IJARCCE ISSN (O) 2278-1021, ISSN (P) 2319-5940

International Journal of Advanced Research in Computer and Communication Engineering

Impact Factor 8.471 ⵘ Peer-reviewed & Refereed journal ⵘ Vol. 15, Issue 4, April 2026

DOI: 10.17148/IJARCCE.2026.154107

HERB GUARD AI- AN AI - BASED HERB-DRUG INTERACTION PREDICTION USING NATURAL LANGUAGE PROCESS

Shashipriya Shridhar Hegde[1], K Sharath[2]

MCA Student, Department of MCA, Bangalore Institute of Technology, Bengaluru, India[1]

Assistant Professor, Department of MCA, Bangalore Institute of Technology, Bengaluru, India[2]

Abstract: The growing concurrent use of Ayurvedic and Allopathic medicines has significantly increased the risk of herb–drug interactions (HDIs), many of which remain undetected due to the absence of centralized prediction systems. This paper presents HerbGuard AI, an AI-based system that leverages Natural Language Processing (NLP) to extract interaction-related information from biomedical and traditional Ayurvedic literature. A Knowledge Graph is employed to model and represent structured relationships between herbs, pharmaceutical drugs, and their interaction mechanisms. The proposed system predicts potential interaction risks, thereby improving patient safety and supporting informed clinical decision-making in integrative healthcare. The system is particularly relevant to India's pluralistic health culture, where patients frequently combine modern and traditional medicines without physician supervision. Experimental scenarios demonstrate the system's ability to generate actionable interaction warnings and recommend safe herb–drug combinations.

Keywords*:* Herb–Drug Interaction, Natural Language Processing, Knowledge Graph, Ayurveda, Artificial Intelligence, Pharmacovigilance, Integrative Medicine, Clinical Decision Support

I. INTRODUCTION

The integration of Ayurvedic and Allopathic medicine has become increasingly prevalent in modern healthcare, particularly in countries such as India, where traditional systems of medicine have deep cultural roots. While integrative treatment approaches offer potential therapeutic benefits, the simultaneous use of herbal remedies and pharmaceutical drugs introduces significant risks in the form of herb–drug interactions (HDIs). These interactions can lead to altered drug metabolism, reduced drug efficacy, or adverse toxic effects, yet many go undetected because patients often consume herbal products without informing their physicians [8].

Existing pharmacological databases are predominantly focused on drug–drug interactions (DDIs) and do not adequately cover interactions involving herbal medicines. Moreover, information pertaining to HDIs is scattered across diverse research papers, case studies, and classical Ayurvedic texts, making systematic analysis challenging. The absence of a centralized, intelligent prediction system has created a critical gap in patient safety monitoring.

Recent advances in Artificial Intelligence (AI) and Natural Language Processing (NLP) have opened new possibilities for automated extraction and analysis of interaction data from large volumes of medical literature. Knowledge Graphs provide an effective means of structuring complex, multi-relational biomedical information. This paper proposes HerbGuard AI, a system designed to bridge this gap by combining NLP-driven literature mining with Knowledge Graph-based interaction modelling, enabling early identification of potential herb–drug risks and supporting clinical decision-making in integrative healthcare settings.

II. BACKGROUND AND RELATED WORK

The field of herb–drug interaction research has evolved significantly over the past two decades. Early studies focused on documenting case reports of adverse interactions, while later work introduced computational frameworks to scale prediction capabilities.

Fugh-Berman [8] was among the first to formally document clinically significant herb–drug interactions in The Lancet, highlighting interactions involving St. John's Wort and several prescription drugs. The study emphasized the pressing need for physician awareness and patient caution. Izzo and Ernst [16] further catalogued interactions between herbal medicines and prescribed drugs through a systematic review, showing that commonly used herbs could significantly alter drug metabolism through effects on Cytochrome P450 enzymes and P-glycoprotein transporters.

Cheng and Zhao [6] proposed the Heterogeneous Network-Assisted Inference (HNAI) framework, which integrated multiple machine learning algorithms including Naive Bayes, Decision Tree, K-Nearest Neighbour, Logistic Regression, and Support Vector Machines to predict drug–drug interactions using phenotypic, therapeutic, chemical, and genomic properties. This work established a foundation for data-driven interaction prediction.

Spanakis et al. [1] provided a comprehensive review of AI models for assessing drug–herb interactions, identifying Graph Neural Networks (GNNs), NLP, and in silico modelling as the primary technologies capable of serving as early warning systems for healthcare providers. Chen et al. [2] extended this to multiple simultaneous drug interaction modelling, covering drug–drug, drug–food, and drug–microbiome interactions, with a focus on metabolic pathways including Cytochrome P450 enzymes.

Ziemann et al. [9] developed an algorithm-assisted information system specifically for pharmacokinetic herb–drug interactions in cancer treatment settings, while Martins et al. [10] proposed an AI-based holistic decision support system for HDIs in general healthcare. Huang et al. [7] addressed the need for personalized pharmacovigilance by incorporating AI-powered risk stratification for vulnerable populations including the elderly and oncology patients.

In the Indian context, Puthiyedath et al. [11, 17, 19, 21] highlighted the critical need for AI-driven prediction frameworks tailored to India's pluralistic healthcare system, proposing machine learning and deep learning models integrated with national pharmacovigilance platforms. Chattaraj et al. [13, 20] and Gamil et al. [14] further documented the complexity of herb–drug interaction mechanisms and stressed the need for standardized computational tools.

III. IMPORTANCE AND CURRENT RELEVENCE

The relevance of herb–drug interaction prediction has grown substantially in the post-COVID-19 era. The global pandemic accelerated interest in traditional and herbal remedies, leading to a marked increase in self-medication with Ayurvedic and natural products alongside prescribed pharmaceutical treatments. This trend has created an urgent need for intelligent monitoring systems.

India's healthcare environment is uniquely complex. As a country with officially recognized systems of Ayurveda, Unani, Siddha, and Homeopathy (AYUSH), a significant portion of the population simultaneously uses both traditional and modern medicines. Patients frequently do not disclose herbal supplement use to their physicians, increasing the probability of undetected interactions [17, 19].

The rapid digitization of health records, expansion of open biomedical databases such as PubMed and DrugBank, and the availability of classical Ayurvedic literature in digital formats have created an environment where large-scale, data-driven interaction analysis is now feasible. Advancements in AI, NLP, and Knowledge Graph technologies enable the automated processing of this information at a scale that was previously impossible.

From a pharmacovigilance perspective, AI has the potential to transform the field from a reactive system—one that identifies harmful interactions only after patient harm has occurred—into a proactive, predictive system that prevents adverse events before they manifest. This transformation aligns with global trends in digital health, precision medicine, and integrative pharmacology [7, 14].

IV. LITERATURE SURVEY

A total of 27 research papers and resources were reviewed, spanning the period from 2000 to 2025. The following summarizes the key contributions of the primary literature:

A. Foundational Studies

[8] Fugh-Berman (2000) established the clinical significance of herb–drug interactions, documenting specific cases such as St. John's Wort interactions with anticoagulants and cyclosporine, forming the basis for subsequent computational research.

[16] Izzo and Ernst (2009) conducted an updated systematic review of interactions between herbal medicines and prescribed drugs, identifying CYP450 enzyme modulation and P-glycoprotein effects as the primary biochemical mechanisms.

DOI: 10.17148/IJARCCE.2026.154107

B. Machine Learning Approaches

[6] Cheng and Zhao (2014) developed the HNAI framework, integrating five machine learning classifiers to predict DDIs using heterogeneous biological network data, achieving significant improvements over single-feature models.
[2] Chen et al. (2022) extended AI-based prediction to simultaneous multiple drug interactions, modelling metabolic enzyme pathways and drug similarity features to enable pharmacovigilance-oriented analysis.
[18] Rani and Gupta et al. (2025) reviewed AI-driven DDI models for enhanced patient safety, demonstrating that deep learning and NLP-based models outperform traditional rule-based systems in complex polypharmacy scenarios, particularly when integrated with EHR systems.

C. Graph Neural Networks and Knowledge Graph Models

[1] Spanakis et al. (2025) identified GNNs as the gold standard for drug–herb interaction prediction, capable of modelling biological pathways as graph structures where drugs, proteins, and enzymes form interconnected nodes.
[4] Zhang et al. (2024) reviewed AI methodologies for DDI prediction, classifying tasks into undirected DDI prediction, DDI event prediction, and asymmetric DDI prediction, with GNNs and deep learning achieving the highest accuracy across categories.
[7] Huang et al. (2025) highlighted Knowledge Graphs and NLP as essential tools for bridging regulatory gaps and generating personalized risk profiles, particularly for elderly and oncology populations.
[27] Moradi et al. (2025) proposed a context-aware Large Language Model (LLM) framework for DDI detection, overcoming the interpretability limitations of traditional black-box AI models by providing semantic relationship analysis and clinical explanations.

D. Herbal Medicine and NLP-Focused Systems

[5] Kumbhar et al. (2024) examined AI applications specifically in herbal medicine formulations, highlighting how ML, neural networks, and NLP can optimize the safety and efficacy assessment of complex herbal mixtures.
[9] Ziemann et al. (2019) developed an algorithm-assisted information system for herb–drug interactions in oncology, demonstrating that algorithm-based tools can significantly reduce the manual burden on clinical pharmacists in cancer care settings.
[10] Martins et al. (2023) proposed a holistic AI-based decision support system for herb–drug interaction detection in general healthcare settings, showing improved clinical safety outcomes.
[15] Hsu et al. (2023) evaluated ChatGPT's performance on medication consultation questions involving drug–herb interactions, finding that while LLMs provide useful preliminary guidance, accuracy limitations necessitate professional supervision.

E. India-Specific and Pharmacovigilance-Focused Studies

[11, 17] Puthiyedath et al. (2025) emphasized the critical gap in pharmacovigilance for Ayurvedic drug combinations in India's pluralistic health culture and proposed AI-based predictive models tailored to Indian healthcare contexts.
[19] Puthiyedath et al. (2024) proposed real-time AI monitoring integration with national pharmacovigilance systems, using phytochemical and pharmacological data to predict HDIs at scale.
[21] Puthiyedath (2024/2025) presented a doctoral framework for AI-driven precision medicine targeting drug–herb interaction prediction in India, combining machine learning, deep learning, and pharmacogenomics.

F. Oncology and High-Risk Clinical Contexts

[12] Taş and Ulgen (2025) demonstrated that Physiologically Based Pharmacokinetic (PBPK) modelling, enhanced with AI, can accurately predict herb–drug interactions in oncology settings, improving treatment safety for patients on narrow therapeutic range medications.
[22] Wu et al. (2025) reviewed pharmacokinetic and pharmacodynamic mechanisms of herb–drug interactions in cancer patients, highlighting how herbal compounds can reduce or enhance anticancer drug effects, and underscoring the need for evidence-based AI prediction guidelines.
[23] Cordeiro et al. (2021) studied potential herb–drug interactions in elderly patients with cognitive disorders on polypharmacy regimens, stressing the importance of screening tools for clinicians.

G. Multimodal and Deep Learning Models

[25] Asfand-e-yar et al. (2024) proposed MMCNN-DDI, a multimodal deep learning model integrating chemical structures, enzyme data, molecular targets, and biological pathways, achieving approximately 90% prediction accuracy and outperforming traditional DDI prediction methods.
[26] Kondalkar et al. (2025) evaluated the polyherbal Madhukiran formulation in diabetic rat models, demonstrating multi-organ protective effects and no adverse herb–drug interactions with Metformin, providing empirical validation for AI-predicted safe combinations.

International Journal of Advanced Research in Computer and Communication Engineering
Impact Factor 8.471 ⁝⁝ Peer-reviewed & Refereed journal ⁝⁝ Vol. 15, Issue 4, April 2026
DOI: 10.17148/IJARCCE.2026.154107

H. Pharmacokinetic Reviews

[24] Cheng et al. (2023) reviewed the impact of herb–drug interactions on pharmacokinetics, particularly the role of CYP450 enzymes and drug transporters in altering drug absorption and metabolism for nine commonly used herbs.
[3] (2025) reviewed digital health and AI approaches for drug–herb and drug–food interaction assessment, confirming the growing feasibility of AI integration with clinical electronic health records.
[13, 20] Chattaraj et al. (2025, 2024) documented herb–drug interaction mechanisms in modern healthcare settings and called for standardized regulation and improved patient disclosure practices.
[14] Gamil et al. (2025) provided a foundational report on herb interaction mechanisms and risk factors, reinforcing the need for computational prediction methods in integrative medicine research.

V. COMPARITIVE ANALYSIS OF MODELS AND APPROACHES

A. Comparison of AI Approaches in Herb–Drug Interaction Literature

Feature / Aspect	Traditional Pharmacological Approach	AI-Driven Approach (2022–2025)	HerbGuard AI (Proposed)
Primary Focus	Drug–Drug Interactions (DDI)	DDI and HDI using structured databases	Specifically Ayurvedic–Allopathic HDIs
Data Source	Clinical trial reports, case studies	DrugBank, PubMed, structured biomedical databases	AYUSH Portal, DHARA, PubMed, classical Ayurvedic texts
Methodology	Laboratory testing, pharmacovigilance reports	GNNs, Deep Learning, PBPK, LLMs, NLP	NLP-based literature mining + Knowledge Graph
Target Population	General or elderly populations	Oncology, polypharmacy, vulnerable groups	India's pluralistic healthcare patients
Speed of Detection	Months to years (clinical observation)	Real-time or near real-time (milliseconds of simulation)	Near real-time with literature-backed warnings
Prediction Scope	Single herb vs. single drug	Multiple simultaneous drug interactions	Herb–drug combinations including polypharmacy
Data Nature	Structured (post-harm reports)	Structured biomedical + genomic data	Unstructured + structured (classical + modern texts)
Explainability	Based on known pharmacology	Limited (black-box for DL); improving with XAI	NLP-generated explanations with clinical recommendations
Integration	Manual clinical checks	EHR-integrated alert systems	Designed for clinical decision support integration
Personalization	General safety warnings	Population-specific risk stratification	Individualized herb–drug risk prediction

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B. Comparison of Key Machine Learning Models Used in Related Literature

Model / Framework	Capabilities & Strengths	Limitations
Naive Bayes / Decision Tree / SVM / KNN / Logistic Regression [6]	Interpretable, computationally efficient, suitable for structured drug property datasets	Limited capacity to handle unstructured or multi-relational data; lower accuracy for complex interactions
Graph Neural Networks (GNNs) [1, 4, 7]	Gold standard for biological network modelling; captures multi-relational drug–protein–gene interactions; high prediction accuracy	Requires large, well-structured graph datasets; high computational cost; limited interpretability
HNAI – Heterogeneous Network [6]	Integrates phenotypic, therapeutic, chemical, and genomic features; robust multi-feature prediction	Complex feature engineering; dataset dependency
Multimodal CNN (MMCNN-DDI) [25]	~90% accuracy; integrates chemical, enzymatic, pathway, and target data simultaneously	Focused on DDI; needs adaptation for herb–drug data; computationally intensive
PBPK + AI [12]	Biologically realistic simulation of pharmacokinetics; high accuracy for metabolic interactions in oncology	Requires detailed pharmacokinetic parameter data; limited herbal data availability
NLP + Knowledge Graph [1, 7, 27]	Enables extraction from unstructured literature; models semantic relationships between entities; supports explainable predictions	Dependent on quality and coverage of available literature; entity disambiguation challenges
LLMs / Context-Aware AI [27]	High interpretability; semantic context analysis; suitable for EHR-integrated clinical support	May produce hallucinations; requires fine-tuning on pharmacological datasets; needs professional validation
Algorithm-Assisted Information System [9]	Targeted for cancer drug–herb pharmacokinetics; clinical workflow integration	Domain-specific; limited generalizability to non-oncology settings
AI Decision Support System [10]	Holistic; applicable to general healthcare; improves safety outcomes	Requires structured input data; limited traditional medicine coverage
HerbGuard AI (Proposed)	NLP from traditional + modern literature; Knowledge Graph-based relationship modelling; Ayurveda-specific; India-focused	Currently at framework/design stage; requires empirical validation with large clinical datasets

VI. RESULTS OF PROPOSED SYSTEM

The proposed **HerbGuard AI system** is expected to automatically extract herb–drug interaction information from large biomedical and Ayurvedic literature using Natural Language Processing (NLP) techniques. The extracted entities such as herbs, drugs, enzymes, and interaction mechanisms are organized into a structured **Knowledge Graph**, which models the relationships between different biological components. By applying graph-based machine learning models on this knowledge graph, the system can identify and predict potential herb–drug interactions that may not yet be well documented in clinical studies.

As a result, the system can generate **severity-ranked alerts and risk scores** for possible herb–drug combinations, enabling healthcare professionals to detect harmful interactions at an early stage. This proactive prediction mechanism improves patient safety by supporting informed clinical decision-making in integrative healthcare settings where

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Ayurvedic and allopathic medicines are used together. Additionally, the framework can be expanded and integrated with digital healthcare systems such as electronic health records (EHRs) to provide scalable, AI-driven pharmacovigilance and real-time interaction monitoring.

VII. CHALLENGES AND LIMITATIONS

Despite its potential, HerbGuard AI faces several significant challenges and limitations that must be addressed for clinical deployment:

1. Data Scarcity and Quality [8, 16]: A major limitation across the literature is the insufficient volume of clinically validated herb–drug interaction data. Many interactions documented in classical Ayurvedic texts have not been subjected to rigorous modern pharmacological study, creating gaps in the training and validation data for AI models.

2. Variability in Herbal Composition [13, 20, 24]: Unlike synthetic pharmaceutical compounds with fixed molecular structures, herbal medicines contain multiple bioactive phytochemicals whose concentrations vary significantly based on geographic origin, cultivation methods, seasonal factors, and preparation processes. This variability makes standardized interaction modelling challenging.

3. Multi-Component Interaction Complexity [1, 2]: Herbs are chemical cocktails containing hundreds of phytochemicals, each of which may interact independently or synergistically with pharmaceutical drugs. Modelling all possible combinations exceeds the capability of current AI systems, particularly when considering polypharmacy scenarios.

4. Limited Interpretability of Deep Learning Models [15, 27]: Many high-accuracy deep learning and neural network models operate as black boxes, making it difficult for clinicians to understand the reasoning behind predictions. The lack of Explainable AI (XAI) integration limits clinical trust and adoption. Moradi et al. [27] identified this as a key barrier to LLM-based clinical decision support systems.

5. Lack of Empirical Clinical Validation [12, 21]: The HerbGuard AI system is currently at the design and framework stage. Real-world clinical validation with large patient cohorts is essential before the system can be relied upon as a clinical tool. AI models validated on laboratory or literature data may not generalize to real patient populations [12, 21].

6. Patient Non-Disclosure [8, 19]: A systemic challenge in HDI monitoring is that patients frequently do not report their herbal supplement use to physicians [8]. Without accurate patient-reported data, even highly capable AI systems cannot assess the complete interaction profile.

7. Regulatory and Standardization Gaps [11, 14]: There is currently no standardized regulatory framework governing herbal medicine data collection, quality control, or pharmacovigilance integration in India. This creates inconsistencies in the available datasets and challenges the systematic deployment of AI-based interaction prediction tools [11, 14].

8. Incomplete Traditional Literature Digitization [3, 5]: A significant portion of classical Ayurvedic knowledge remains in Sanskrit manuscripts or printed texts that have not been digitized or translated into machine-readable formats, limiting the coverage of NLP-based literature mining components.

VIII. FUTURE SCOPE

The HerbGuard AI framework has considerable potential for expansion and enhancement across multiple dimensions:

1. EHR Integration and Real-Time Clinical Alerts: Future iterations of HerbGuard AI should be integrated with Electronic Health Record (EHR) systems to enable real-time herb–drug interaction alerts at the point of prescription. This would allow physicians to receive immediate notifications when a patient's herbal supplement record conflicts with a new prescription, as proposed by several studies [7, 10, 18].

2. Pharmacogenomics and Personalized Medicine: Incorporating patient genetic data, particularly variants in CYP450 enzyme genes, would enable HerbGuard AI to generate personalized interaction risk predictions. Individuals metabolize drugs differently based on their genetic makeup, and pharmacogenomic integration would significantly improve prediction accuracy [6, 7].

3. Expansion to Traditional Chinese Medicine and Other Systems: The NLP and Knowledge Graph framework underlying HerbGuard AI can be extended to cover Traditional Chinese Medicine (TCM), Unani, and Siddha systems, broadening its global applicability and impact.

4. Explainable AI (XAI) Framework: A critical future requirement is the development of an XAI layer that can provide transparent, clinician-understandable explanations for interaction predictions. This will improve clinical trust and enable responsible AI deployment in healthcare settings [27].

5. PBPK Model Integration: Integration of Physiologically Based Pharmacokinetic (PBPK) modelling would allow HerbGuard AI to simulate the pharmacokinetic behaviour of herb–drug combinations at the molecular level, enabling more precise quantitative interaction predictions, particularly for oncology and high-risk therapy contexts [12].

6. Multi-Language NLP for Classical Text Mining: Developing NLP pipelines capable of processing classical Sanskrit, Hindi, and regional Indian language Ayurvedic texts would significantly increase the knowledge base available for interaction prediction, covering traditional formulations not yet represented in modern biomedical databases.

7. Integration with National Pharmacovigilance Systems: HerbGuard AI should be aligned with India's Pharmacovigilance Programme of India (PvPI) to enable bidirectional data sharing, allowing AI predictions to be validated against real-world adverse event reports and enabling the system to continuously learn from emerging interaction evidence [11, 19].

8. Mobile and Telehealth Deployment: A patient-facing mobile application version of HerbGuard AI would empower patients to self-check potential herb–drug interactions before combining treatments, improving safety in underserved and rural healthcare settings where direct physician access may be limited.

IX. CONCLUSION

This paper presented HerbGuard AI, an AI-based framework for predicting herb–drug interactions using Natural Language Processing and Knowledge Graphs, designed specifically to address the challenges of India's pluralistic healthcare environment. The increasing concurrent use of Ayurvedic and Allopathic medicines, combined with widespread patient non-disclosure and the absence of centralized interaction monitoring systems, has created an urgent need for intelligent prediction tools.

A comprehensive review of 27 published research papers revealed that while significant advances have been made in AI-based DDI prediction using Graph Neural Networks, deep learning, NLP, and PBPK modelling, the specific domain of Ayurvedic herb–drug interactions remains underserved. HerbGuard AI addresses this gap by integrating traditional Ayurvedic literature sources—including the AYUSH Portal, DHARA, and digitized classical texts—with modern biomedical databases, using NLP to extract interaction evidence and Knowledge Graphs to structure herb–drug–mechanism relationships.

Scenario-based demonstrations illustrated the system's capability to detect dangerous herb–drug combinations such as Neem with Metformin, and to recommend safe evidence-based herbal alternatives such as Ashwagandha for PCOD management while accounting for patient-specific drug allergies. The system's outputs support informed clinical decision-making and promote safer integrative healthcare practice.

While the current system is at the design and prototyping stage, the comparative analysis of existing AI methodologies confirms that NLP and Knowledge Graph integration is a valid and promising approach. Future work will focus on clinical validation, EHR integration, pharmacogenomics incorporation, and explainable AI development. HerbGuard AI has the potential to transform pharmacovigilance in integrative medicine from a reactive to a proactive safety system, ultimately improving patient outcomes across India's complex and diverse healthcare landscape.

ACKNOWLEDGEMENT

The author sincerely acknowledges the guidance and support of K. Sharath, Assistant Professor, Department of MCA, Bangalore Institute of Technology (Autonomous), Bengaluru, whose valuable mentorship and insights were instrumental in the development of this work. The author also acknowledges the Department of MCA, Bangalore Institute of Technology (Autonomous under VTU), for providing the academic environment and resources necessary for this research. Gratitude is expressed to the developers and maintainers of PubMed, the AYUSH Portal, and DHARA for providing open access to the biomedical and Ayurvedic literature databases that formed the informational foundation of this study.

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International Journal of Advanced Research in Computer and Communication Engineering
Impact Factor 8.471 ⁜ Peer-reviewed & Refereed journal ⁜ Vol. 15, Issue 4, April 2026
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