

PharmaGraph: Safe Drug Interaction Intelligence using Knowledge Graphs & LLMs



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Agenda

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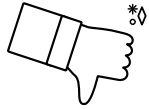
I Problem Statement



Problem Statement



Some drugs can be **dangerous** when taken **together**.






Doctors **don't** always have quick tools to check for this.

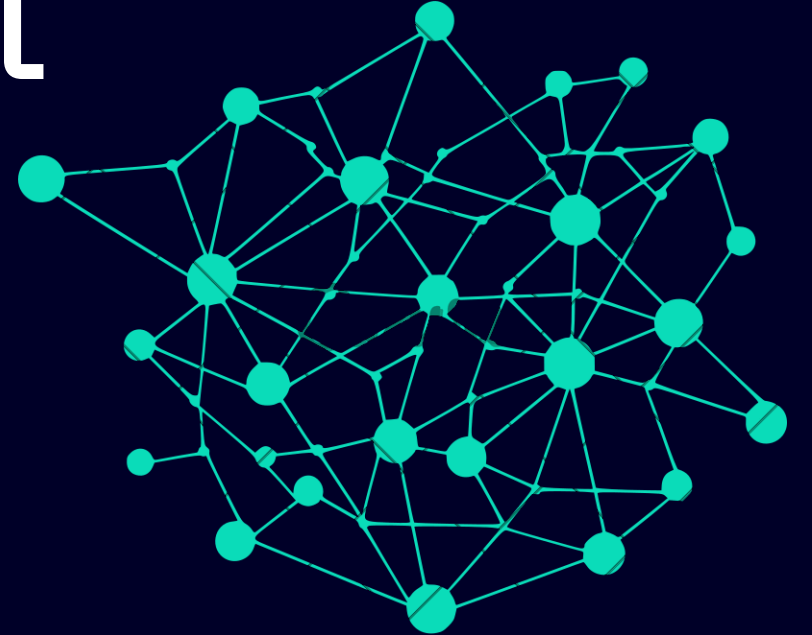


We aim to build an **AI system** that answers **drug interaction** questions clearly, using trusted medical data.

System Overview

- **PharmaGraph** is a hybrid AI system.
- It processes natural language questions.
- Combines:
 -  → **Named Entity Recognition**
 -  → **Knowledge Graph search**
 -  → **LLM-based explanation or recommendation.**

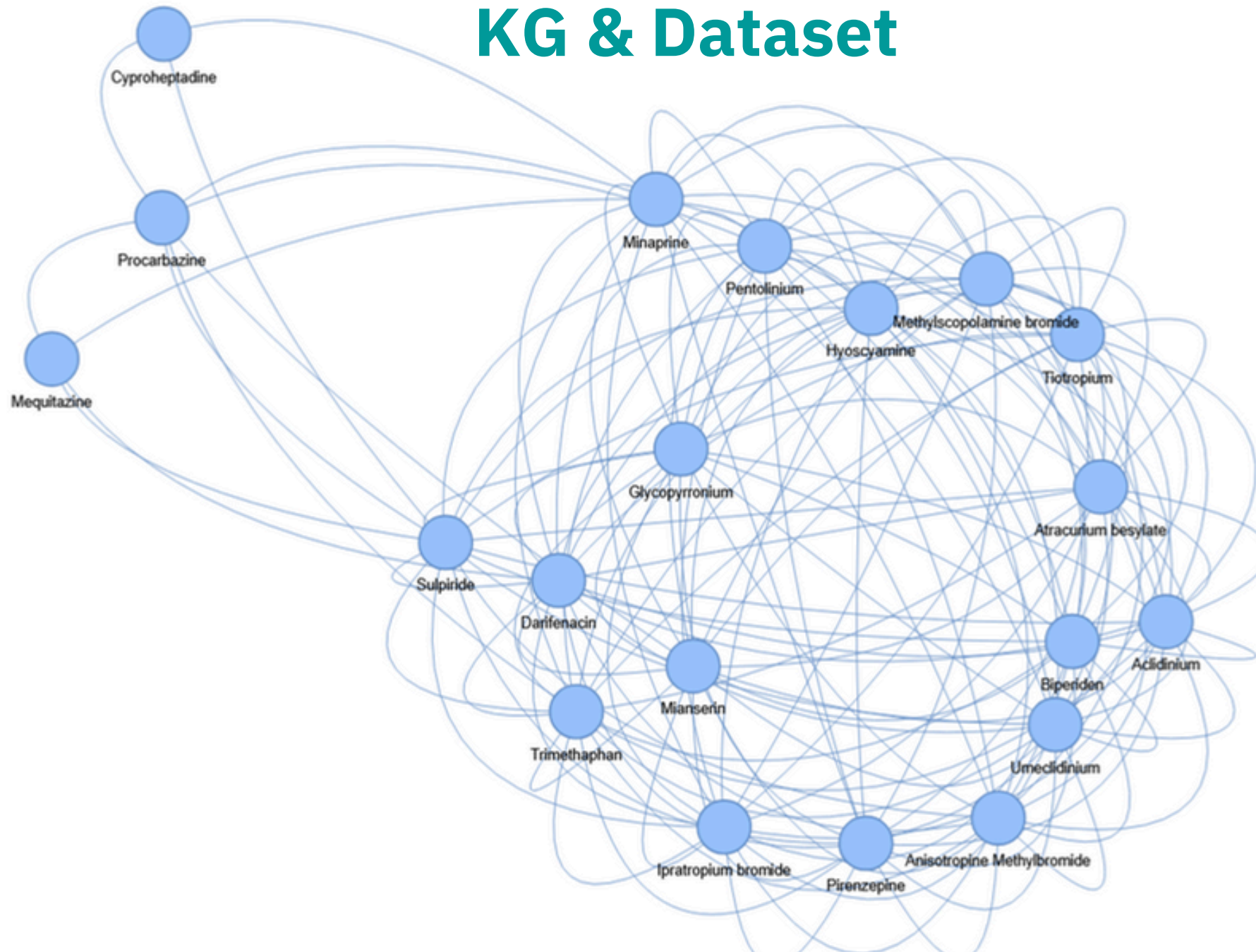
| Knowledge Graph & Dataset



KG & Dataset

- Dataset Source: **DrugBank**
- Files Used:
 - Drug-drug interactions (**DrugBank_known_ddi.txt**)
 - Approved drug details (**Approved_drug_Information.txt**)
 - Interaction descriptions (**Interaction_information.csv**)
- Graph Construction:
 - Each node = **Drug**
 - Each edge = **Known interaction** (labeled by severity/class)
- Tool Used: **NetworkX** (Python)
- Purpose: Build a searchable **graph** of drug **interactions** for clinical reasoning

KG & Dataset



Entity Recognition & Normalization

We use **SciSpaCy** (BC5CDR model) to extract:

 → **Drug names**

 → **Conditions**

Normalized to DrugBank IDs via synonym mapping.
Ensures query compatibility with KG nodes.

| Search Strategies in the KG



Direct RAG (Direct Edge Search)

- ✔ Checks if two drugs have a **direct** interaction in the graph
 - Simple **1-hop** check between nodes
 - Very fast and reliable
- ✔ Accurate for known interactions
- ✗ Cannot detect indirect links

For Undirected Graph

Light RAG

First checks for a **direct interaction**

- Then checks for **indirect links** via shared neighbors (1-hop path)
- Adds more context without increasing complexity

✓ **Lightweight** but smarter than direct lookup

✗ Misses **long** paths in the graph

(1-Hop Expansion)

GraphRAG

Finds the **shortest path** between two drugs

- Can explain the path step-by-step (**2 or 3 hops**)
- Ideal for complex, **multi-step** interactions



✓ Deep graph reasoning

✗ Slower than light methods

Multi-Hop Reasoning

RQ-RAG (Refined Query RAG)

LLM first **rephrases** or clarifies unclear user input

- Then apply the **graph search** method(GraphRAG)
- Good for handling messy, unclear, or long questions
-  Flexible and context-aware
-  Adds an extra LLM step → slower

Query Refinement

LightGraphRAG (Combined Method – Ours)

Combines the best of Light RAG + GraphRAG

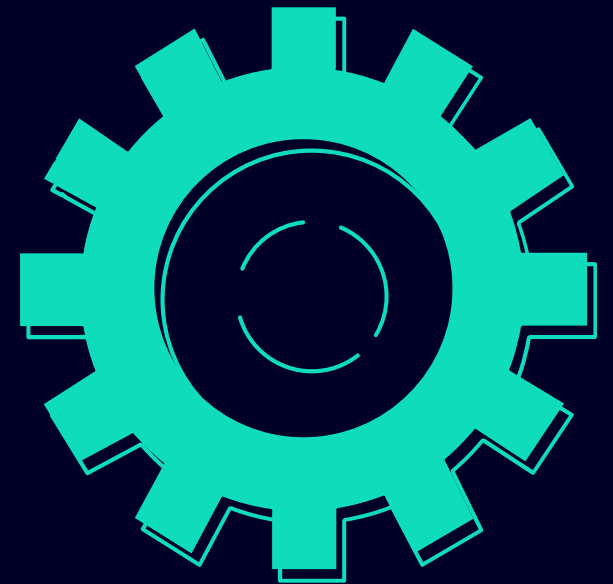
- Handles **direct edges**, **1-hop neighbors**, and **short paths**
- Used in **all 4 functionalities** in PharmaGraph

✓ **Best** performance (F1, Precision, Coverage)

✓ Unified and reliable across query types

Hybrid Strategy

| Core Functionalities of PharmaGraph




Two-Drug Check

- Checks if two drugs interact
- Returns a clear yes/no with reasoning

Describe your situation involving two drugs:

I'm taking Hyoscyamine and Pirenzepine together. Is it safe?

Analyze

 **Response:**

Based on the provided background knowledge:

- Hyoscyamine and Pirenzepine should not be taken together due to a potential for increased risk or severity of adverse effects.

Show Knowledge Graph Raw Result ^

- **Hyoscyamine and Pirenzepine:** Direct interaction: The risk or severity of adverse effects can be increased when #Drug1 is combined with #Drug2.


Full Interaction List

- Finds all drugs that interact with a given drug
- Helps assess its interaction profile


Enter the drug name:

Umeclidinium

Find Interactions

 **Result:**

- Umeclidinium and Abiraterone: Serum concentration of Abiraterone increases.
- Umeclidinium and Acridinium: Umeclidinium may enhance Acridinium's anticholinergic effects.
- Umeclidinium and Alfentanil: Risk or severity of side effects may be heightened when combined.
- Umeclidinium and Ambenonium: Therapeutic efficacy of Ambenonium can be diminished when used alongside Umeclidinium.
- Umeclidinium and Amiodarone: Metabolism of Amiodarone can be suppressed when combined with Umeclidinium.
- Umeclidinium and Amoxapine: Therapeutic efficacy of Amoxapine can be compromised when combined with Umeclidinium.
- Umeclidinium and Anisotropic Methylbromide: Umeclidinium may enhance Anisotropic Methylbromide's anticholinergic effects.
- Umeclidinium and Atomoxetine: Metabolism of Atomoxetine can be impaired when combined with Umeclidinium.
- Umeclidinium and Atracurium besylate: Umeclidinium may enhance Atracurium besylate's anticholinergic effects.
- Umeclidinium and Atropine: Umeclidinium may enhance Atropine's anticholinergic effects.

Show Knowledge Graph Raw Result 

List Check

- "Is Drug X safe with [Drug A, B, C]?"
- Checks one drug against a list of others
- Flags any unsafe combinations


Enter the main drug:

Mianserin

Enter a list of other drugs (comma-separated):

Trimethaphan, Sulpiride, Mequitazine

Check Against List


 **Result:**

Drug Interactions Findings:

- Mianserin has a **direct interaction** with Trimethaphan, potentially increasing the anticholinergic activities.
- Mianserin has an **indirect interaction** with Sulpiride through Pirenzepine, potentially increasing the anticholinergic activities.
- Mianserin has an **indirect interaction** with Mequitazine through Darifenacin, potentially decreasing the metabolism of Mequitazine.

Therefore, caution is advised when combining Mianserin with Trimethaphan, Sulpiride, or Mequitazine.

Please consult your doctor for further guidance and personalized recommendations regarding potential drug interactions.

Show Knowledge Graph Raw Result 

Safe Recommendation

- Suggest a non-interacting drug for [condition]
- Suggests a non-interacting drug for a condition
- Considers patient's current medications


Enter a list of current drugs the patient is taking (comma-separated):

Losartan, Amlodipine, Aspirin

Describe the patient's diagnosis and situation:

Patient is diagnosed with Hypertension and needs a safe new drug.

Recommend Safe Drug

 **Recommended Drug(s):**

Recommended Medication:

- Enalapril - Effective for treating hypertension with minimal side effects.

Summary: The recommended medication is Enalapril, an FDA-approved drug safe for treating Hypertension.

Show Forbidden Drugs List ^

Forbidden drugs: Amlodipine, Aspirin, Carbamazepine, Fosphenytoin, Losartan, Lumacaftor, Nafcillin, Nevirapine, Pentobarbital, Phenobarbital, Phenytoin, Primidone, Rifabutin, Rifampicin, Rifapentine, Secobarbital

| Model Hosting & Integration



Model Hosting & Integration

LLMs Used:

- **Gemma 7B** → Handles Tasks 1–3
- **MedExpert** → Specialized for Task 4 (Safe Drug Recommendation)

About MedExpert:

- A domain-specific model trained on **drug** safety data, **clinical pharmacology**, and **drug interactions**
- Designed to recommend safe alternatives grounded in biomedical context

Deployment:

- Hosted on **Google Colab**
- Exposed as an API via **ngrok** for easy local access

I Results & Evaluation



Results & Evaluation

Compared 5 Search Methods

→ Direct, LightRAG, GraphRAG, RQ-RAG, **LightGraphRAG**

Evaluated on:

→ F1 Score, Precision, Coverage

Best Performer:

→ LightGraphRAG

✓ **Highest** F1 & coverage

✓ Reliable across all **4 tasks**

I Conclusion



Conclusion

- PharmaGraph checks drug interactions and gives safe suggestions.
- Combines NER, knowledge graph, and LLMs.
- LightGraphRAG was the most effective search method.
- All 4 tasks were handled accurately and clearly.

| Thank you!

