MedPharma AI: Bridging Gap between General Physicians and Pharmacologists

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We accept the work contained in the report titled "MedPharma AI: Bridging Gap between General Physicians and Pharmacologists", written by Muhammad Talha and Syed Zain Ul Abadeen Hussain Naqvi as a confirmation to the required standard for the partial fulfillment of the degree of Bachelor of Science in Artificial Intelligence.

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Abstract

The MedPharma AI project addresses the critical issue of polypharmacy related Drug to Drug Interactions (DDIs) where current reactive detection methods often fail to prevent adverse effects. The proposed solution is an AI-driven framework utilizing Graph Neural Networks (GNNs), Explainable AI (GNE), and Large Language Models (LLMs) to proactively predict DDIs using the DDInter and DrugBank datasets. The methodology involves representing drugs as nodes in a graph structure for complex interaction analysis with GNE providing textual justifications for transparency. The model's results show high performance, achieving an overall accuracy of 88% and strong F1-scores across all severity categories, notably 89% for 'Major' interactions. In conclusion, MedPharma AI offers a robust, scalable, and proactive clinical decision support system designed to reduce adverse drug reactions and significantly improve patient safety.

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Acronyms and Abbreviations

ADR	Adverse Drug Reaction
AI	Artificial Intelligence
API	Application Programming Interface
BNF	British National Formulary
DB	Database
DDI	Drug–Drug Interaction
DDInter	Drug–Drug Interaction Database
DrugBank	DrugBank Database
GNE	Graph Neural Explainability
GNN	Graph Neural Network
GPU	Graphics Processing Unit
LLM	Large Language Model
ML	Machine Learning
NLP	Natural Language Processing
UI	User Interface
XAI	Explainable Artificial Intelligence

Chapter 1

Introduction

1.1 Project Overview

Polypharmacy or the simultaneous prescription of several medications for a single patient is a major issue in contemporary medical care, particularly effects the elder patients. While multiple drugs are often necessary for treating complicated illnesses, taking them together increases the risk of Drug-Drug Interactions (DDIs), which can cause Adverse Drug Reactions (ADRs), reduce treatment efficacy, or even lead to life-threatening complications. Research has pointed out that a significant part of the hospital admissions of older persons is due to preventable drug interactions, which calls for the implementation of detection mechanisms that would be proactive in nature. Historically, DDIs have been recognized through clinical studies, pharmacovigilance research, and manual cross-checking by medical professionals through the use of fixed drug databases. Such traditional techniques, however, are reactive, slow, and have limited scalability; they often do not suffice in timely identifying new interactions that might have come up. The growth and development of the pharmaceutical sectors are not only a blessing but also a challenge for the medical practitioners and pharmacists who are to use the new drugs and their combinations. The MedPharma AI project intends to overcome these limitations by creating an AI-based predictive system that can promptly detect and explain possible drug-drug interactions. The architecture will use machine learning and graph neural networks (GNNs) as the primary means of working with large medical datasets, particularly the DDInter one, which is connected to the database DrugBank directly to have a more profound pharmacological information and better data integrity. The explainable AI (GNE) is also used in the system to provide the transparency of the model and confidence of the users as the interaction should be presented in a decomontable manner. The system has integrated a large language model (LLM) as a smart conversational agent into it. The integration helps the physicians to inquire about the interaction and they receive replied responses which are similar to

human like and easy to comprehend. The combination of the explainability and predictive modeling and the prompting of communication is intended to bridge this gap between AI technology and clinical applicability to improve patient safety and reduce ADRs and help healthcare workers make more informed and data-driven decisions.

1.2 Problem Statement

The rise in the count of prescribed drugs has made it more cumbersome to identify harmful drug interactions by applying the conventional rule based regimes. Such traditional methods of functioning are slow to respond, are prone to errors, and cannot support clinical reasoning much. In addition, because new pharmaceutical products are gradually being introduced quite fast, it has become even more difficult to maintain the interaction information. As a result, an intelligent, explainable and proactive DDI prediction framework is required to help healthcare professionals.

1.3 Problem Description

In spite of polypharmacy being the main aspect of contemporary medicine, it has been further augmented. The risk of drug interactions is exceedingly high. In case of the interaction of several drugs able to interfere with the properties of each other including pharmacodynamics or pharmacokinetics causing unpredictable side effects, or even treatment failure.As an example, another drug can react with one and can either make the other drug more toxic, or in the opposite scenario, can influence the metabolism. The healthcare specialists must face numerous issues in the healthcare industry, such as interactions management that contains, among others, limiting access to real-time information, understanding issues related to AI creation, and the non-user-friendliness of visualization tools for interaction effects. The MedPharma AI system will aim at reducing these obstacles through a multi-layer AI system. It is able to foretell interactions and, at the same time, may give explanations which are significant in clinical terms, therefore establishing trust among medical professionals and resulting in their approval of the tool.

1.4 Project Objectives

The objective of the project is to design an AI-driven drug to drug interaction prediction and explanation system that will help healthcare professionals avoid adverse drug reactions and, therefore, safer prescription decisions. The objectives of the study are:

- To create an explainable AI (GNE) model offering a prediction and the clarification of the rationale behind each choice.

- To develop a ChatGPT-based LLM system that enables physicians and doctors to enable natural language query into drug interaction prescription..

1.5 Project Scope

The project's scope defines the boundaries of the MedPharmaAI solution, outlining the features that are included, excluded, and the considerations made during development. This ensures focused execution, realistic expectations, and alignment with project objectives.

Included

- AI and GNN models for predicting drug-drug interactions.
- Merging of DDInter and DrugBank datasets.
- Usage of Explainable AI (GNE) for interpretability and visualization.
- Creation of ChatGPT-based communication module for pharmacist interaction.
- Making a web interface for healthcare professionals that is user-friendly.

Not Included

- Monitoring of prescriptions for individual patients in real-time.
- Systems for compliance with legal, ethical and regulatory requirements.
- Hospital EHR (Electronic Health Record) systems integration.
- Clinical deployment or extensive pharmaceutical testing.

Assumptions

- The DDInter and DrugBank datasets are accessible and organized perfectly.
- Sufficient computing power (for example, GPU systems) is ready for training the model.
- Users (pharmacists/clinicians) are expected to know drug terms and AI system outputs at a basic level.

Summary

This chapter gives an overall idea of the MedPharma AI project, which is aimed at an AI-based detection and explanation system for drug-drug interactions due to polypharmacy. It highlights the issue of ADRs caused by the use of multiple medications, characterizes

the drawbacks of the conventional detection techniques, and asserts the necessity for a smart, explainable, and interactive AI system. The chapter goes on to state the goals and the range of the system, presenting the unification of GNN, Explainable AI (GNE), and ChatGPT based interaction as a means to close the divide between data driven expectations and clinical decision making. The project in the end aspires to deliver a tool that is scalable, transparent, and user-friendly for the healthcare professionals to use in the area of medication safety assurance and patient outcome enhancement.

Chapter 2

Literature Review

2.1 Introduction

The co-administration of drugs sometimes leads to interactions, termed drug-drug interactions (DDIs). DDI is one of the leading cause of patient safety problems, especially in patients taking multiple medications.Studies such as [1] have established this concern,and global health reports including [2] continue to alert health care systems to the risks of adverse drug reactions, hospitalization,and therapeutic failure resulting from medication combinations.Notably,even highly trained and experienced health care providers find it challenging to detect drug interactions. Therefore, there is an urgent need for computational systems that can detect DDIs while being intelligent,scalable,and interpretable. The existing literature has tackled the DDI analysis in different ways, among them are rule-based clinical databases,bio medical text mining,graph-based modeling,and molecular deep learning.Although considerable advancements have been made,most existing systems suffer from common limitations: lack of interpretability,inability to combine different data sources,dependency on static datasets,and limited usability for clinicians. This chapter provides a comprehensive examination of the literature in these fields and describes MedPharma AI system within this research landscape.

2.2 Polypharmacy and Clinical Significance of DDIs

The literature on polypharmacy always states that the unintentional mixing of drugs is still an important reason for hospital emergency visits, especially in the case of older patients. The research by [1] indicates a great clinical significance of drug interactions on the patients' results, whereas the World Health Organization (WHO) standards point out the monitoring as a preventive measure against the negative events prevention [1, 2].

DDI detection, classical methods of the past, depend largely on top-notch rule-based databases of known drug interactions that have been meticulously compiled. These systems are still favored in clinical practice but possess a lot of limitations: not only can they not

spot new interactions, but they also do not have any predictive power, and they do not adjust to the new findings in the biomedical field.

2.3 Drug–Drug Interaction Detection in Biomedical Text

NLP techniques were applied widely by the researchers to retrieve drug-drug interactions from both clinical and scientific literature. Deep learning architectures, like those demonstrated by [3], have proven to be much more efficient than rule-based systems as they can learn contextual and semantic representations from the unstructured text.

According to [4], machine learning classifiers used on biomedical literature can be very accurate in prediction. Nevertheless, these systems, which are based on text, are limited to the processing of text and are not able to perform molecular-level reasoning.

Text-extraction-based methods are effective in retrieving interactions found in literature or clinical notes and report very high precision and recall on the textual data. On the other hand, they lack the molecular context and thus give only a limited view to the clinicians regarding the interpretability. Moreover, these methods rely on the presence of high-quality text sources which may restrict the recognition of newly occurring interactions that have not yet been reported in the literature.

2.4 Knowledge Graphs and Graph Databases in Drug Safety

Knowledge graphs (KGs) provide a systematic method for representing biomedical relationships. Research by [5] demonstrates that knowledge graphs can effectively model and represent semantic relationships among drugs, proteins, and diseases, resulting in more comprehensive interaction modeling.

Graph databases enable efficient storage, querying, and reasoning over complex biomedical networks. While earlier work like [6] explored these technologies for genome-scale networks, their application to drug interaction analysis has expanded the potential for knowledge integration across multiple data modalities.

2.5 Graph Neural Networks for Molecular Prediction

Graph neural networks (GNNs) have emerged as a powerful approach for representing molecular architectures and their pharmacological relationships. [7] pioneered the application of multimodal graph convolutional networks (GCNs) for predicting polypharmacy side effects, demonstrating the superiority of graph-based learning over conventional statistical models.

Subsequent advancements include GNN architectures for molecular property prediction [8], GNN-based DDI modeling [9], and attention-based molecular transformers [10]. These

models utilize graph representations derived from SMILES strings, typically processed using tools such as RDKit [11].

GNN-based systems excel at molecular reasoning and can represent intricate chemical structures to identify potential interactions with high predictive accuracy. Furthermore, they effectively illustrate structural characteristics of molecules relevant to interactions. However, these models are frequently described as "black-box" approaches, which restricts their interpretability for clinical end-users and limits meaningful integration with textual and clinical knowledge.

2.6 Explainable Artificial Intelligence in Medicine

Explainability is a critical factor enabling AI technology deployment in hospitals and clinics. Medical XAI reviews [12] and pioneering research [13] emphasize that trust and transparency are compromised by black-box models.

2.7 Large Language Models in Clinical Decision Support

Large language models (LLMs) including ChatGPT have demonstrated near-expert-level performance in medical reasoning. Research presented by [14] and [15] reveals high accuracy in medical question-answering, patient counseling, and clinical explanation generation.

The integration of LLMs with predictive models creates interactive clinical tools capable of explaining model outputs, assisting clinicians, and enhancing interpretability. This combination of computational prediction with natural language explanation represents a significant advancement toward clinically deployable AI systems.

2.8 Comparison of Existing DDI Detection Methods

Table 2.1 summarizes major studies on DDI detection methods, their approaches, strengths, and limitations. This comparison identifies research gaps that the proposed MedPharma AI system aims to address.

Table 2.1: Summary of existing DDI detection methods, their strengths, and limitations

Study	**Method/Model**	**Strengths**	**Limitations/Notes**
Zhang et al. [3]	Deep learning survey	Comprehensive review of DDI extraction methods	Review article; no novel implementation

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Study	**Method/Model**	**Strengths**	**Limitations/Notes**
Lee et al. [4]	Deep learning for DDI prediction	High accuracy; learns from biomedical data	Text-based only; cannot integrate molecular information
Zhao et al. [5]	Knowledge graph-based DDI detection	Interpretable relationships; structured data	KG completeness issues; static datasets
Balaur et al. [6]	Graph DB for networks	Scalable; flexible for integration	Requires complex schema design
Zitnik et al. [7]	GCN for polypharmacy effects	Strong predictive accuracy	Limited interpretability; clinical integration limited
Jin et al. [9]	GNN-based DDI prediction	High molecular feature performance	Dense feature engineering; computationally intensive
Liu et al. [8]	GNN for molecular properties	Good molecular representation	Lacks direct clinical application
Maziarka et al. [10]	Attention-based transformer	Captures complex molecular structures	Heavy computational cost
Holzinger et al. [13]	Explainable AI for medicine	Provides transparency	Not specific to DDI; general domain
Singhal et al. [14]	LLM-based medical QA	High accuracy in medical reasoning	Limited real-world DDI prediction
Thirunavukarasu et al. [15]	LLM clinical support	Interactive explanations	Dependent on large text corpora; not molecular
Liu et al. [16]	AI for ADR automatic coding	Validates AI on real-world pharmacovigilance data	Uses French national data only; specific to coding task
Maher et al. [1]	Polypharmacy epidemiology	Clinical relevance; evidence-based	Observational; not predictive
WHO [2]	Medication safety guidelines	Global perspective; policy guidance	Policy document; not computational

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Study	Method/Model	Strengths	Limitations/Notes
Landrum [11]	RDKit cheminformatics	Standardized molecular processing	Requires programming knowledge

2.9 Research Gap Summary

Current DDI detection approaches have significant limitations that restrict their clinical applicability. Text-based methods operate exclusively on textual data and cannot infer molecular-level information. Knowledge graph-based strategies, while interpretable, typically depend on static datasets and cannot dynamically incorporate new drug data or emerging interactions. Machine learning models trained solely on structured datasets may identify molecular patterns but lack the interpretability required for healthcare applications.

The proposed MedPharma AI system addresses these gaps by integrating multiple complementary approaches:

- **Molecular graph prediction**: Leverages GNNs to predict interactions from molecular structure
- **Knowledge graph reasoning**: Combines structured knowledge about drugs, SMILES and formulas.
- **Explainability**: Employs explainable GNNs to identify molecular features driving predictions
- **Natural language generation**: Uses LLMs to translate complex predictions into clinician-friendly explanations
- **Dynamic prediction**: Enables real-time incorporation of new or previously unseen drug combinations

This integrated approach ensures that DDI predictions are not only accurate but also interpretable and actionable for clinical decision-making. By combining predictions from molecular, textual, and knowledge-graph-based methods, the system provides comprehensive coverage of potential drug interactions while maintaining transparency in its reasoning.

Summary

Current literature is well-established in NLP-based extraction, molecular graph modeling, and knowledge graph reasoning. However, most existing systems address these components

separately, resulting in limited explainability, interactivity, and cross-modal integration. The proposed MedPharma AI system advances the field by unified integration of GNN-based molecular prediction, explainable AI mechanisms, graph databases, and LLM-powered user interaction within a single clinical decision support framework.

This chapter has demonstrated the maturity of individual components and the critical gap in their integration. The following chapters will present the architecture, implementation, and evaluation of MedPharma AI as a solution to this research gap.

Chapter 3

Requirement Specifications

Introduction

The awareness of drug administration becoming more complex as polypharmacy cases increase, together with the need for DDIs to predict and elucidate, calls for the use of higher-end DDI systems. Chapter 2 pointed to the existing methods involving DDI extraction from texts, knowledge graphs, graph neural networks, and explainable AI as well as the corresponding limitations in today's systems, such as dependence on static databases, lack of interpretable results, and inadequate coupling of molecular and clinical data.

Drawing on the above, this chapter sets out the **requirement specifications** for the MedPharma AI system to be developed. It first identifies the drawbacks of current DDI detection systems, secondly, shows the workflow and benefits of the AI-supported solution, and lastly, specifies both functional and non-functional requirements. Moreover, it presents **use cases** that serve to explain the interaction between the system and its end-users i.e., pharmacists, researchers, and clinicians thus, providing a basis for future system design and implementation.

3.1 Existing System

The currently used systems for recognition of Drug to Drug Interactions (DDIs) predominantly use rule-based and database-driven techniques that depend on predefined lists of known interactions. Widely used platforms like DrugBank, Medscape, and Drugs.com heavily rely on these manually curated datasets to find and inform about interactions among the prescribed medications. The functioning of these systems involves searching for entered drug names in the unchanging records of the previously recognized interactions and showing their degrees of severity.

3.1.1 Limitations

The aforementioned traditional systems, though they have been quite useful in clinical practice, come with a number of drawbacks that made them less effective and less adaptable to modern healthcare applications. Below are the main drawbacks identified:

- The over-reliance on manually curated and static databases that need to be updated regularly and this makes it difficult to collect new or developing drug interactions.
- The systems are unable to predict unknown or potential interactions since the information these systems can only retrieve is already present in the database.
- Absence of learning capability because they are based on fixed rules instead of adaptive or data-driven algorithms.
- The interaction results come without explanation or reasoning making them less useful for research and clinical interpretation.
- The interaction of the user is limited since most systems offer only static textual outputs that do not involve natural language understanding or conversational support.
- There is limited accessibility as many existing drug interaction platforms can only be used upon purchasing or subscribing through institutions which limits access for individual researchers and smaller healthcare facilities.
- They are heavily dependent on the accuracy and completeness of the underlying datasets which increases the risk of having outdated or missing information.

The existing DDI systems are limited by these drawbacks and, therefore, cannot manage the increasing intricacy of cases of polypharmacy and the fast emergence of new drugs correctly. Hence, a smart, explainable, and data-driven system that can predict and interpret drug-drug interactions dynamically must be created.

3.2 Proposed System

The suggested system, MedPharma AI, presents a framework for AI-powered and interpretable drug-drug interaction (DDI) prediction that aims to get rid of the restrictions that are associated with classical database-based systems. It incorporates Machine Learning (ML), Graph Neural Networks (GNNs), Explainable AI (GNE), and a ChatGPT-based Large Language Model (LLM) in order to predict, visualize, and explain the possible interactions between drugs. The system is running in a preventive and interactive way, thus offering the medical staff trustworthy and easy-to-grasp insights.

3.2.1 System Workflow

The workflow of the proposed system includes the following key points:

1. **Data Integration:** Joins the information of both DDInter and DrugBank data sets, combining the information.
2. **Graph Representation:** A graph model is used in which drugs are the dots (nodes) and their interaction with one another in the form of lines (edges) to enhance relational learning.
3. **Explainable AI (GNE) Module:** Visualises the reason behind the model and identifies the relevant aspects on which the prediction of the interaction relies, thereby making it higher to trust and interpretable.
4. **ChatGPT-driven Conversational Interface:** Strengthens the communication of pharmacists and physicians with the overlay in colloquial language, people-like, individual clarifications of each outcome.
5. **Web Application Interface:** Reveals a user interface that runs on Python and has been developed with Streamlit, MongoDB and dashboards on neo4j, with real-time forecasts possible and representation of drug interactions.

It is proposed that the given system will permanently transform the DDI detection as a conventional one proactive, dynamic, and open-minded approach of the clinical decision-support tool.

3.2.2 Advantages of the Proposed System

- **Predictive Intelligence:** Machine learning models to detect drug to drug interactions.
- **Explainability:** Each predicted interaction is followed by textual pathway explaination through the GNE module.
- **Interactive Communication:** ChatGPT enables natural language interaction making the system user friendly to physicians.
- **Data Integration:** Combines two or more credible datasets (DDInter and DrugBank) to absolutely encompass drug coverage.
- **User Friendly Interface:** Web-based application is easy to access and lucid interaction graphs visualization..
- **Efficiency:** Time and manual work on the verification of complex polypharmacy interactions are lowered, thereby hastening the decision making process and being safe.

3.3 Requirement Specifications

3.3.1 Customer Requirement

In the eyes of a clinician, especially a pharmacologist or a general physician, the most important requirement is a dependable and smart system that would help to spot possible drug-drug interactions (DDIs) both quickly and precisely. The system must have the following features:

- **Analyze multiple prescribed drugs and detect interactions:** The system would inherently check all medications prescribed together, determine interactions, and indicate any mixes that might be unsafe for patients.
- **Present adverse effects, severity, and clinical implications clearly:** The interactions that were detected should be provided with thorough details on ear- marked adverse reactions, their clinical significance, and the precautions that are suggested, thus enabling the healthcare professionals to take well-informed decisions.
- **Explain predictions using XAI modules:** A prediction should always be backed up with an explanation that is made by the explainable AI algorithms that would be spotlighting the reasoning underlying the potential interaction risks.
- **Visualize interaction graphs and textual explanations:** The system would deliver graphical views of drug interaction networks accompanied by textual sum- maries, thus helping users to get a fast understanding of complicated relations.
- **Allow natural language queries via ChatGPT interface:** The users would be able to put forth their questions in simple terms such as “What is the effect of Drug A when combined with Drug B?” and get evidence-based, contextually young responses.
- **Ensure data security, accuracy, transparency, and user-friendliness:** The system would ensure the security of the interactions, the reliability of the predictions, the clarity of the explanations, and the intuitiveness of the system in use for the busy healthcare professionals.

3.3.2 Functional Requirements

The functional requirements of MedPharma AI are summarized in Table 3.1, describing the key modules, their inputs, and the processes they perform.

Table 3.1: Functional Requirements of MedPharma AI

Module	**Input/Trigger**	**Function/Process**
User Authentication	Username, password, email	Register new users, hash passwords, login existing users, secure session management.
Data Integration and Preprocessing	DDInter and DrugBank datasets	Map identifiers, clean and normalize data, convert into graph format for GNN training.
Model Training and Prediction	Preprocessed drug graph, molecular features	Train GNN, apply GNE for interpretability, predict interactions with severity levels.
Explainable AI Visualization	Model predictions and interaction graph	Generate subgraph visualizations, highlight key contributing features, provide textual explanations.
ChatGPT-LangChain Interaction	Natural language queries	Extract drug entities, retrieve predictions and database info, generate context-aware response.
Web Interface	Drug names or textual queries	Provide input forms or chat interface, display predictions, severity levels, and visualizations.

3.3.3 Non-Functional Requirements

Table 3.2 lists the non-functional requirements of MedPharma AI, detailing performance, usability, security, and other operational aspects.

Table 3.2: Non-Functional Requirements of MedPharma AI

Aspect	**Requirement**
Performance	Predictions should be returned within five seconds for standard drug pair queries.
Accuracy	Target prediction accuracy of at least 87% on validation datasets.
Scalability	Support multiple users simultaneously without affecting performance.
Security	Encrypt all communications and protect user data with secure authentication.
Usability	Interface must be intuitive and simple for non-technical healthcare users.
Reliability	Ensure consistent results across repeated predictions.
Maintainability	Modular system architecture to support updates, retraining, and feature addition.
Accessibility	Web-based system accessible across desktop, tablet, and mobile devices.
Documentation	Provide comprehensive user and developer documentation for system use and maintenance.

3.4 Use Cases

The following use case tables describe various user interactions and scenarios within the **MedPharma AI** system.

1. **Access Home Page**

Table 3.3: Use Case Specification: Access Home Page

Use Case ID	MEDPHARMA-UC-001
Use Case Name	Access Home Page
Actors	Researcher, Pharmacist, System User
Basic Flow	(a) The user is directed to MedPharma AI web application. (b) The home page is loaded, and main features are shown by the system such molecule upload, DDI analysis, and AI assistant. (c) The user may explore information about the system or proceed to log in/register.
Alternative Flow	If the user is already authenticated, the system redirects directly to the dashboard.
Pre-conditions	• User has a stable internet connection. • The MedPharma AI platform is online and accessible.

2. **Drug Interaction Prediction**

Table 3.4: Use Case Description: Drug Interaction Prediction

Use Case ID	MEDPHARMA-UC-002
Use Case Name	Drug Interaction Prediction
Actors	Researcher, System
Basic Flow	(a) The researcher logs into the MedPharma AI platform. (b) Uploads two drug names. (c) The system processes molecular data using RDKit and GNN-based models. (d) The system predicts possible drug to drug interactions. (e) The prediction and interaction scores are displayed to the user.
Alternative Flow	If the molecular format is invalid, the system requests re-upload with a valid file type.
Pre-conditions	• The researcher has valid login credentials. • The system's AI models and databases are operational.

3. **Molecular Visualization and Explanation**

Table 3.5: Use Case Description: Molecular Visualization and Explanation

Use Case ID	MEDPHARMA-UC-003
Use Case Name	Molecular Visualization and AI Explanation
Actors	Pharmacist, Researcher, System
Basic Flow	(a) The user selects a drug molecule from the dashboard. (b) The system visualizes its 2D or 3D molecular structure using RDKit. (c) The system displays predicted molecular interactions via graph representation. (d) A language model (LLM) generates an explanation for the observed interactions. (e) The user reviews visualizations and explanations for decision support.
Alternative Flow	If data retrieval fails, the system displays a retry prompt.
Pre-conditions	• User is logged in. • Interaction prediction has been completed. • LLM module is active and connected.

4. **Knowledge Graph Integration and Analysis**

Table 3.6: Use Case Description: Knowledge Graph Integration and Analysis

Use Case ID	MEDPHARMA-UC-004
Use Case Name	Knowledge Graph Integration and Analysis
Actors	System, Researcher
Basic Flow	(a) The system retrieves molecular and interaction data from the database. (b) It builds a graph-based representation using Neo4j. (c) The researcher queries or explores the relationships between drugs. (d) The system visualizes the graph with links and properties.
Alternative Flow	If the database connection fails, the system retries or displays an error.
Pre-conditions	• Valid database connection to Neo4j and MongoDB. • Processed molecular data available for analysis.

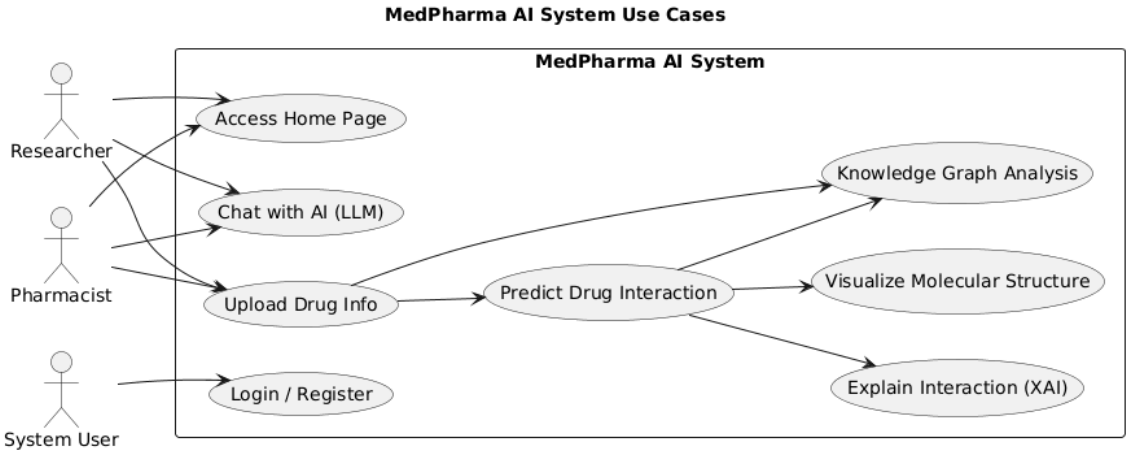


Figure 3.1: Use Case Diagram for MedPharma AI System

Summary

Chapter 3 forms the basis of the MedPharma AI system by unambiguously stating its requirements and use cases. The chapter started with the analysis of the current DDI systems, pointing out the limitations in terms of static data, no predictive power and low explainability. Then it showed the new system with its AI-powered workflow, combining several datasets, GNN predictions, explainable AI visualizations, and ChatGPT-driven conversational interface as the main points.

Chapter 4

Design

4.1 System Design

The MedPharma AI design stage consists of a theoretical approach to a structured, functional, and efficient system that can predict, explain, and visualize drug-drug interactions (DDIs). The system has emphasized modularity, scalability and interpretability to assure technical strength and medical stability. MedPharma AI plays upon the three technologies: Graph Neural Networks (GNNs). Prediction, explainable AI (XAI) to interpretability, and Large Language Models. There has been a dominance of technologies in a single framework that allows the MedPharma AI to provide a data-driven, smart, and interactive solution to determine possible interaction of adverse drugs reactions, where drugs are administered concomitantly. The system takes a modular model comprising of interconnected layers that execute such duties as preprocessing of the data, model prediction, generation of explanations, and user interaction. The interaction between the parts is carried out via pre- data pipelines which are defined, it can be altered or updated by individual modules independently.

4.2 System Architecture

The architecture of the MedPharma AI is designed as a hybrid multi-layered design that. combines AI prediction, explainability and natural language interaction. The principal parts are:

1. **Input Layer:** The system accepts drugs names as input for processing.
2. **Preprocessing Layer:** The system uses RDKIT library to convert drugs input into structured molecular graphs.
3. **GNN Layer:** This layer based on the graph of drug-drug interactions predicts them.

4. **Explainable AI Layer:** Use Graph Neural Explainer (GNE) to identify the important pathway.
5. **LLM Layer:** Rely on ChatGPT via LangChain for the purpose of natural language interpretation.
6. **Database Layer:** MongoDB for structured data, Neo4j for relational graphs are the storages.
7. **Interface Layer:** The user graphical options were from Streamlit with ease and interaction.

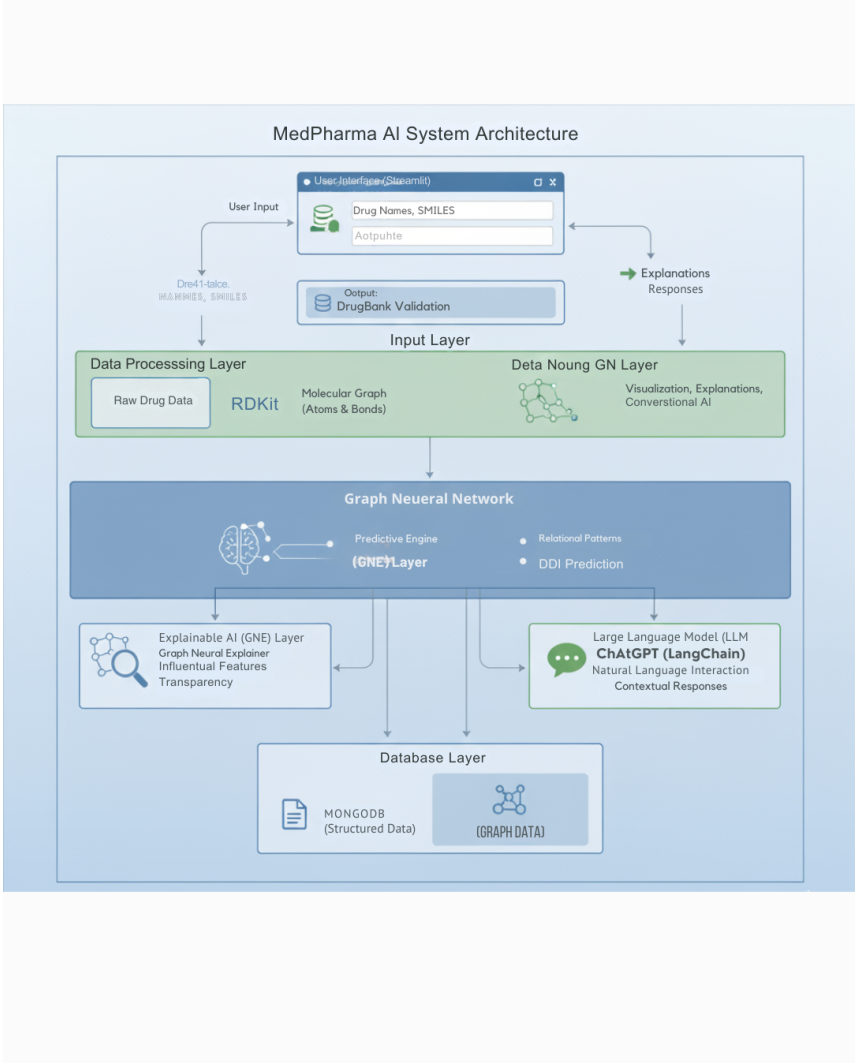


Figure 4.1: System Architecture of MedPharma AI

4.3 Design Constraints

The system architecture has to deal with several constraints:

1. **Hardware Limitations:** Due to the high computation demand, GPU resources are the only option for GNN training.
2. **Software Limitations:** The implementation is based on the combination of Python, PyTorch Geometric, RD-Kit, LangChain, Streamlit, MongoDB, and Neo4j.
3. **Data Limitations:** The datasets lack information about the patients' dosages and concentrations.
4. **Performance Limitations:** To be efficient, graph computations go through the process of being batch-processed and normalized.
5. **Security Limitations:** Sensitive information is protected through encryption in queries and logs; proper authentication is required for accessing the database.

Figure 4.2: Design Constraints of MedPharma AI

4.4 Design Methodology

The design methodology incorporates an AI pipeline structured into modules for being efficient and interpretable:

1. **Data Collection:** Obtain data related to drugs from the DDInter and DrugBank.
2. **Preprocessing:** Transform SMILES into graphs and standardize the features.
3. **Model Training:** The GNN is trained to detect the structure-related dependencies between drug pairs.
4. **Explainability:** GNNExplainer is applied for the model's transparency.
5. **LLM Integration:** ChatGPT is used for the natural language explanations.
6. **Deployment:** Streamlit, along with MongoDB and Neo4j are the tools used to integrate the modules together.

Figure 4.3: Design Methodology of MedPharma AI

4.5 High-Level Design

4.5.1 Flowchart

The workflow of the system is depicted in the diagram:

1. The user inputs the drug names
2. Data is verified and then converted to a graph type.
3. The GNN gives a prediction about the probability of interaction.
4. The explainability module uncovers the pathway that had the most impact.
5. The results are stored in MongoDB and can be visualized via Neo4j.
6. The Large Language Model (LLM) provides a captivating explanation.

4.5.2 Activity Diagram

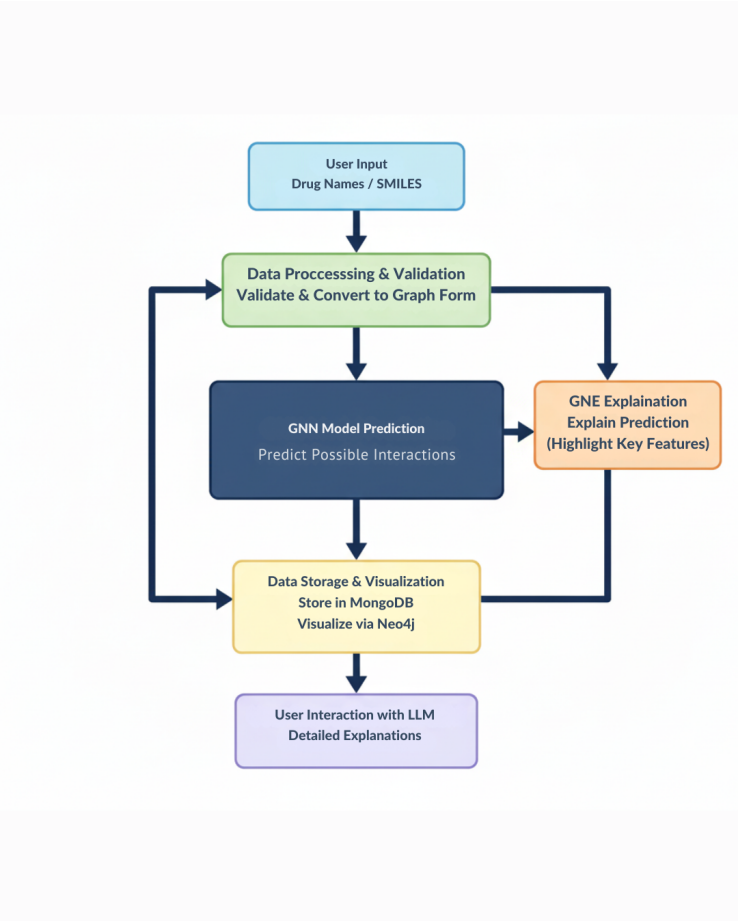


Figure 4.4: Activity Diagram of MedPharma AI

4.5.3 Sequence Diagram

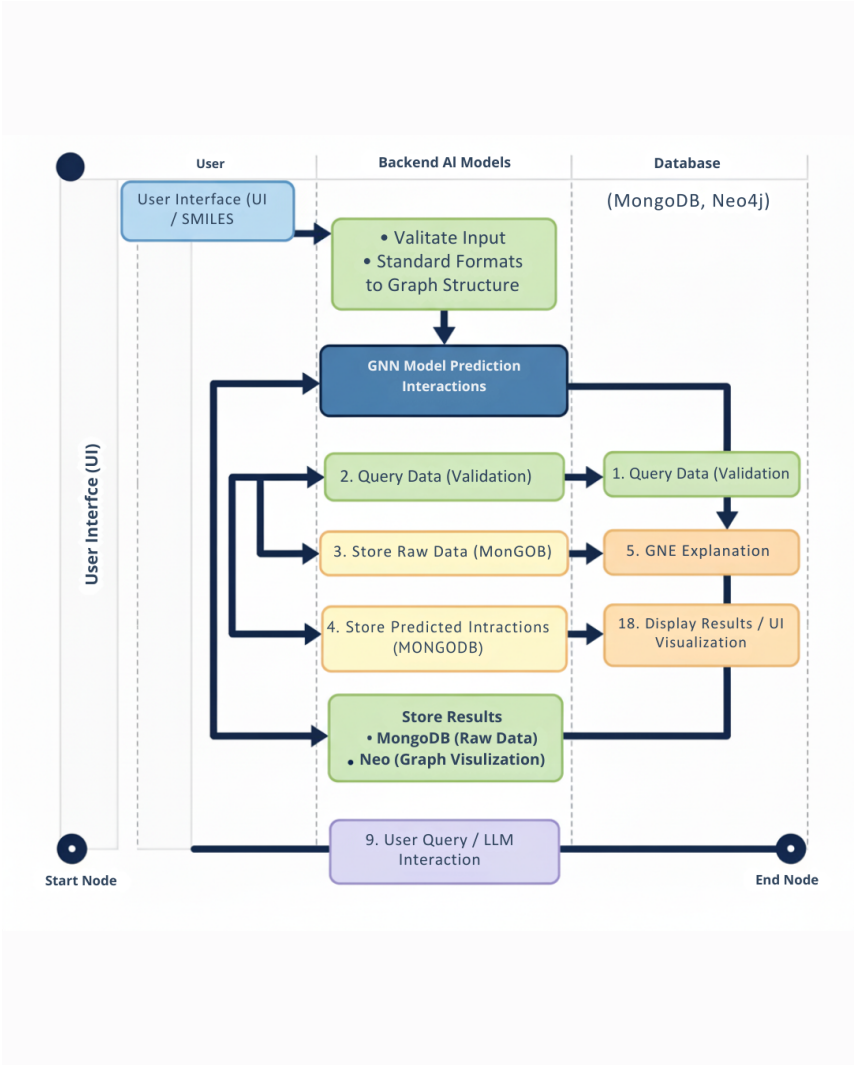


Figure 4.5: Sequence Diagram of MedPharma AI

4.6 Low-Level Design

The low-level design indicates the interior responsibilities of every module:

- **Preprocessing Module:** Parsing of SMILES, the building of graphs, and extraction of features.
- **Prediction Module:** Processing through GNN and scoring by probability.
- **Explainability Module:** GNNExplainer gives the outputs of the interpretable subgraphs.
- **Conversation Module:** Interaction and explanations based on LLM.

- **Database Module:** For structured storage, MongoDB is used; Neo4j for graph traversal.
- **Interface Module:** The UI of Streamlit is for visualization and query handling.

4.7 Database Design

MedPharma AI employs a mixed database architecture:

- **MongoDB:** Keeps track of medicine titles, SMILES notation, forecasts, and time stamps.
- **Neo4j:** Maintains drug interactions and visual representations of the graph.

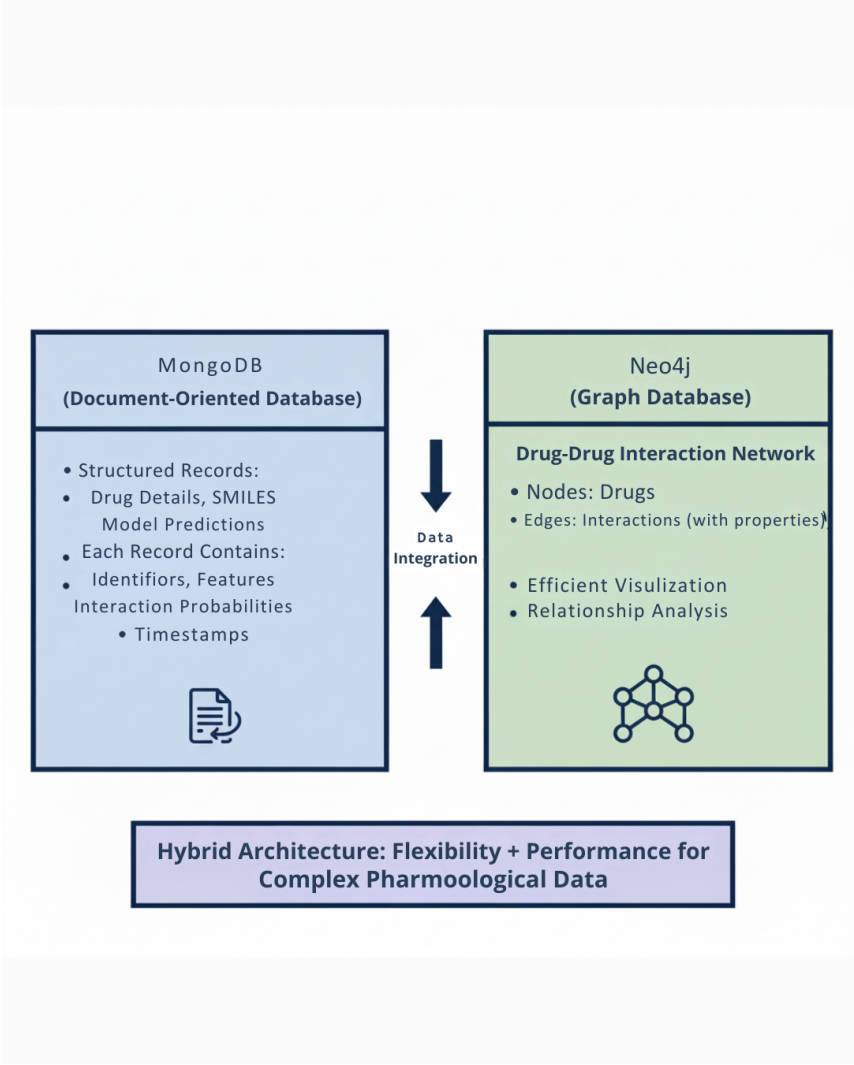


Figure 4.6: Database Design of MedPharma AI

4.8 External Interfaces

The system components are linked through external interfaces:

- **User Interface:** Streamlit dashboard for user interaction and data visualization.
- **Database Interface:** API links to MongoDB and Neo4j.
- **LLM Interface:** ChatGPT incorporation through LangChain middleware.

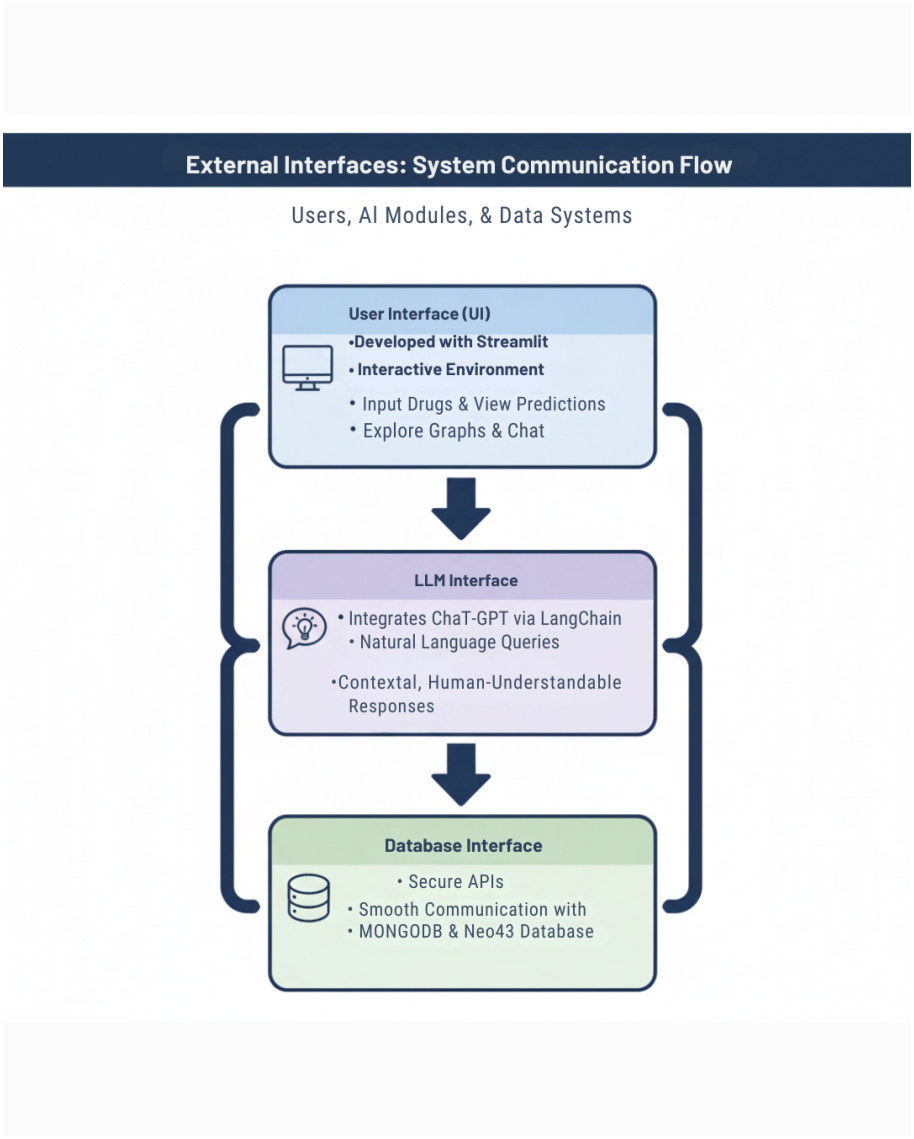


Figure 4.7: External Interfaces of MedPharma AI

Summary

The design of MedPharma AI has been discussed in this chapter, which includes architecture, constraints, design methodology, high- and low-level designs, and database schema. The modular system of the application is the main feature that guarantees support for clinical decision making, and it is also highly interpretable and expandable. The following chapter deals with implementation and experiments with results obtained.

Chapter 5

System Implementation

5.1 System Architecture

MedPharma AI's architecture is outfitted with the best technology to combine AI models, pharmaceutical datasets, and a user-friendly web interface without any disruption. It is built in a modular way thus, making it easier for the different parts of the system to be efficient in their predictions, be interpretable and interact with one another.

The system has several important layers which are:

1. **Data Layer:** It sources data from DDInter and DrugBank and integrates it, preprocesses it, and performs normalization, mapping, and deduplication.
2. **Machine Learning Layer:** A Graph Neural Network (GNN) is implemented to predict drug-drug interactions based on the molecular and pharmacological features represented as graph nodes and edges.
3. **Explainable AI Layer:** It uses a Graph Neural Explainer (GNE) to interpret the predictions made by the model and to point out the features or nodes that had the most impact in helping that specific prediction.
4. **Interaction Layer (LLM):** Through LangChain, it links the ChatGPT model which allows natural and interactive communication with the users.
5. **Web Interface Layer:** The users can input drug names, view predictions, and analyze model outputs through an explanation on a Streamlit-based platform.

5.2 Functionality of the Components

- **Data Preprocessing Component:** Cleans, integrates, and converts drug datasets into graph structures. Drugs are nodes, interactions are edges.

- **GNN Model Component:** Learns drug representations from graph data and predicts interaction probability and severity (mild, moderate, severe).
- **Explainability Component (GNE):** Identifies subgraphs and molecular features responsible for predictions, improving transparency.
- **LLM Component:** Processes user queries, retrieves model predictions, and returns natural language explanations via ChatGPT.
- **Web Application Component:** Manages user interaction, displays results, visualizations, and explanations securely.

5.3 Communication Between Components

Communication is modular and efficient between layers:

- Data Layer → Machine Learning Layer: Preprocessed structured datasets are passed.
- Machine Learning Layer → Explainable AI Layer: Predictions are provided for interpretation.
- Explainable AI Layer → Interaction Layer (LLM): Results that are interpretable are sent for natural language explanation.
- Web Interface Layer → Backend APIs: Predictions and visualizations are displayed to users through Streamlit.

5.4 Tools and Technologies Used

Table 5.1: Tools and Technologies Used in MedPharma AI

Category	**Technology Used**
Programming Languages	Python
Frameworks	VSCode, LangChain
Libraries	PyTorch, PyTorch Geometric, TensorFlow, NetworkX, Matplotlib
Models	Graph Neural Network (GNN), Graph Neural Explainer (GNE), ChatGPT
Datasets	DDInter, DrugBank
Frontend Tools	Streamlit
Database	MongoDB, Neo4j
Hardware	NVIDIA RTX 2060 GPU (8 GB), Intel i7 Processor, 16 GB RAM
Operating System	Windows 11 / Ubuntu 22.04

5.5 Development Environment

Python 3.10 was used along with VSCode for backend and model training to develop the system. Web app was made on Streamlit and LangChain along with ChatGPT integration was used for interactive queries. Matplotlib and NetworkX were used for visualization and debugging. The development workstations comprised an NVIDIA RTX 2060 GPU, an Intel Core i7 processor, and 16 GB RAM.

5.6 Processing Algorithms

1. **Data Processing Algorithm**
    - Gather data from DDInter and DrugBank sources.
    - Process datasets by cleaning, normalizing, and merging them.
    - Create a graph $G = (V, E)$ where V represents drugs and E represents their interactions.
2. **Model Training Algorithm (GNN)**
    - Graph G is the input.
    - Implement graph convolutional layers to acquire node embeddings.
    - Train the model with the Adam optimizer and binary cross-entropy loss.
    - Return: Probability of interaction and its severity predicted.
3. **Explainability Algorithm (GNE)**
    - Trained GNN model and drug pair are the input.
    - Locate subgraphs and attributes that influence the prediction.
    - Produce a visualization and a textual explanation.
4. **LLM Interaction Logic**
    - User query via web interface is the input.
    - Drug names are extracted using LangChain.
    - GNN predictions are retrieved and a context-aware response is generated via ChatGPT.

5.7 Application Access Security

The safe opening of MedPharma AI is very important to keep safe medical and drug interaction data which are sensitive. In order to protect the accounts of users and guarantee their privacy, the system has put in place various security measures at different levels:

- **User Authentication:** Prior to system access, users must first go through the registration and login process. Passwords are hashed with industry-standard algorithms and are kept in a secure manner to avoid unauthorized access.
- **Session Management:** The system uses secure tokens to encrypt active sessions, which will automatically expire in case of inactivity or when the user logs out, thus minimizing the threat of session hijacking.
- **Data Protection:** User data and interaction data considered sensitive are encrypted at all times (both at rest and in transit) through the use of TLS/SSL protocols, which means that data cannot be intercepted or altered.
- **Role-based Access Control:** Users are given different levels of access according to their roles (e.g., admin, healthcare professional). Predictive models and sensitive results are only accessible to the authorized users, thus applying the least privilege principle.
- **Audit and Monitoring:** System logs keep records of user activity, login attempts, and administrative changes. This allows monitoring of possible suspicious activities as well as compliance with security best practices.

5.8 Database Security

The MedPharma AI system makes use of secure databases (MongoDB and Neo4j) to hold orderly drug facts, interactions, and user passwords. Different methods are employed for securing the databases, and one of the methods is:

- **Encrypted Storage:** The most confidential information, like credentials and medical records, is encrypted at the database level with the goal of avoiding unauthorized access.
- **Access Control:** Administrative rights are limited to only those users authorized; thus, the number of persons who can alter the database is small, which in turn decreases the probability of unintentional or ill-intentioned changes.
- **Data Validation:** The combination of input validation and sanitation is a must in order to block injection attacks and to keep the database entire.
- **Backup and Recovery:** Regular automated backups guarantee that data can be restored in case of hardware failure, corruption, or accidental deletion.
- **Monitoring and Alerts:** Database activity is constantly monitored, and alerts are issued for unusual access patterns or failed login attempts, which allows for the proactive managing of security.

5.9 Graphical User Interface (GUI)

The MedPharma AI system offers a highly intuitive user interface that is extremely easy to use and is primarily aimed at the healthcare professionals. The GUI allows for the effortless transition among the different functions, the straightforward input of data, and the easy-to-understand presentation of forecasts and justifications. User interfaces have been devised with the consideration of being accessible, transparent, and interactive, thus enabling the non-technical users to tap into the AI power.

Figure 5.1: MedPharma AI Home GUI: Home page offers an overview of the app, and it includes access to the modules of the app

Figure 5.2: About Us Page:Shows details on the developers.

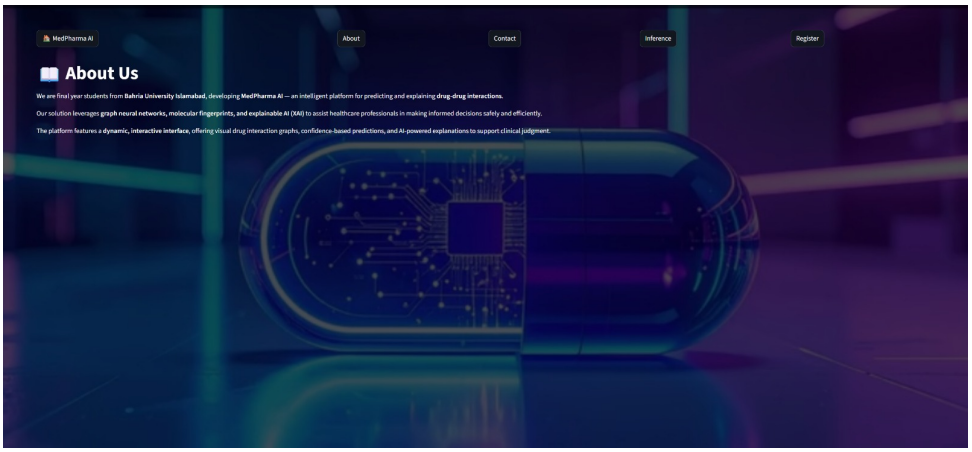


Figure 5.3: Contact Us Page: This offers a medium through which users can give comments on the site, request support, or report problems.

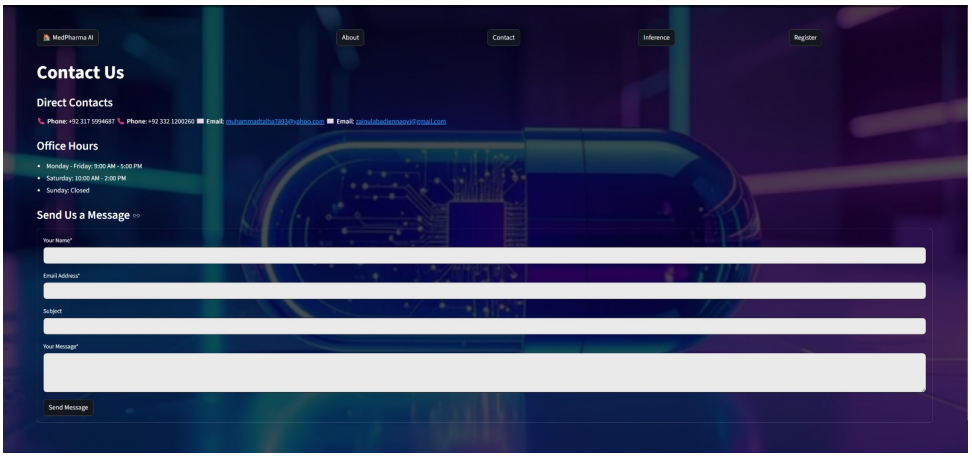


Figure 5.4: Authentication Page: It assures the accessibility of the system with a new user option and registration.

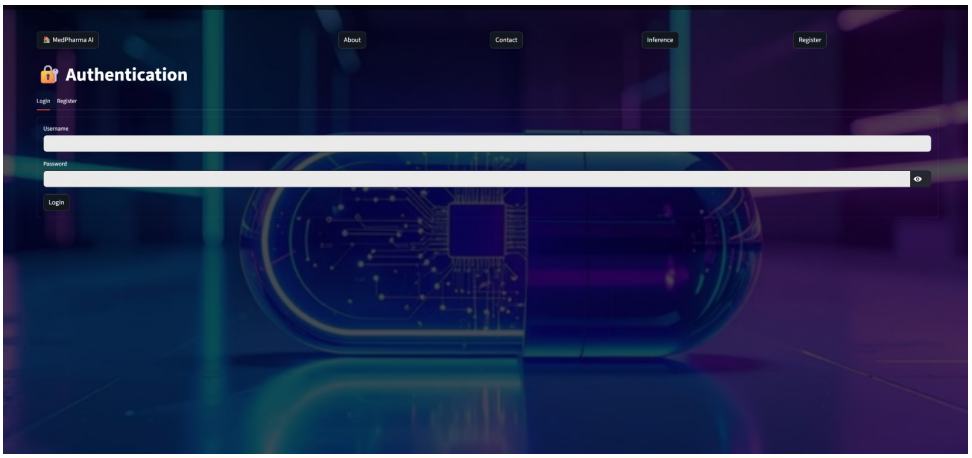


Figure 5.5: Login Page: Provides secure login functionality for registered users with multi-factor authentication support.

Figure 5.6: Enter Drug Name for Prediction: Allows users to input drug names, select interaction parameters, and initiate the prediction process.

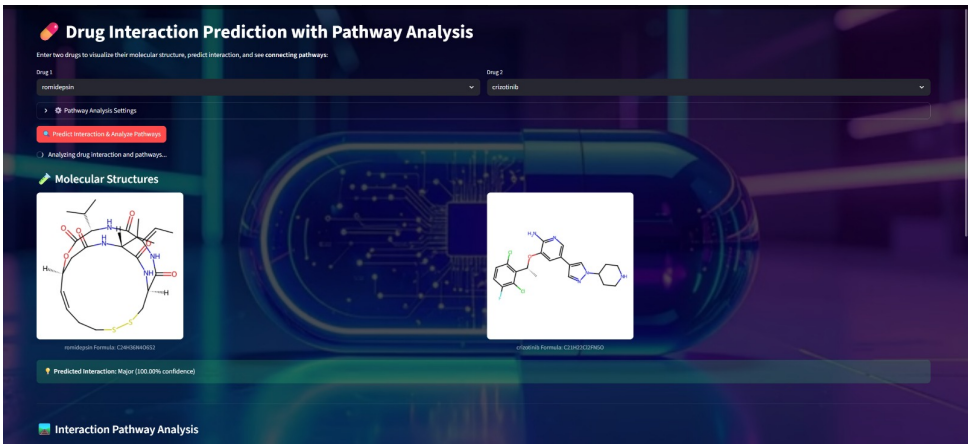
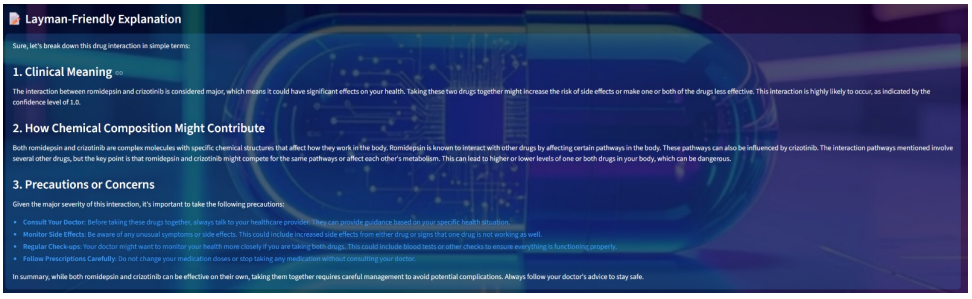


Figure 5.7: Analysis of Results: Displays predicted interaction result and confidence score .

Figure 5.8: Result Interpretation and Visualization: Provides detailed explanations of model predictions using Graph Neural Explainer visualizations, highlighting important pathways.



Summary

The specific aspects of the MedPharma AI system implementation were given in detail in Chapter 5, with special attention to the security of the application, the integrity of the database, and the use of the system by the users. The system guarantees access security by means of user authentication, session management, data protection, role-based access control, and activity auditing thus permitting only authorized users to access the secure functionalities and data. The database is secured by using an encrypted form of storage, limiting access only to authorized personnel, validating inputs, performing regular backups, and having a recovery process in place, and also monitoring the database all the time with alerts in place, thus providing data integrity and preventing unauthorized or malicious activities. Moreover, the graphical user interface (GUI) is a platform for healthcare professionals that is very straightforward and easy to use, allowing them to easily navigate through the application (drug input, prediction analysis, visualization of results, and even understanding through explainable AI features). To sum up, the implementations described in this chapter show that MedPharma AI is a secure, user-friendly, and reliable platform for predicting and interpreting drug-drug interactions, thus upholding the reliability of the system and the safety of sensitive data in both clinical and research settings.

Chapter 6

System Testing and Evaluation

6.1 Graphical User Interface Testing

MedPharmaAI's GUI was evaluated in terms of its ability to provide an intuitive, responsive, and visually consistent experience. Testing was done on accessibility, layout uniformity, input interactions, and quality of chemical images.

People from the pharmaceutical and data science sectors worked with the modules of drug upload, similarity prediction, explanation generation, and visualization. Input was gathered to enhance ease of use.

Table 6.1: User Feedback from GUI Testing

Participant	Experience	Suggestions for Improvement
Dr. Junaid	Interface well-organized and interactive. Drug upload and visualization were intuitive.	Add option to visualize both molecular structures simultaneously.
Faisal	Appreciated minimalistic layout and real-time results.	Include tooltips or help messages for new users.
Dr. Saman	Smooth navigation; explanation section informative.	Add dark mode for better visibility during extended use.

Summary of GUI Testing

The graphical user interface is very easy to use and nice to look at. It has been proposed to add small features such as tooltips, dark mode, and better molecule comparison views.

6.2 Usability Testing

Usability testing assessed the extent to which users were able to interact with MedPharmaAI and understand its outputs. The participants were doctors, medical students, and AI researchers.

The following tasks were performed:

- Drug names were uploaded.
- Molecular structures were visualized.
- Interaction predictions were generated.
- LangChain-generated explanations were interpreted.

Table 6.2: Usability Framework Evaluation

Framework Aspect	**Evaluation**	**Rating (1–5)**
Learnability	Easy to learn and understand	5
Efficiency	Tasks completed quickly with minimal steps	4
Memorability	Interface and actions easy to recall	4
Errors	Few operational errors encountered	5
Satisfaction	Users were highly satisfied	5

Summary of Usability Testing

The system showed excellent usability and hardly any user confusion. The combination of interaction design and interpretability of AI outputs makes it appropriate for research and teaching.

6.3 Compatibility Testing

The testing of the system took place on various devices, operating systems, and browsers:

- **Devices:** Laptops, desktops, GPU workstations
- **Operating Systems:** Windows 10, Ubuntu 22.04
- **Browsers:** Google Chrome, Microsoft Edge, Mozilla Firefox

Table 6.3: Compatibility Testing Results

Platform	**Status**	**Comments**
Windows 10 – Chrome	Passed	Fully functional and responsive
Windows 10 – Edge	Passed	Minor delay in molecule rendering
Ubuntu – Firefox	Passed	Smooth visualization and inference
Streamlit Cloud	Passed	Stable deployment and access
Local GPU Server	Passed	Fast inference and graph generation

Summary of Compatibility Testing

MedPharmaAI disclosed fantastic cross-platform compatibility. The performance has been slightly varied due to the rendering speeds of the different browsers, however, no functionality issues were faced.

6.4 Exception Handling

In one system test, the tests checked the system's ability to handle output gracefully while under different stress conditions.

Table 6.4: Exception Handling Test Results

Test Scenario	Status	Comments
Invalid Drug SMILES Input	Passed	Error message displayed; processing prevented
Network Connectivity Loss	Passed	User prompted to reconnect; no crash
Missing Drug Name Input	Passed	Alert displayed for valid input
Model Timeout during Inference	Failed	Minor crash under high latency; optimization needed
Database Access Denied	Passed	Exception handled with message to user

Summary of Exception Handling

In many cases, exception handling should be a factor in the preservation of system stability. Timeouts in the current model during heavy load conditions need improvement.

6.5 Load Testing

Emulated a multitude of concurrent users for performance and scalability assessment.

Table 6.5: Load Testing Results

User Load	Concurrent Users	Average Response Time	System Response
Low Load	10–20	1–2 seconds	Normal operation
Moderate Load	50–100	3–4 seconds	Slight delay in prediction output

Summary of Load Testing

The system was effective under moderate load conditions. Inference time was longer with high loads, indicating resource allocation or distributed deployment optimization.

6.6 Security Testing

User data and model outputs were protected by security testing, which encompassed the following aspects:

- **Authentication:** logging in through JWT
- **Authorization:** access control based on roles
- **Data Security:** encryption via HTTPS
- **Session Management:** timeout and secure log-off

Table 6.6: Security Testing of MedPharmaAI System

Security Aspect	**Details**
Authentication	Secure token-based login sessions via JWT
Authorization	Role-based access control prevents unauthorized module access
Data Security	HTTPS encryption protects data in transit
Session Management	Secure session tracking and automatic timeout

Summary of Security Testing

This conclusion was reached on the basis of the interpenetration of unexpected phenomena, ensuring that securing the system was safe and reliable.

6.7 Test Cases

Test Case: Access Home Page

Table 6.7: Test Case - Access Home Page

Test Case ID	MEDPHARMA-TC-001
Function to be Tested	Home Page display
Initial State	Application deployed and running
Test Setup	User opens system URL
Input	Launch system
Expected Output	Home page with navigation menu, “Predict”, “Explain”, “About” buttons
Actual Output	As expected
Status	Pass

Table 6.8: Test Case - Drug Upload and Prediction

Test Case ID	MEDPHARMA-TC-002
Function to be Tested	Upload drug SMILES or name and predict interactions
Initial State	User logged in
Test Setup	Navigate to prediction module
Input	Enter two valid drugs or SMILES codes
Expected Output	Interaction prediction and molecular graphs
Actual Output	As expected
Status	Pass

Test Case: Drug Upload and Prediction

Test Case: Generate Explanation

Table 6.9: Test Case - Generate Explanation

Test Case ID	MEDPHARMA-TC-003
Function to be Tested	Generate natural-language explanation
Initial State	Prediction completed
Test Setup	Click “Explain Interaction”
Input	Select interaction pair
Expected Output	Human-readable explanation generated
Actual Output	As expected
Status	Pass

Test Case: Visualization of Molecules

Table 6.10: Test Case - Visualization of Molecules

Test Case ID	MEDPHARMA-TC-004
Function to be Tested	Display molecular structures and interaction graph
Initial State	Valid drug inputs uploaded
Test Setup	Click “Show Molecule Graph”
Input	Trigger visualization
Expected Output	2D molecular structure and graph correctly displayed
Actual Output	As expected
Status	Pass

Summary

The evaluation and testing of MedPharmaAI have been discussed in Chapter 6. The processes of GUI, usability, compatibility, exception handling, load, and security testing were confirming the system’s efficiency, accuracy, and stability. There were slight problems

with the application during high load situations, but otherwise all the modules worked as anticipated. The application is secure, user-friendly, and able to deliver trustworthy drug–drug interaction predictions with explainable outputs, thereby becoming a powerful tool for pharmaceutical research and decision-making support.

Chapter 7

Conclusion

The MedPharma AI system is one of the significant steps along the path to the use of AI in the sphere of pharmaceutical research, as well as informatics in healthcare. The platform is a deep-learning, cheminformatics and smart-data management framework that provides an end to end solution to drug-drug interactions prediction. The system is reliable and scalable because it uses sophisticated technologies such as RDKit to process molecular structures, Neo4j to visualize knowledge graphs, and MongoDB to store data and make it secure and efficient. This combined effort by both GNNs and predictive algorithms has caused MedPharma AI to be able not only to screen the chemical properties but also to identify the most probable molecular interactions as well as to guide researchers to the most promising drug candidates. The interactive interface of Streamlit transforms the complicated AI processes into the easy and user-friendly version. The system also uses smart reasoning by use of large language models to give explanations based on situations and direct the users on how to interpret the behavior and suggestions of the drug. MedPharma AI in a word is an automated, explicable, and user-friendly platform, which bridges AI and pharmaceutical sciences. It saves time in the drug analysis, minimizes the occurrence of human error, and enhances improved decision-making in clinical and research processes since it supports researchers, pharmacists and medical practitioners.

7.1 Future Work

Although MedPharma AI is an excellent platform for pharmaceutical analysis driven by AI, its full potential still needs some improvements in the future. Among the proposed ideas are:

- **Integration of Real-World Clinical Data:** One of the key developments will be the introduction of electronic health records (EHRs) and clinical trial data to tailor drug

interaction predictions to individual patients and thus, enhance clinical relevance.

- **AI-Based Drug Recommendation System:** The new versions will contain a drug recommendation engine that will recommend the most suitable drug combinations and treatment plans based on the properties of the drug molecules and patient-related factors.
- **Enhanced Molecular Visualization:** The application can be augmented with 3D molecular rendering and similarity analysis to share with researchers and pharmacists deeper chemical insights than initially foreseen.
- **Reinforcement Learning for Drug Optimization:** MedPharma AI can be powered through incorporating reinforcement learning models capable of suggesting structural changes in the event of molecules to enhance the therapeutic effect or minimize side effects.
- **Deployment as a Cloud-Based API:** By positioning MedPharma AI to research institutes and healthcare organizations, it can be deployed as a cloud service with secure authentication and API endpoints for accessibility.

MedPharma is planning to stay on its evolutionary path and hence becoming an intelligent pharmaceutical partner that will always be available for drug discovery, safety evaluation, and precision medicine. The reduction in the time and cost of pharmaceutical research along with the improvement of the quality and safety of the medications available for the patients is the ultimate goal to be achieved.

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Medpharma AI: 3:20 pm

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