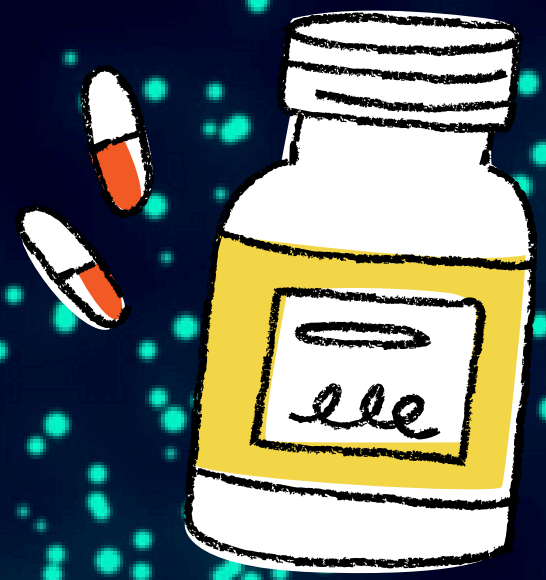
PharmaGraph: Safe Drug Interaction Intelligence using Knowledge Graphs & LLMs



Team Member

Youssef Hassan, Ahmed Kamal, Ziad Moataz

Supervisor

Dr. Ensaf Hussien

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Agenda

- Problem Statement
- Knowledge Graph & Dataset
- Entity Recognition & Normalization
- Search Strategies in the KG
- LightGraphRAG: Our Unified Method
- Core Functionalities (1–4)
- Model Hosting & Integration
- Results & Evaluation
- Conclusion & Future Work

Problem Statement

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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

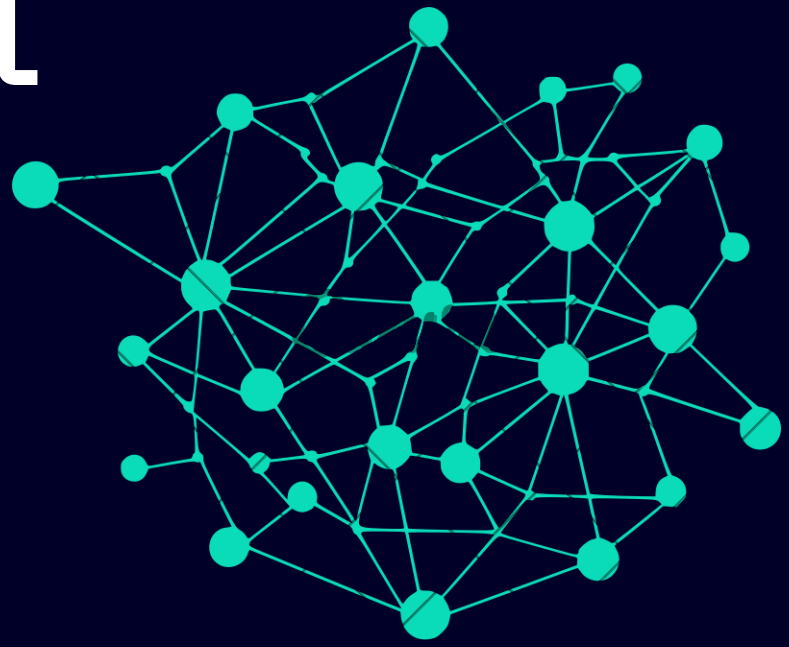
- **PharmaGraph** is a hybrid AI system.
- It processes natural language questions.
- Combines:

 → **Named Entity Recognition**

 → **Knowledge Graph search**

 → **LLM-based explanation or recommendation.**

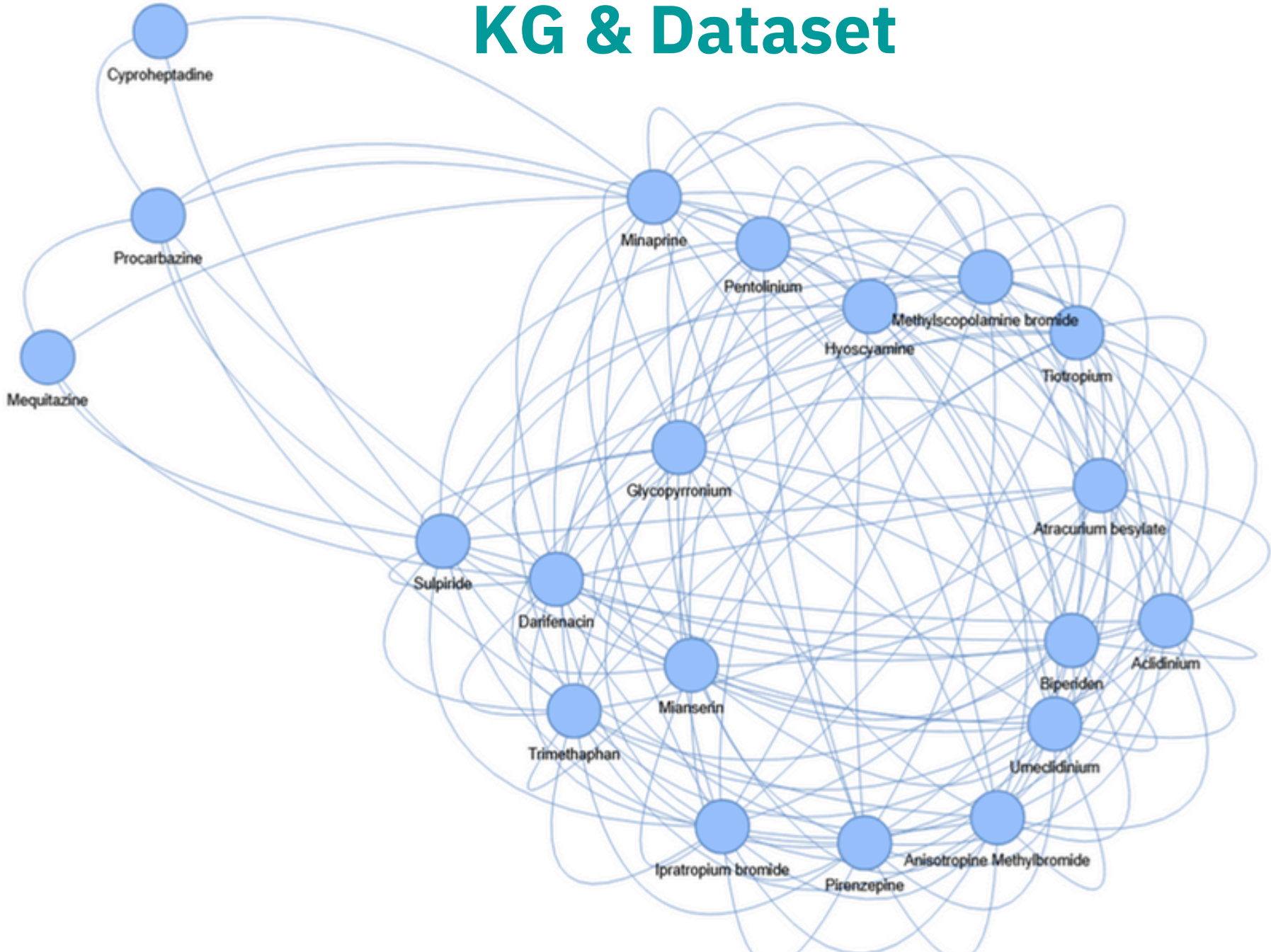
Knowledge Graph & Dataset



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


Cyproheptadine
Procarbazine
Mequitazine
Minaprine
Pentolinium
Hyoscyamine
Methylscopolamine bromide
Tiotropium
Glycopyrronium
Atracurium besylate
Sulpiride
Darifenacin
Aclidinium
Biperiden
Mianserin
Trimethaphan
Umeclidinium
Ipratropium bromide
Pirenzepine
Anisotropine Methylbromide

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

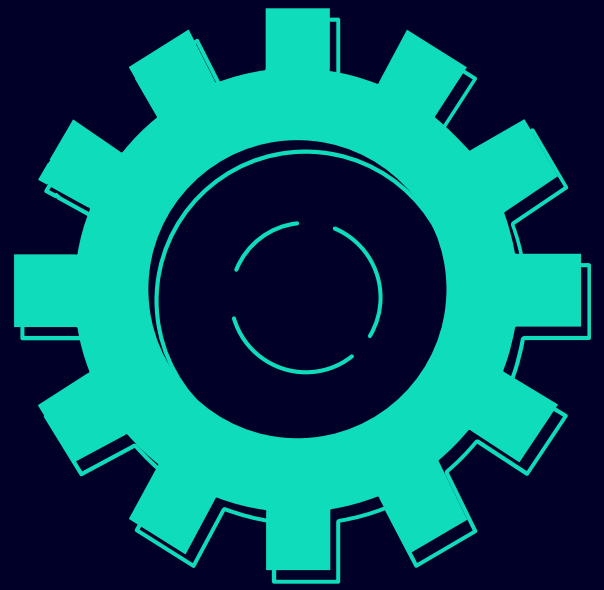
- Handles **direct edges**, **1-hop neighbors**, and **short paths**
- Used in **all 4 functionalities** in PharmaGraph

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

✅ Unified and reliable across query types

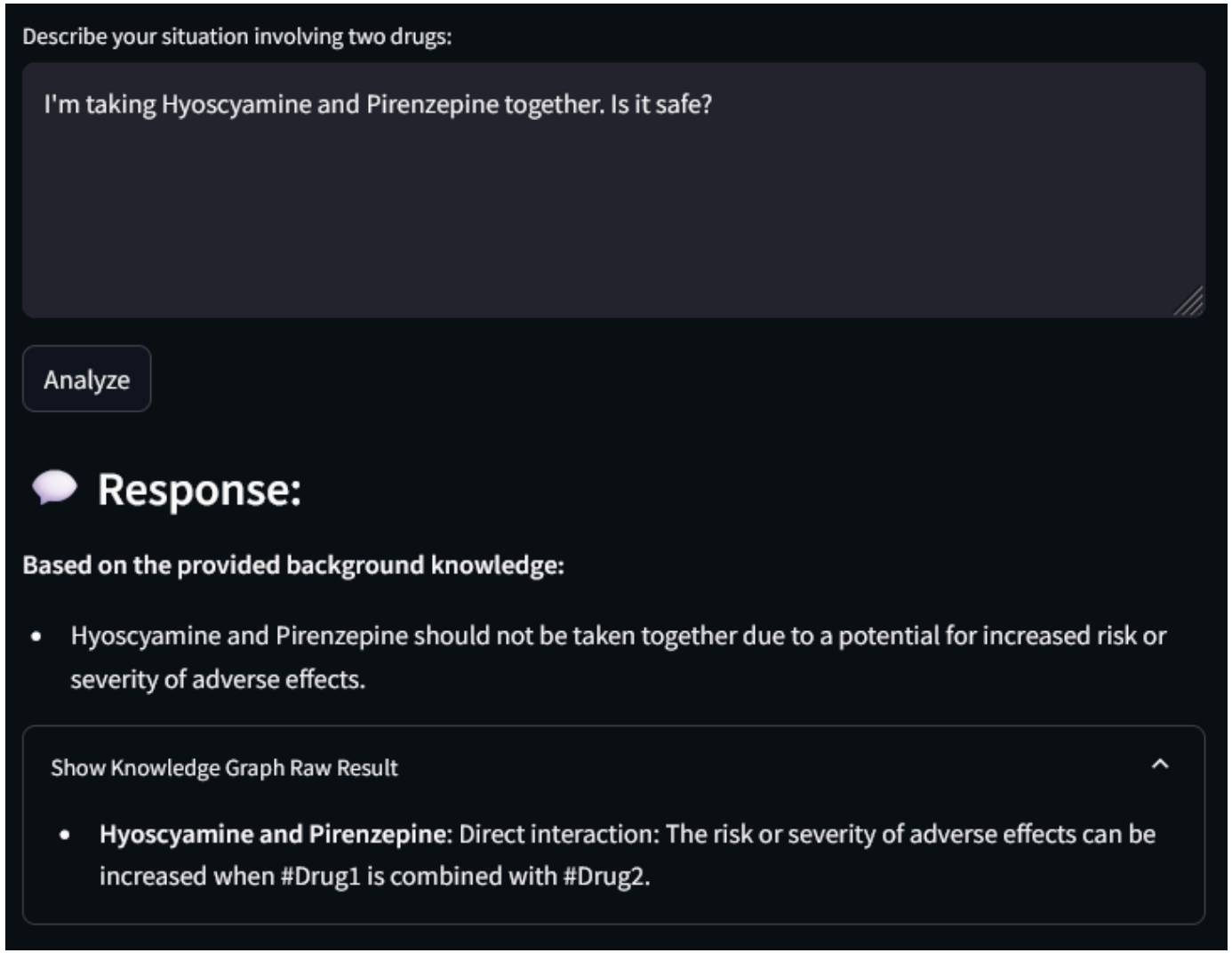
Hybrid Strategy

Core Functionalities of PharmaGraph



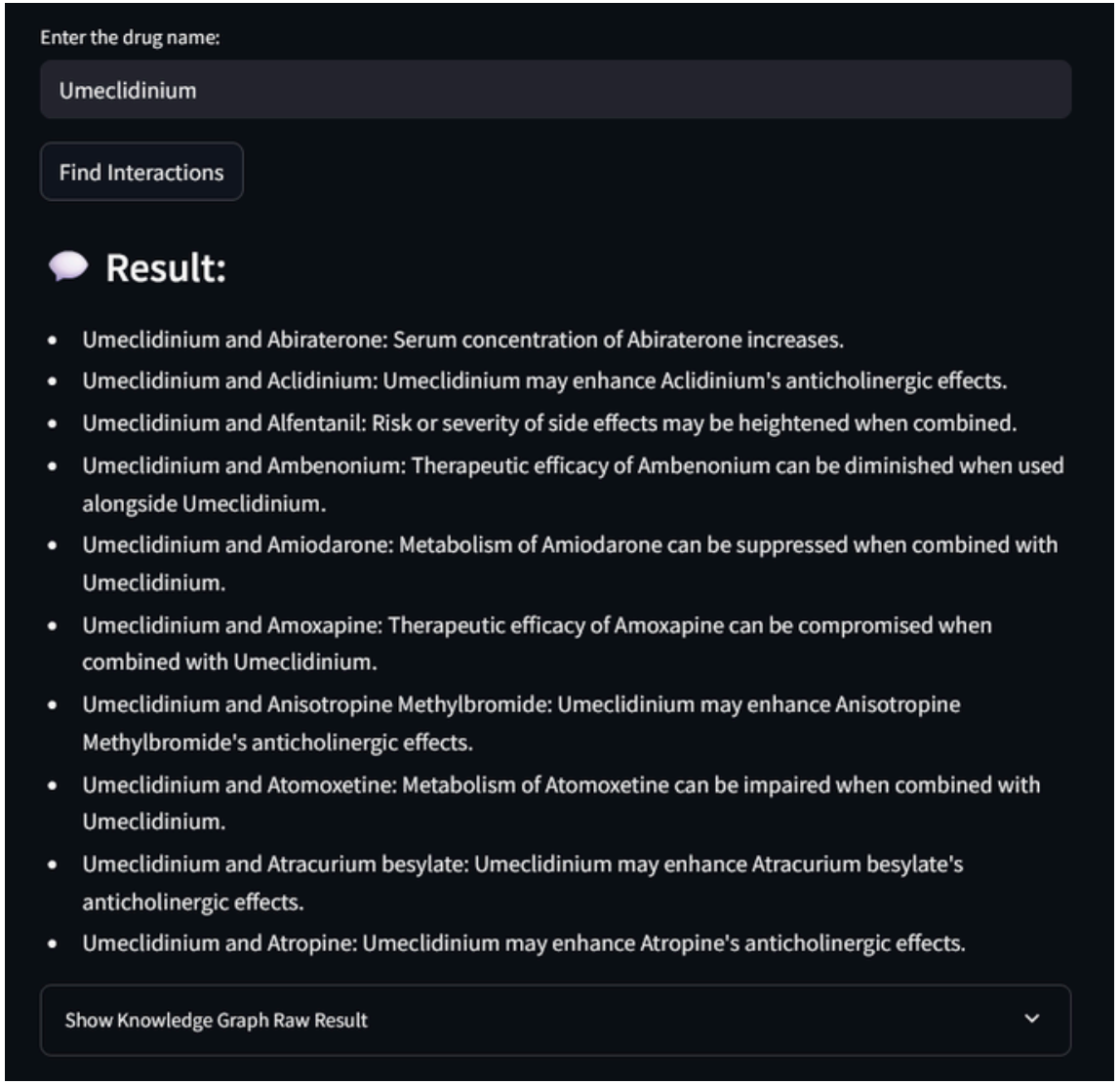
Two-Drug Check

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



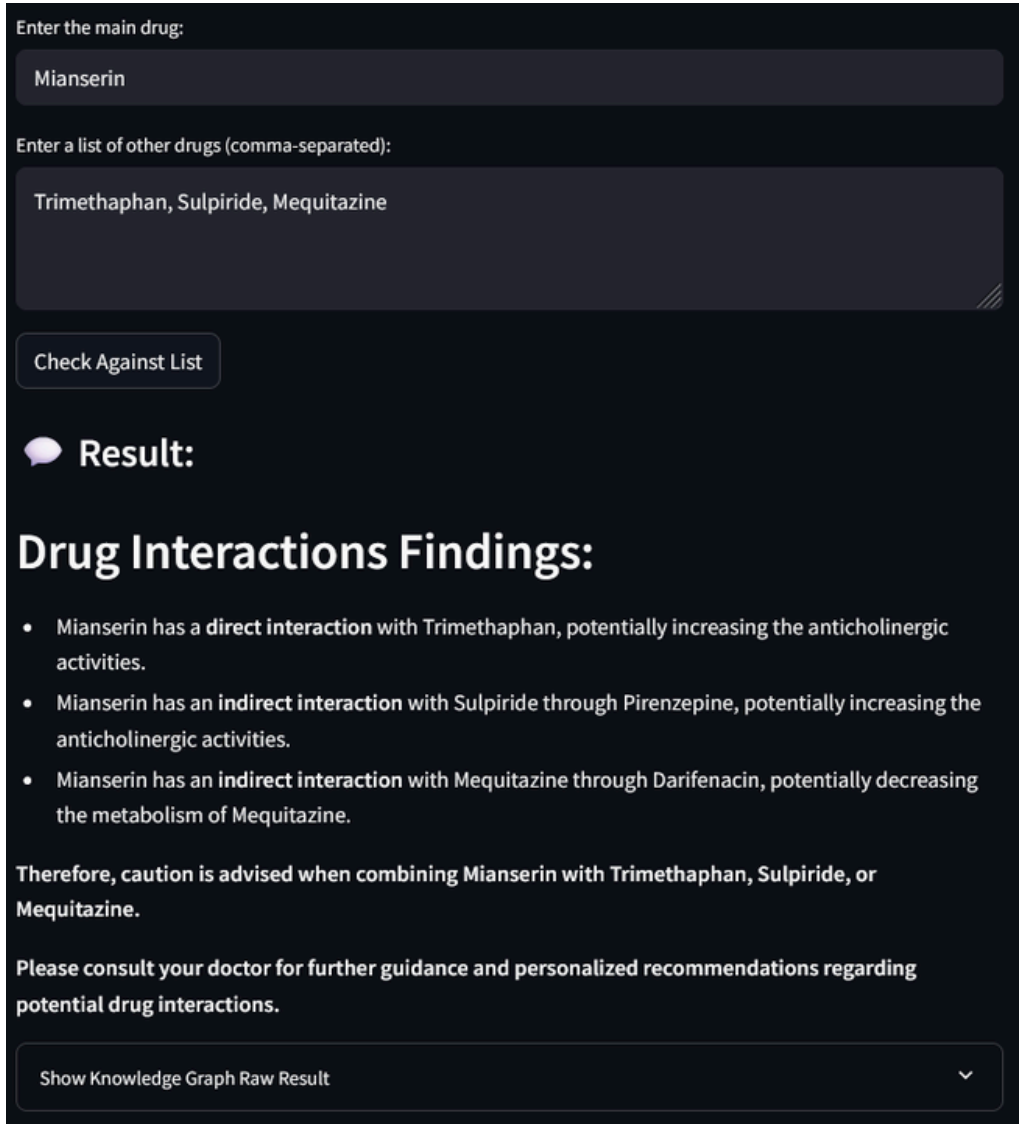
Full Interaction List

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



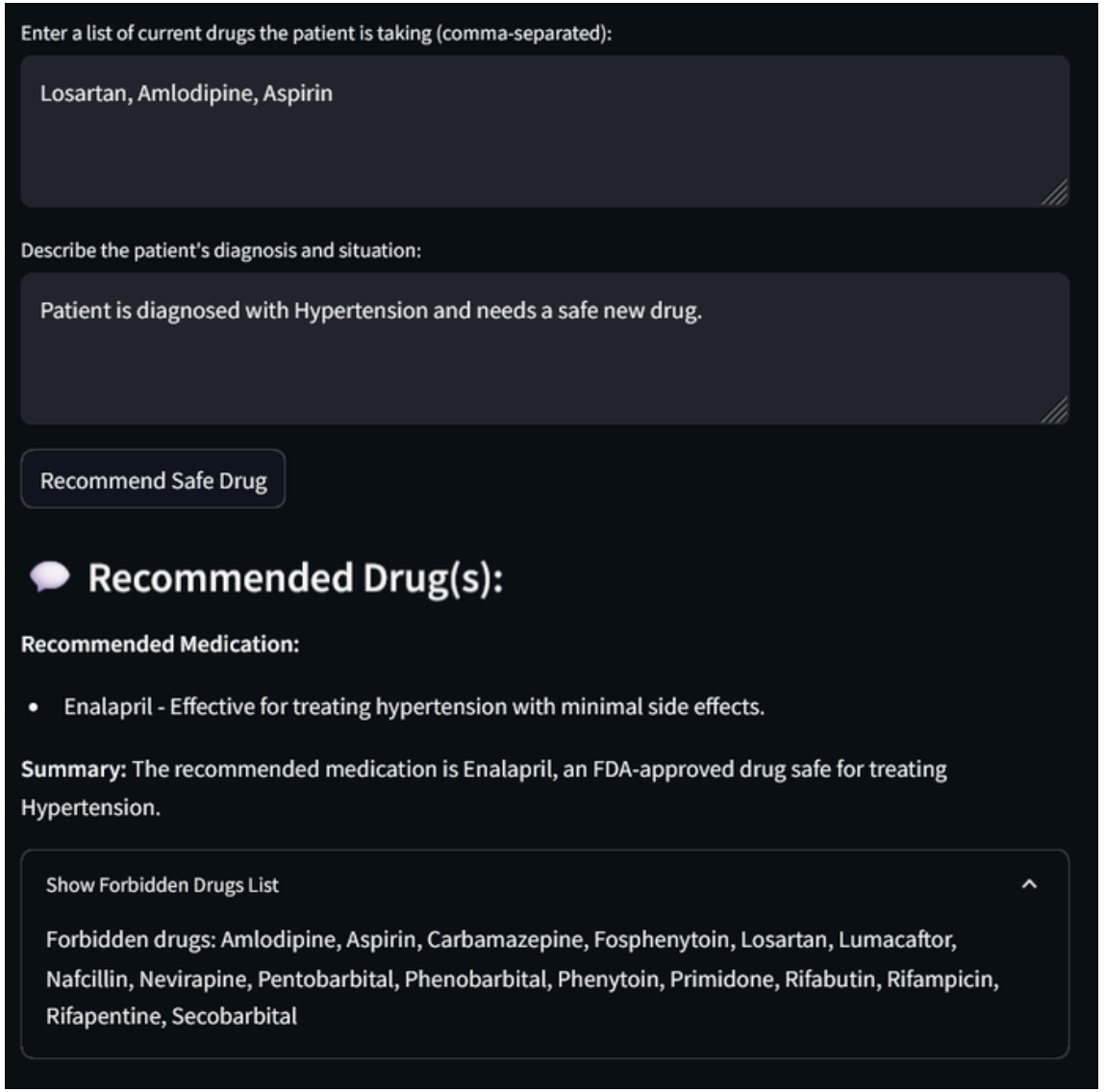
List Check

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



Safe Recommendation

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



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

Results & Evaluation

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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**

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!