for benchmarking and method transfer, but data access is sometimes restricted by commercial incentives or inconsistent data formats. Standardized preprocessing (baseline correction, alignment, normalization) and robust validation against reference standards are essential for reliable AI-driven quality assessments.

2.6 Clinical, Real-World, and Pharmacovigilance Data Real-world data (RWD) from electronic health records, pharmacovigilance databases, and observational studies provide evidence on safety, herb–drug interactions, and clinical outcomes. Integrating RWD with mechanistic AI models enables translational insights but poses privacy, bias, and confounding risks. Phenotype harmonization, standardized adverse event coding, and careful causal inference methods are needed to derive trustworthy signals from noisy, heterogeneous data.

2.7 Data Standardization, Interoperability, and Provenance Adherence to FAIR principles (Findable, Accessible, Interoperable, Reusable) and robust provenance tracking are foundational for reproducibility. Adoption of shared ontologies, such as disease and pathway ontologies, herb taxonomies, and standardized chemical identifiers, supports cross-study integration. Interoperability requires consistent metadata schemas and versioned data, enabling researchers to reproduce analyses and compare results across studies and traditions.

2.8 Data Accessibility and Curation Practices Open-access datasets and community-curated resources accelerate reproducibility and method benchmarking. Controlled-access resources balance data utility with privacy and intellectual property concerns, particularly for traditional knowledge. Transparent curation practices, including documentation of inclusion criteria, data cleaning steps, and confidence levels for annotations, are essential for trustworthy AI-driven conclusions.

III. AI/ML/NLP/DS METHODOLOGIES

3.1 Data Preprocessing and Feature Extraction for Herbal Data Effective AI analysis begins with appropriate preprocessing of heterogeneous data. Techniques include standardization of chemical identifiers, taxonomic reconciliation of herbs, normalization of activity measures, and alignment of clinical endpoints. Feature extraction for phytochemicals may involve molecular fingerprints, physicochemical descriptors, and predicted ADME properties. For textual resources, NLP pipelines must address multilingual corpora, archaic terminology, and nonstandard spellings, employing named entity recognition (NER), relation extraction, and concept normalization to construct structured knowledge graphs.

3.2 Network Pharmacology and Multi-Target Modeling Network pharmacology offers a paradigm for understanding multi-component, multi-target interactions characteristic of traditional formulations. Constructing herb–phytochemical–target–disease networks enables discovery of potential mechanisms and synergy patterns. Graph-based models (including graph neural networks, GNNs) facilitate learning over such networks, supporting tasks such as link prediction, node classification (e.g., target prioritization), and pathway-level inference. A rigorous evaluation framework requires careful consideration of sampling bias, network sparsity, and biological plausibility.

3.3 QSAR and Quantitative Pharmacology for Phytochemicals Quantitative structure–activity relationships (QSAR) and related pharmacology models enable prediction of bioactivity for phytochemicals with limited experimental data. Descriptor selection, model interpretability, and robust cross-validation are essential. When extending QSAR to natural products, challenges include chemical diversity, complexity of multi-target interactions, and potential activity modulation in multi-component mixtures. Hybrid models that integrate QSAR with network-based priors can improve predictive performance and interpretability.

3.4 Multi-Omics Integration and Systems Pharmacology Integrating genomics, proteomics, metabolomics, and pharmacokinetics with herb-derived data facilitates systems-level insights into mechanism, synergy, and safety. Multi-omics fusion strategies range from early integration (concatenating feature vectors) to late integration (ensemble models) and intermediate architectures (multi-view learning). Causal inference and perturbation analysis can help disentangle direct phytochemical effects from network-level secondary responses, offering a more robust foundation for translational hypotheses.

3.5 Graph Neural Networks and Knowledge Graphs Knowledge graphs capture entities (herbs, constituents, targets, diseases) and their relationships, enabling scalable reasoning over complex biomedical knowledge. Graph neural networks (GNNs) propagate information across nodes to predict interactions, infer missing links, and uncover hidden associations. For herbal medicine, KG-based approaches support hypothesis generation for new formulations, adverse-event prediction, and literature-based evidence synthesis. Challenges include constructing high-quality graphs with accurate provenance, handling missing data, and maintaining interpretability.

3.6 NLP and Literature Mining for Traditional Knowledge NLP-driven literature mining unlocks insights from centuries of pharmacopoeias, modern clinical trials, and ethnobotanical reports. Core tasks include multilingual NER for herbs and phytochemicals, relation extraction for herb–drug–disease associations, sentiment and outcome extraction from clinical narratives, and summarization of mechanistic hypotheses. Ontology-driven approaches improve cross-lingual transfer and ensure semantic consistency. Reproducibility hinges on transparent data sources, annotation schemas, and evaluation benchmarks.

3.7 Computer Vision for Botanical Identification and Quality Assessment Computer vision (CV) models classify plant species, detect morphological features, and assess quality attributes from images of plant material and products. CV methods support authentication, adulteration detection, and standardization of raw materials before downstream analyses. Important considerations include dataset diversity (species variants, growth stages, processing methods), robust evaluation under real-world imaging conditions, and annotation reliability to ensure model accuracy.

3.8 Spectroscopy-Based ML for Quality Control and Adulteration Detection Spectroscopic modalities (NIR, MIR, Raman, UV-Vis) coupled with ML enable rapid, non-destructive quality control and adulteration screening. Calibration models, spectral preprocessing, and chemometrics techniques underpin robust performance. Transferability of models across instruments and batches remains a key challenge; domain adaptation strategies and external validation are critical for practical deployment.

3.9 Model Interpretability, Explainability, and Trust Trustworthy AI in traditional medicine requires interpretability aligned with domain knowledge. Approaches include post-hoc explanation methods (SHAP, LIME), inherently interpretable models (sparse regression, attention-based networks with meaningful explanations), and visualization of networks and pathways. Clear communication of confidence, uncertainty, and limitations is essential for acceptance by clinicians, regulators, and traditional knowledge holders.

3.10 Reproducibility, Benchmarking, and Toolchains Reproducible research depends on transparent data provenance, versioned code, and shared benchmarks. Standardized evaluation protocols and publicly available datasets enable meaningful cross-study comparisons. Toolchains should cover data preprocessing, model training, evaluation, and reproduction of results. Open science practices, including preregistration of analysis plans and sharing of computational notebooks, enhance credibility and accelerate progress.

IV. APPLICATIONS IN TRADITIONAL AND HERBAL MEDICINE

4.1 Diagnosis Support and Decision-Making Aids AI-enabled diagnostic aids utilize clinical data, symptom patterns, and literature-derived associations to support decision-making in contexts where traditional formulations are employed. Multimodal models integrating clinical measurements, patient-reported outcomes, and herbal regimen data can aid differential diagnosis, treatment selection, and monitoring of therapeutic responses. Careful validation in diverse populations, attention to cultural context, and alignment with traditional diagnostic frameworks are essential.

4.2 Formula Optimization and Synergy Modeling Formulation optimization seeks to balance efficacy, safety, and manufacturability in multi-component herbal prescriptions. AI approaches incorporate network pharmacology insights, omics-derived mechanism hypotheses, and empirical dose–response data to predict synergistic interactions and potential antagonism. Optimization under constraints (safety margins, regulatory limits, quality-control considerations) can guide the refinement of traditional formulas or the design of novel multi-component combinations.

4.3 Herb–Drug Interactions and Pharmacovigilance Herbal–drug interactions (HDIs) pose safety concerns, particularly when herbal products accompany conventional medications. AI-driven HDI prediction models leverage target overlap, pathway crosstalk, and pharmacokinetic considerations to flag potential interactions. Post-market surveillance models integrating spontaneous adverse event reports, social media signals, and pharmacovigilance databases can uncover safety signals associated with herbal products, informing regulatory actions and clinician guidance.

4.4 Quality Control, Adulteration Detection, and Authentication Quality assurance encompasses botanical authentication, adulteration detection, and constituent quantification. AI-enabled spectroscopy, CV, and ML pipelines offer rapid screening and batch-level inspection of raw materials and finished products. Robust datasets, instrument

standardization, and cross-laboratory validation are necessary to ensure consistent performance and regulatory acceptance.

4.5 Safety Assessment and Toxicology Predictions Predictive models for toxicity risk, hepatotoxicity, and organ-specific adverse effects can complement traditional safety assessments. Integrating toxicology data with phytochemical properties and network-based mechanistic insights enhances the ability to flag risky constituents and refine safety profiles. Transparent reporting of model uncertainties and validation against independent datasets strengthens the reliability of such predictions.

4.6 Translation into Clinical Practice and Evidence Generation Translational pathways require rigorous clinical evaluation, standardized reporting of outcomes, and alignment with regulatory expectations. AI-facilitated evidence generation—from pilot studies to pragmatic trials—can help move traditional/herbal therapies toward evidence-informed adoption. Stakeholder engagement, harmonized outcome measures, and robust data governance are key enablers of credible translation.

V. NETWORK PHARMACOLOGY AND CASE STUDIES

5.1 Case Study A: Ayurvedic Formulations for Metabolic Syndrome A network pharmacology approach can model multi-component Ayurvedic formulations against targets implicated in metabolic syndrome (e.g., insulin signaling, lipid metabolism, inflammatory pathways). By constructing herb–constituent–target–disease networks and applying graph-based inference, researchers can identify combinations predicted to modulate key pathways with favorable safety profiles. Validation across *in vitro* assays and limited clinical data provides iterative refinement with a focus on safety.

5.2 Case Study B: TCM Network Pharmacology for Cancer-Related Pathways Traditional Chinese medicine (TCM) formulations often claim multi-target mechanisms relevant to cancer biology. GNN-driven analyses of herb–target associations and disease networks can propose plausible mechanisms and prioritize constituents for experimental validation. Emphasis on interpretability (e.g., mapping network motifs to known signaling cascades) enhances plausibility and guides experimental follow-up.

5.3 Case Study C: NLP-Driven Extraction of Herb Safety Signals NLP pipelines can synthesize evidence from pharmacopoeias, case reports, and post-market literature to surface safety signals and potential HDIs. Through relation extraction and temporal trend analysis, such approaches help regulators and clinicians monitor evolving safety profiles and identify topics warranting deeper study.

VI. TRANSLATIONAL PATHWAYS, REGULATORY, AND ETHICAL CONSIDERATIONS

6.1 International Regulatory Frameworks and Quality Standards Herbal products traverse different regulatory landscapes, including those for dietary supplements, traditional medicines, and phytopharmaceuticals. A robust AI-enabled translational workflow must incorporate regulatory expectations for quality control, validation, and post-market surveillance. Harmonization efforts—where feasible—facilitate cross-border collaboration while preserving local regulatory sovereignty and traditional practice.

6.2 Quality Control Standards for Herbal Products Quality standards address identity, purity, potency, and safety. AI-assisted methods contribute to rapid, non-destructive screening, whereas standardization of reference materials, solvent systems, and instrument calibration enhances comparability. Documentation of batch-specific data, provenance, and analytical conditions is essential for regulatory review.

6.3 Pharmacovigilance in Herbal Medicine Systematic safety monitoring complements preclinical and clinical testing. AI-enabled pharmacovigilance can enhance signal detection, trend analysis, and causal inference for HDIs and product adulteration. Transparent reporting of limitations and uncertainties is critical to ensure that safety signals are interpreted appropriately in clinical and regulatory contexts.

6.4 Intellectual Property, Benefit-Sharing, and Traditional Knowledge Respect for traditional knowledge and equitable benefit-sharing are essential when translating AI-derived insights into commercial products or clinical

practice. Clear governance structures, community engagement, and compliance with international frameworks (e.g., the Nagoya Protocol) help balance innovation incentives with respect for source communities and cultural heritage.

6.5 Ethical Guidelines for AI-Assisted Traditional Medicine Research Ethical considerations include informed consent for data use, privacy protections, avoidance of exploitation, and transparent disclosure of AI limitations. Researchers should articulate the boundaries of AI in decision-making, ensure clinician and patient oversight, and actively address potential biases introduced by data gaps or cultural contexts.

6.6 Risk–Benefit Considerations in AI-Enabled Translational Pathways A deliberate risk assessment framework should weigh potential benefits (improved safety, more rapid discovery, better standardization) against risks (misinterpretation, overreliance on black-box models, data privacy concerns). Iterative, human-in-the-loop designs and predefined thresholds for clinical applicability help mitigate risk while advancing innovation.

VII. REPRODUCIBILITY, OPEN SCIENCE, AND DATA SHARING

7.1 Protocols, Data Licensing, and Versioning Transparent reporting of data sources, preprocessing steps, model architectures, hyperparameters, and evaluation procedures is essential. Versioned datasets and code repositories enable reproducibility, while clear licensing clarifies data usage rights and distribution constraints.

7.2 Benchmark Datasets and Evaluation Metrics Community-accepted benchmarks and standardized metrics (e.g., AUROC, precision-recall, F1 for classification tasks; MAE/MSE for regression; network-based metrics for link prediction; interpretability scores for explainable AI) support fair comparisons across studies. Publicly available benchmarks, with baseline models and train/test splits, accelerate methodological progress.

7.3 Reproducibility Challenges in Herbal AI Key obstacles include sparse data for rare herbs, inconsistencies in taxonomic naming, and variability across laboratories and instruments. Meta-analytic approaches and cross-lab replication studies, alongside robust uncertainty quantification, can help address these issues.

VIII. GAPS, LIMITATIONS, AND FUTURE DIRECTIONS

8.1 Methodological Gaps While AI methods show promise, gaps remain in causal inference for multi-component systems, scalability of network models to very large herb–disease networks, and robust evaluation of interpretability in biological terms. Hybrid modeling that combines data-driven learning with mechanistic reasoning remains a priority.

8.2 Data Gaps and Standardization Expected data gaps include limited high-quality clinical trial data for many traditional formulas, inconsistent ontologies, and incomplete pharmacovigilance data for certain regions. Investments in data curation, standardization, and sharing infrastructure are essential.

8.3 Translational Gaps Bridging bench to bedside—particularly for complex polyherbal formulations—requires rigorous clinical validation, standardized outcome measures, and regulatory alignment. Collaborative networks spanning researchers, clinicians, traditional practitioners, regulators, and patient communities are crucial.

8.4 Roadmap for Integration A pragmatic roadmap includes: (i) developing shared, openly accessible benchmarks and datasets; (ii) building interoperable AI pipelines with clear provenance; (iii) fostering cross-cultural collaborations to respect traditional knowledge; (iv) implementing regulatory-informed evaluation frameworks; (v) prioritizing reproducibility and transparency in published work; and (vi) designing training and education programs to cultivate a new generation of researchers capable of integrating AI with traditional medicine in a responsible manner.

IX. CONCLUSIONS

Artificial intelligence (AI), machine learning (ML), natural language processing (NLP), and data science (DS) are reshaping how traditional and herbal medicines are understood, evaluated, and translated into contemporary healthcare. This global, cross-cultural review demonstrates that AI-enabled approaches can illuminate the complex, multi-component nature of herbal formulations, reveal mechanistic pathways through multi-omics and network pharmacology, and enhance practical aspects such as quality control and safety monitoring. The overarching message

is not that AI replaces traditional knowledge or empirical validation, but that it provides rigorous, transparent, and scalable tools to augment evidence-based practice while respecting cultural contexts and intellectual property.

Key takeaways from this synthesis include:

- Data landscape and interoperability are foundational. The power of AI rests on high-quality, well-annotated, and interoperable data. Harmonized identifiers for herbs and constituents, standardized ontologies, and FAIR data practices are essential to enable meaningful cross-dataset analyses and reproducible results across traditions.
- Methodological breadth is advantageous. The most impactful work integrates diverse AI/ML/NLP/DS techniques—graph neural networks and knowledge graphs for multi-target and network pharmacology analyses, multi-omics data fusion for mechanism discovery, NLP for literature-based knowledge synthesis, and spectroscopy/computer vision for quality control and authentication. Interpretable models and robust uncertainty quantification are critical to foster trust among clinicians, regulators, and traditional practitioners.
- Translational and regulatory realities shape research trajectories. Quality control, pharmacovigilance, and clear pathways to regulatory acceptance must be embedded early in AI-driven studies. Ethics, benefit-sharing, and protection of traditional knowledge are equally integral to responsible innovation and long-term societal impact.
- Collaborative, cross-cultural ecosystems accelerate progress. Effective translation requires multi-stakeholder partnerships among researchers, traditional practitioners, clinicians, regulators, industry, and patient communities. Transparent data governance, shared benchmarks, and open science practices will enhance reproducibility and accelerate safe adoption.
- Practical roadmaps emerge from synthesis. A staged approach is advised: (i) invest in data standardization and provenance; (ii) develop interoperable AI pipelines with rigorous validation; (iii) establish global benchmarks and open datasets; (iv) emphasize regulatory-aware evaluation and reporting; (v) cultivate training programs that equip researchers with both AI literacy and traditional-medicine expertise; and (vi) foster ethical frameworks that protect communities and ensure equitable access to innovations.

Looking forward, the most impactful research will bridge gaps between discovery and clinical translation in ways that are culturally sensitive and regulatorily credible. Priority areas include causal inference in multi-component systems, scalable evaluation of network-based hypotheses, robust cross-instrument and cross-lab transferability for spectroscopy- and CV-based QA/QC, and the development of consensus reporting standards tailored to AI-assisted traditional medicine research. A practical, globally inclusive research roadmap—grounded in transparent methodologies, open data, reproducible workflows, and ethical governance—will maximize the potential of AI to deliver safe, effective, and evidence-based benefits from traditional and herbal medicines.

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