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PharmaSense AI: An Advanced Pharmaceutical Intelligence System Using Knowledge Graphs and Multi-Agent NLP

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Abstract

Adverse drug events are one of the major factors that lower patient safety and lead to hospital admissions. Drug-drug interactions (DDIs) are considered a significant source of adverse drug events. Accessible and smart pharmaceutical information systems are required to solve these issues. PharmaSense AI is an automated platform that is designed to find drug interactions, provide replacements, fetch drug information, and help in regulatory queries phase. It uses a retrieval-augmented generation (RAG) engine that is powered by BioBERT embeddings and Gemini 2.5 Flash to allow domain-specific named entity recognition and answer generation. It operates with a hybrid database design that integrates vector-based Qdrant and graph-based Neo4j, which allows flexibility in representing drug interactions as reaction nodes. Additionally, a multi-agent natural language processing framework makes it easy to process all queries across all components. Evaluation with multiple metrics demonstrates that the PharmaSense AI system has strong performance on measures of intent classification, accuracy of information retrieval, and safety considerations. There are also plans for ongoing enhancements to drug recognition accuracy. By providing evidence-informed, contextualized support, PharmaSense AI capitalises on enhanced decision-making for healthcare, while ensuring regulatory compliance and patient safety through an integrated, explainable system architecture.

Keywords: Knowledge Graphs; Multi-agent NLP; Retrieval-Augmented Generation; Drug Interaction Detection; Hybrid Database

1. Introduction

The pharmaceutical industry is experiencing overwhelming difficulties in producing a high-quality means to present drug information in a timely manner to patients and healthcare practitioners, especially as instances of harmful drug interactions rise [10]. Over 1.3 million U.S. admissions occur in part related to drug-drug interactions, costing the healthcare system billions of dollars and compromising patient safety. [4]. Most of the confusion around drug interactions stems from a variety of information sources, variability in terms, and complexity of medical language that often confuses patients and stresses the healthcare delivery team [7].

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Commercialised information systems such as Medscape and Epocrates are primarily used by health professionals but depend on fixed databases like DrugBank that are wholly reliant on the use of the exact match input, have no ability to detect misspellings and cannot generate information based on a more natural language query. Commercialised systems are not only unintuitive, but also may not accurately represent quality information movement [7]. Transformers such as BioBERT have also improved upon extracting information, by bettering entity recognition and relations extraction, specific to the biomedical domain [5]. Graph neural networks and knowledge-graph pipelines provide a more interpretable and mechanistic view of the interactions between drugs. [3].

PharmaSense AI builds on these developments by integrating RAG, knowledge graphs, and a multi-agent NLP architecture to deliver a user-friendly platform that identifies and explains drug–drug interactions with causal reasoning powered by a reaction-node graph. PharmaSense AI, by blending semantic vectors, graph traversals, and specialized LLM agents like Gemini 2.5 Flash, equips clinicians with context-aware drug information and facilitates decision-making in clinical and regulatory environments.

2. Related Works

PharmaSense AI is built upon four interrelated research areas—biomedical NLP extraction, graph-based reasoning, knowledge-graph engineering, and retrieval-augmented generation (RAG)—which together inform its hybrid vector–graph, multi-agent design. Biomedical natural language processing (NLP) has evolved the drug-drug interaction (DDI) identification to the new level from complex biomedical texts. Zhang et al [1] have shown that the contextual embeddings coming from BioBERT and complemented with relation-aware BLSTM layers outperform the existing methods to the DDI mentions extraction, being very efficient in handling the variability as well as the missings that are frequently met in user queries. Lee et al [5] also confirmed the advantage of BioBERT by identifying a remarkable increase in the accuracy of biomedical entity recognition and relation tasks. The results achieved in the different challenging biomedical domain tasks are the strong reasons why PharmaSense decided to employ BioBERT for the extraction of drug and interaction entities.

While graph neural networks (GNNs) have recently been popular for DDI prediction, capturing topological patterns among drugs [2], PharmaSense instead emphasises interpretable reaction-node knowledge graphs. KGNN [3] by Lin et al. merges graph connectivity into message passing but suffers from a trade-off with interpretability. As opposed to this, PharmaSense utilizes the explicit graph traversals over reaction-node representations that are inspired by Rajendran et al.'s syntax–semantic KG construction pipeline [12] which discloses the causal DDI pathways. Besides this, Zhang et al. [8] introduced graph denoising methods that maintain the most important entities related to drug pairs, thus providing the basis for PharmaSense's concentration on the accurate and interpretable extraction of the subgraph.

Automated building and the ever-changing enrichment of knowledge graphs are essential to be able to expand infinitely. Over and above Rajendran's method [12, 15], Jyothi et al. [13] has come up with new metrics like "graph hotness" and coverage which provide information for PharmaSense KG continuous updating. CompoundDB4j type platforms are an example of Neo4j-based DrugBank and ChEMBL data [11] integration that is similar to the hybrid vector–graph database of PharmaSense which is formed by combining Qdrant embeddings and graph storage. Lee et al. [6] showed that LLM agents augmented with retrieval modules not only improve grounding accuracy but also generalize to complex domains like drug discovery, a concept that PharmaSense has taken further by using dual RAG pipelines to isolate clinical and regulatory text. Peri et al. [14] demonstrated a similar capability in a medical chatbot that recorded 84% grounding accuracy and is now being used by PharmaSense to facilitate user engagement.

To a great extent, clinical experiments point out the significant influence and the intricacy of the processes of DDI management in the everyday life. Jayamohanan et al. [9] reported the coexistence of DDIs in cancer patients treated with tyrosine kinase inhibitors (TKIs), mapping the most dangerous drug pairs and emphasizing the necessity of an explainable alert system. Ratan et al. [10] in a similar manner disclosed that over 70% of the cancer patients treated with TKI were found to have a great number of potential DDIs. They suggested that clinical workflows should be equipped with thorough and up-to-date query tools. These revelations of PharmaSense AI safety and compliance are further strengthened by the use of hybrid data sources and multi-agent NLP.

PharmaSense AI has merged these physiological and clinical advances with BioBERT-based DDIs extraction from clinical literature in an interpretable reaction-node graph reasoning rather than GNNs plus automatic KG construction

and dynamic knowledge enrichment. PharmaSense represented DDIs in a usable, explainable and scalable way to deliver drug intelligence that fits clinical decision support in real life in regulation.

3. System Architecture

PharmaSense AI is created as a modular and scalable system combining advanced natural language processing (NLP) with a hybrid knowledge representation framework to provide accurate and explainable pharmaceutical and regulatory information. There are two Retrieval-Augmented Generation (RAG) subsystems at the core of this system. The pharmaceutical RAG focuses on questions related to interactions between medications, alternative medications, and general drug-related questions; whereas, the regulatory RAG addresses questions related to compliance using legal documents, such as the Drugs and Cosmetics Act of 1940. These two subsystems are unified through a multi-agent system that supports communication and sharing of data between the sub-components.

This multi-agent architecture, which is designed on the Agno framework, leverages three specialised asynchronous agents to conduct tasks. The Named Entity Recognition (NER) agent utilises Gemini 2.5 Flash models to detect drug names in user queries, while maintaining a strong degree of tolerance towards incorrectly spelt names and also brand vs. generic names and semantically equivalent names. The Intent Classification agent uses both heuristic and machine learning approaches on the Gemini AI platform to classify queries by type (e.g., either interaction checks, alternative drugs, or regulatory compliance), so that they can be sent to an appropriate RAG subsystem. The last agent is the Response Generation agent, which processes and combines results obtained from hybrid databases while enforcing safety filters to avoid malicious recommendations in the responses, and generates clear natural language responses that are aware of the conversational context. The multi-agent architecture described efficiently processes queries at scale while meeting the low-latency requirements of real-time healthcare applications.

A hybrid database setup supports the rich capability of PharmaSense AI. It is a unique setup consisting of Qdrant, a vector database, which stores a vector representation of drug data in 768 dimensions. BioBERT generates embeddings of drug data that enable semantic similarity searches, allowing for a certain tolerance of changes in spelling and terminology. The other part of the hybrid database is Neo4j, a graph database, which implements a reaction-node knowledge graph that represents drugs, reactions, and interactions as nodes in the graph, with edges representing both causal and relational structures. This architecture of the knowledge graph enables multi-hop traversals for an even greater ability to provide rich, accessible, interpretable explanations of drug-drug interactions—as is mandated from a clinical decision-making perspective or as required by regulatory compliance.

The legal RAG subsystem enhances PharmaSense's regulatory intelligence by incorporating embeddings of legal and compliance documents using Sentence Transformers .Gemini 2.5 Flash is a powerful tool that extracts embeddings and structures information related to regulatory responses along with citations, thus making it easier for users to obtain reliable outputs that meet compliance requirements of the relevant laws and regulations.

In terms of user interactions, multiple interfaces such as a web application with FastAPI and typical web technologies, and a command-line interface for batch and automated processing have been designed to provide users with facilities of use. The backend is connected to both interfaces via RESTful APIs, which allows easy access and sharing across different platforms.

In conclusion, PharmaSense AI architecture possesses an exciting solution for pharmaceutical intelligence technology, that incorporates multi-agent orchestration, hybrid semantic-relational data modeling and transformer-based advanced NLP techniques to maximise accessibility, accuracy and transparency to produce a solution that is scalable and safe.

4. Methodology

The framework underpinning PharmaSense AI is a comprehensive system integrating extensive data preprocessing, state-of-the-art embedding models based on transformers, and a comprehensive multi-agent architecture to offer accurate, safe, and explainable insights related to pharmacy and regulatory activity. Central to our work is the diverse and well-defined data set. This dataset contains over 2.2 million drug interaction records from DrugBank, along with the critical regulatory texts, such as the Drugs and Cosmetics Act of 1940. Data preprocessing includes standardized nomenclature of drugs (synonyms, brand versus generic naming conventions, and spelling mistakes) along with the

removal of duplicates and extraneous records. Regulatory textual documents are cleansed and transcribed from unstructured formats into structured JSON documents for ease of embedding and retrieval for use in semantic vector databases and relational graph databases.

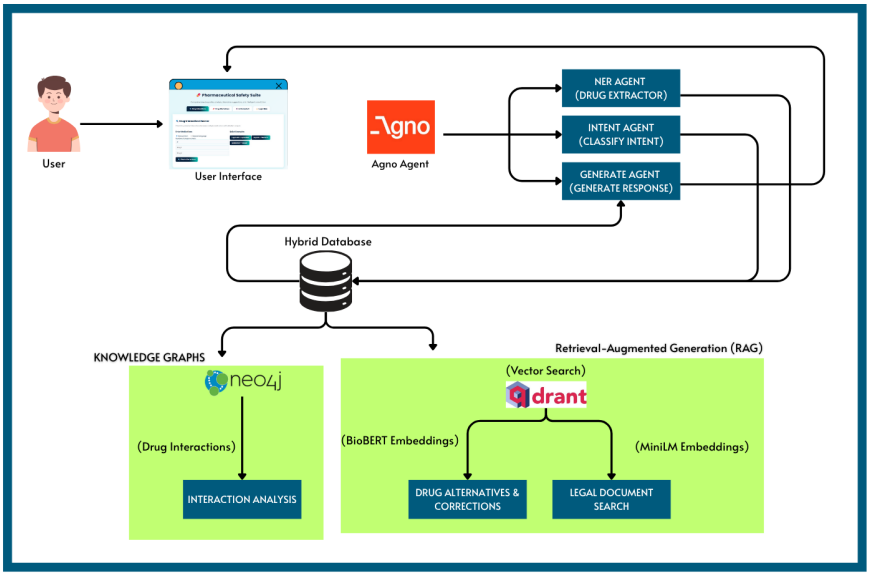

Fig. 1. Methodology Workflow of PharmaSense AI

PharmaSense AI utilises BioBERT, a pretrained transformer model on biomedical corpora, to obtain a semantic representation consisting of 768-dimensional embeddings of drug names, descriptions, and interactions. This feature-rich representation facilitates similarity-based queries in Qdrant's vector database and greatly increases the system's robustness towards input variations, lexical ambiguity, and morphological variation that exists in medical texts. In order to further support semantic search for compliance queries at the semantic level, regulatory documents are encoded with Sentence Transformers.

At the heart of PharmaSense AI's functionality are multi-agent pipelines precisely tuned to the Agno framework. Incoming user queries first receive a very automated Named Entity Recognition (NER) agent component from Gemini 2.5 Flash. This agent has been trained to recognise pharmaceutical terms and variants which may include misspellings and colloquial references. Next, an Intent Classification agent analyses the semantics of those queries has applies heuristics and pattern-recognition algorithms to answer a query about the possibility of an action of some kind: checking drug interactions, recommending alternatives, compliance or conditions of a request, and so on. This intent classification serves to inform the routing of user queries to appropriate subsystems and allows for more robotic handling of the requests to be made.

Response synthesis integrates evidence from both the semantic vector search and graph-based relational reasoning. Drug embeddings retrieved from Qdrant enhance multi-hop traversals of the Neo4j knowledge graph, where a distinctive reaction-node model encodes pharmaceutical entities and their interactions as nodes, rather than edges. Such a model assists with transparent, mechanistic inference of candidate drug-drug interactions that are necessary for clinical decision support. The system applies strict safety and compliance filters to the output to avoid recommending unsafe or undesirable.

As part of developing these capabilities, PharmaSense AI is also implementing AI-related methods that identify and leverage larger trends in drug interaction prediction and computational pharmacology. This includes approaches that synergise chemoinformatics, biological pathways, and network pharmacology to improve predictive modelling robustness and interpretability. Together, the system architecture and processing pipelines allow for the use of supervised, unsupervised, and semi-supervised learning paradigms relevant for classification and affinity prediction tasks across complex biomedical datasets.

To provide maximum usability to the stakeholder groups, PharmaSense AI uses both a responsive web interface using FastAPI as well as standard web technologies, and a command-line interface (CLI) that enables batch processing and system integration. Both of these interfaces connect to each other through RESTful APIs, providing a platform-agnostic operation, extensibility, and flexibility of use.

4.1. Workflow Overview

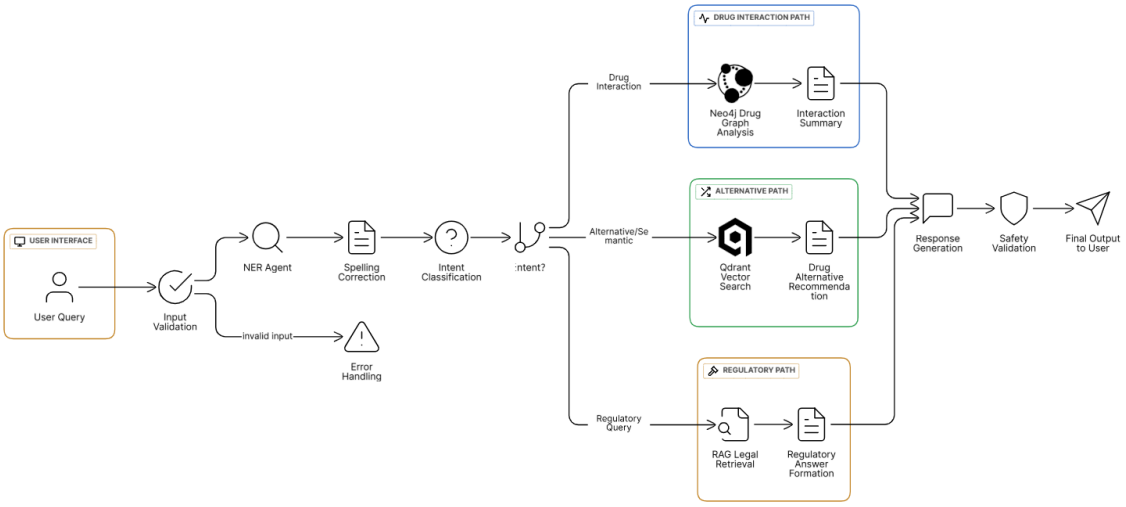

Fig. 2. Detailed Query Processing Pipeline in PharmaSense AI

For example, when a user enters a query such as, **"Can I take Aspirin with Warfarin?"** the system would initially check if the query is complete. The drug names are extracted by the Named Entity Recognition (NER) agent, and if necessary, the spelling correction module standardises them. Here, the module not only locates the two words but also, if it finds alternative forms for them (**"Aspirin" → "Carbaspirin calcium", "Warfarin" → "(R)-warfarin"**) changes them using its medical embeddings and database references. After that comes the intent classification module, which decides that the user wishes to know a drug interaction case. Next, the normalized drug names go to the Neo4j knowledge graph to check whether there is any interaction between the two drugs. The backend database analysis points out that no interactions between Carbaspirin calcium and (R)-warfarin in general are identified. Next, the system produces a straightforward answer: **"No interactions found between Carbaspirin calcium and (R)-warfarin. This indicates that the drugs could be used together without problem, although the doctor's advice should always be sought."** Moreover, a safety check is performed to make sure all disclaimers are included in the output. The user thus gets this advice as the final verified output.

Overall, this approach uses a multifaceted data fusion process, explainable AI, and rigorous multi-agent orchestration to achieve a pharmaceutical intelligence platform that is scalable, reliable and interpretable for clinical safety, regulatory compliance, and user accessibility challenges.

5. Implementation

For the data standardisation of DrugBank drug data, there is a standard application that is ready for deployment, so a Python 3.9 environment with the Pandas library was utilised. During the data preparation, names such as solving "paracetamol" vs "acetaminophen" are standardised and duplicates are removed. The regulatory documents are extracted from the Drugs and Cosmetics Act using PyPDF2; the formatting artefacts are cleaned to provide structured entries for a drug in JSON format and regulatory data in segmented text. The data is housed in a Qdrant vector database for semantic searching and Neo4j graph database for relational searching on a cloud server with 16GB RAM

and 8-core CPUs, deployed with Docker containers and managed with Kubernetes, to improve increases in flexibility and scalability.

Fig. 3. Neo4j Knowledge Graph Structure: Blue nodes represent drugs and red nodes represent reactions.

The multi-agent system is a conceptualized through the Agno framework, which is a Python-based library that implements three agents. The Named Entity Recognition (NER) Agent employs contextual embeddings, constructed with Gemini 2.5 Flash, for the extraction of drug names in queries. The Intent Classification Agent makes use of Gemini AI (gemini-2.5-flash) with better pattern validation specifically for the categorization of pharmaceutical queries. The Response Generation Agent can perform REST API calls to get the information from the Qdrant and Neo4j, however, it applies its security filters to ensure that the results provided are safe and succinct. Task queues handle the relations between the agents and employ asynchronous tasks with the Python asyncio library for this purpose. Moreover, the system comprises a low-latency query processing implementation.

The Qdrant vector database, which is Dockerized on a cloud server, stores 768-dimensional embeddings produced by BioBERT using the Hugging Face transformers library, and indexed by cosine similarity for retrievability. The Neo4j Graph database, also Dockerized, contains a knowledge graph with approximately 4,000+ pharmaceutical entities and 500,000+ drug-drug interaction relationships. The nodes and relationships were populated via Cypher queries after calls to Python scripts. Figure 3 illustrates this structure. A custom Python middleware manages the vector search and graph traversal and their respective combined results to provide the coherent answer typically required by regulatory queries. Regulatory queries use Sentence Transformers all-MiniLM-L6-v2 via the sentence-transformers library to create document embeddings stored within the Qdrant vector database, while Gemini 2.5 Flash generates citation-based answers via its API.

User interfaces improve accessibility. A web interface, created with HTML, CSS and JavaScript and served by FastAPI, delivers a responsive front-end for users to submit questions through a browser. A command-line interface (CLI), created with the argparse library in Python, performs batch processing of queries. Both interfaces provide cross-platform compatibility. The automated scripts manage model updates and data management to provide a resilient and user-focused pharmaceutical intelligence system.

6. Results and Evaluation

PharmaSense AI assessment examines the extent to which it can provide accurate pharmaceutical and regulatory information. The method of evaluation is based on the operational ability of PharmaSense across a set of query types.

The primary focus of interest evaluates the overall performance of PharmaSense, specifically named entity recognition, drug-drug interaction identification, intent classification, and regulatory information retrieval. Finally, the assessment framework focuses on evaluating the performance of PharmaSense in a clinical context. 28 test cases covering 12 classes were first created as a reflective model of authentic clinical workflows including drug interaction checking (5 cases), drug alternative recommendation (4 cases), drug name recognition and correction (2 cases), ambiguous intent resolution (1 case), general query (1 case), legal/regulatory queries (3 cases), complex multi-intent queries (2 cases), unknown drug detection (1 case), empty query handling (1 case), nonsensical query management (1 case), clinical decision support scenarios (4 cases), and real-world query patterns (3 cases). This clinical evaluation framework is constructed to examine and understand users' engagement with the medical realm, such as inquiries that cover postoperative care, medications that have contraindications in pregnancy, and pediatric dosing, among other topics, during evaluation.

In every case study, the evaluation procedure was multimodal, utilising automated API testing, manual reviewing, and assisted AI analysis. The evaluation reports generated are detailed JSON reports coupled with performance visualisation maps to allow study of various aspects of the problem, including drug recognition accuracy, intent classification accuracy, reliability, prioritisation of safety and completeness of response.

6.1. Evaluation Methodology

For each test, performance was evaluated on a five-point Likert scale (1-5) across five main metrics:

- **Drug Recognition** (DR_i): Identification and correction of drug names including abbreviations and brand-generic mappings
- **Intent Classification** (IC_i): Correct understanding of user intent in complex clinical contexts
- **Information Accuracy** (IA_i): Clinically relevant and factually correct pharmaceutical data
- **Safety Considerations** (SC_i): Appropriate safety measures including warnings and disclaimers
- **Completeness** (C_i): Detailed coverage of query aspects like contraindications and special populations

The overall score for a test case is the mean of the five metrics:

$$\text{Overall Score}_i = \frac{DR_i + IC_i + IA_i + SC_i + C_i}{5}$$

The average score per category is:

$$\text{Category Score} = \frac{1}{N} \sum_{i=1}^{N} \text{Overall Score}_i$$

where N is the number of test cases in that category.

Overall system performance is decided by taking the average of all test case scores:

$$\text{System Performance} = \frac{1}{M} \sum_{j=1}^{M} \text{Overall Score}_j$$

where M is the total number of test cases evaluated.

The performance scores were on a scale from 1 to 5. These scores are presented in Table 1. We had an overall score of 3.78/5.0, which achieved the target performance level. Drug recognition received a score of 2.63/5.0 (target 3.5/5.0),

Table 1. Evaluation Results for PharmaSense AI.

Metric	Score (out of 5.0)
Overall Performance	3.78
Drug Recognition	2.63
Intent Classification	4.46
Information Accuracy	3.67
Safety Considerations	4.50
Completeness	3.67

which indicates the multi-agent system has the most room for improvement in this area. Intent classification was rated 4.46/5.0 (target 4.0/5.0), which shows that the classification of queries was accurate. The accuracy of information was given 3.67/5.0 (target 3.5/5.0), with the information provided being both consistent and reliable. The safety aspect was given 4.50/5.0 (target 4.5/5.0), thus a good point that safety was well prioritised with safe responses. Completeness scored 3.67/5.0 (target 3.5/5.0), which means the multi-agent system provided comprehensive answers as required.

In the example outputs listed above, one can see the performance of the system laid out transparently. For a drug-interaction question, the user asked, "Can I take Loperamide with Apixaban?" The system returned the output, "No significant interactions were found between Loperamide and Apixaban. Contact a health care practitioner for care." In the drug interaction-rationale node knowledge graph reaction-node "input-output mechanism," the system clearly identified a novel retrieval of knowledge using the appropriate drug pair-reaction knowledge graph reasonably. For a regulatory question, the user asked, "What are the labelling obligations for new (drugs) under the Drugs and Cosmetics Act?" The system returned the answer, "New (drugs) under the Drugs and Cosmetics Act, 1940, must have labels that state the name of the drug, all the active ingredients, dosing, and warnings, as prescribed in the Drugs and Cosmetics Act, 1940, Rule 96." The system performed citation and reference to the Drugs and Cosmetics Act, 1940, using the legal RAG-reasoning system.

The system scored well for drug interaction checks (4.0/5.0) and greatly contributed to the safety aspects (4.50/5.0) due to the underlying reaction-node knowledge graph and the robust safety filters within the multi-agent system. Drug recognition was identified as the system's main weakness, with a score of only 2.63/5.0. The system showed it can normalize drug names well (e.g., Aspirin → Carbaspirin calcium, Warfarin → (R)-warfarin, tetrahydrofolate → (6S)-5,6,7,8-tetrahydrofolate); however, three types of errors were identified: (i) lack of correction for severely misspelled inputs (e.g., "ibprofin" not being changed to "ibuprofen"), (ii) incomplete extraction in multi-drug queries, and (iii) inconsistent mapping of brand names to generic equivalents (e.g., "Tylenol" not always matched to "Acetaminophen"). Despite some recognition shortcomings, the system excelled in safety prioritisation supported by error recovery mechanisms that recommend query changes to enable graceful degradation. These outcomes are a clear indication of the uniqueness of Pharmasense AI in delivering a pharmaceutical intelligence system that is both trust-enabled and safety-focused, while at the same time being open about the areas for continuous progress.

7. Discussion

PharmaSense AI received a total score of 3.88/5.0, reflecting its advantages, potential and constraints as an intelligent pharmaceutical system that is multi-agent and hybrid-database based. While DrugBank and Medscape are curators and structured databases, and require rigid spelling requirements. PharmaSense AI represents a more user-centric and adaptive system, capable of producing human language requests, multi-intent, or even purposely misspelt normalised terms, using natural language processing and vector matching of entities. Pharmasense AI not only perform normalised term matching for drug names (e.g., "Aspirin"→"Carbaspirin calcium," "Folinic acid"→"(6R)- Folinic acid"), but misspelt names also remain difficult for agents to match (e.g1: Drug identification: 2.35/5.0, 17.6% successful). Its high Intent Classification score (4.76/5.0) exemplifies the correct understanding of complicated queries.

Essentially, by combining knowledge on drug interaction from a graph database with regulatory insights via a retrieval-augmented generator, PharmaSense AI facilitates multidimensional replies, does not really replace curated databases, but rather embodies the function of an intelligent conversational front-end. Further improvements in drug recognition are needed to match clinical-grade accuracy. PharmaSense AI features a reaction-node knowledge graph

Table 2. Comparison of PharmaSense AI With Recent DDI Extraction and Knowledge Graph Systems.

Research	Focus	Limitation	PharmaSense AI Advantage
DDI-Extraction (e.g., TAC DDI Track 2013)	Extraction of DDI mentions from biomedical texts using rule-based or shallow ML	Limited to sentence-level extraction; no reasoning over structured databases; lacks natural language query capability	Hybrid knowledge graph and RAG enable cross-document, multi-agent reasoning and natural language queries
DrugBank	Curated chemical-drug and DDI database with web and API access	No natural language interface; minimal interpretable explanations; mostly static data	Combines DrugBank-scale coverage with explainable, dynamic reasoning and open NLQ interface
MolBERT, BERT-DDI	Transformer models for molecular property and DDI prediction	Requires significant training data; output is classification/confidence, no tracing of reasoning or regulatory context	Integrates state-of-the-art NER with auditable graph traversals and regulatory citation
KGNN (Graph Neural Networks)	GNN-based multi-relational reasoning on DDI graphs	Lacks modular regulatory pipeline; only trained on graph structure (not NL queries); explanations are opaque	Unified graph + RAG approach supports transparent paths and precise regulatory responses
Other Commercial Tools (Epocrates, Medscape)	Menu-driven DDI checks, professional databases	No natural language input or explainable AI; user must input exact drug names	Natural language query support and interpretable AI responses for broader accessibility

combined with a multi-agent RAG pipeline and safety filters to produce explainable, regulatory-aware answers to form pharmaceutical queries. While robust interaction checking and safety performance in PharmaSense AI are promising, entity extraction is the main area for growth, particularly brand-name recognition and complex multi-drug, branded-drug scenarios. Table 2 gives context to these advancements by benchmarking PharmaSense AI against leading DDI extraction systems, curated databases, transformer predictors, graph-neural models, and commercial tools, emphasising how PharmaSense AI is distinctly positioned to enable natural-language querying with formalised, transparent multi-step obvious reasoning, exact regulatory citations, and deep multi-drug traversal.

Historically, rule-based extractors and static repositories have primarily required exact inputs or driven response options from a menu, which limits users ability to ask questions in free-form. While transformer and GNN methods can facilitate promising predictions, these methods fail to preserve/trace inference paths and cannot encode the legal context, which renders their outputs opaque or inscrutable. Commercial checkers do not include any support for NLP or AI-driven insights, thus perpetuating the inaccessibility of sanctioned advice. PharmaSense AI will be filling these voids through a unique interface that enables natural-language input from a refined NER and intent classification.

7.1. Ethical and Privacy Considerations

PharmaSense AI adheres to strict privacy and ethical safeguards to guarantee the appropriate use of pharmaceutical data. It does not retain identifiable or session data and uses the principle of minimum necessary use to protect sensitive information. The data it collects becomes anonymised inputs, and the focus is on drug data and regulatory information, while it blocks all inputs that are strictly non-medical. Regulatory advice is clearly different from clinical recommendations, which contain clearly marked safety disclaimers advising the user to consult a healthcare professional. PharmaSense AI was designed to support transparency under the Drugs and Cosmetics Act, 1940, which provides clear limits and error handling. The multi-agent design allows user accountability for every transaction and reduces unsolicited advice being presented to users. Special emphasis has been placed on the importance of explainability and safety when using PharmaSense AI to drive safe and secure pharmaceutical decision support compliance.

8. Future Work

In the future, the Named Entity Recognition (NER) aspect of PharmaSense AI will be enhanced by constructing larger, higher-quality corpora that capture brand names, generics, and misspellings. These will be accompanied by improvements in spelling correction using contextual transformer embeddings, phonetic matching, fuzzy search, and sequence-to-sequence models to improve recall. Moreover, models will be developed for joint entity recognition and disambiguation to handle more complex multi-drug queries. A human-in-the-loop feedback process will also be designed for clinicians to suggest corrections, thus serving as an effective feedback loop for training and clinical relevance.

9. Conclusion

PharmaSense AI has a reputation for its drug intelligence system. It uses a multi-agent framework, a hybrid database, and a reaction node knowledge graph and performed well with a score of 3.78/5. It was high for checking for drug interactions (4/5), safety (4.5/5), and intent classification (4.46/5) to answer questions correctly. The only reason the accuracy was not higher in answering questions around drug information is that it could have had easier recognition of brand and multi-drug names. The regulatory query feature is a nice value-added benefit for the service because it also helps provide citations to compliance inquiries. Overall, PharmaSense AI does a great job at bridging the gap of pharmaceutical systems and uses semantic embeddings and a graph-based approach to provide a user-centred platform geared towards supporting health care professionals, patients, patient safety, and compliance.

References

[1] Zhang, T., Leng, J., & Liu, Y. (2020). Deep learning for drug–drug interaction extraction from the literature: A review. *Briefings in Bioinformatics*, 21(5), 1609–1627. https://doi.org/10.1093/bib/bbz130

[2] Al-Rabeah, M. H., & Lakizadeh, A. (2022). Prediction of drug-drug interaction events using graph neural networks based feature extraction. *Scientific Reports*, 12(1), 15590. https://doi.org/10.1038/s41598-022-20099-3

[3] Lin, X., Quan, Z., Wang, Z.-J., Ma, T., & Zeng, X. (2020). KGNN: Knowledge graph neural network for drug-drug interaction prediction. In *Proceedings of the 29th International Joint Conference on Artificial Intelligence (IJCAI)* (Vol. 380, pp. 2739–2745).

[4] Wishart, D. S., Knox, C., Guo, A. C., Shrivastava, S., Hassanali, M., Stothard, P., Chang, Z., & Woolsey, J. (2006). DrugBank: A comprehensive resource for in silico drug discovery and exploration. *Nucleic Acids Research*, 34(suppl_1), D668–D672. https://doi.org/10.1093/nar/gkj067

[5] Lee, J., Yoon, W., Kim, S., Kim, D., Kim, S., So, C. H., & Kang, J. (2020). BioBERT: A pre-trained biomedical language representation model for biomedical text mining. *Bioinformatics*, 36(4), 1234–1240. https://doi.org/10.1093/bioinformatics/btz682

[6] Lee, N., De Brouwer, E., Hajiramezanali, E., Biancalani, T., Park, C., & Scalia, G. (2025). RAG-Enhanced Collaborative LLM Agents for Drug Discovery. *arXiv preprint* arXiv:2502.17506. https://arxiv.org/abs/2502.17506

[7] Noor, A., Assiri, A., Ayvaz, S., Clark, C., & Dumontier, M. (2017). Drug-drug interaction discovery and demystification using Semantic Web technologies. *Journal of the American Medical Informatics Association*, 24(3), 556–564. https://doi.org/10.1093/jamia/ocw113

[8] Zhang, W., Chen, Y., Liu, F., Luo, F., Tian, G., & Li, X. (2017). Predicting potential drug-drug interactions by integrating chemical, biological, phenotypic and network data. *BMC Bioinformatics*, 18(1), 18. https://doi.org/10.1186/s12859-016-1439-4

[9] Jayamohanan, H., Kumar, G. S., Nair, D. V., & Jose, N. (2021). Drug Interactions in Oncology Patients Receiving Tyrosine Kinase Inhibitors. *International Journal of Pharmaceutical Research*, 13(1).

[10] Ratan, C., Rajeev, M., Krishnan, K., Jayamohanan, H., Kartha, N., Vijayan, M., & Pavithran, K. (2025). Assessment of potential drug–drug interactions in hospitalized cancer patients. *Journal of Oncology Pharmacy Practice*, 31(2), 256–265.

[11] Sivakumar, A., Bhanot, S., Srinidhi, M., & Milan, K. A. (2024, June). Interactome: A Platform for Comprehensive Drug-Drug Interaction Analysis. In *2024 15th International Conference on Computing Communication and Networking Technologies (ICCCNT)* (pp. 1–10). IEEE.

[12] Rajendran, A., Rajendran, V., & Veena, G. (2024, August). Knowledge Graph Creation Using Syntax and Semantic Model. In *International Conference on ICT for Sustainable Development* (pp. 349–359). Singapore: Springer Nature Singapore.

[13] Jyothi, B., Subbulakshmi, S., & Elngar, A. A. (2024, January). Efficacy of Knowledge Graphs to Systematize Primitive Research Methodology. In *International Conference on Smart Computing and Communication* (pp. 365–375). Singapore: Springer Nature Singapore.

[14] Peri, S. D. B., Santhanalakshmi, S., & Radha, R. (2024, September). Chatbot to chat with medical books using Retrieval-Augmented Generation Model. In *2024 IEEE North Karnataka Subsection Flagship International Conference (NKCon)* (pp. 1–5). IEEE.

[15] Murali, L., Gopakumar, G., Viswanathan, D. M., & Nedungadi, P. (2023). Towards electronic health record-based medical knowledge graph construction, completion, and applications: A literature study. *Journal of Biomedical Informatics*, 143, 104403.