CASE STUDIES: AI & Computational Chemistry for BioPharma R&D

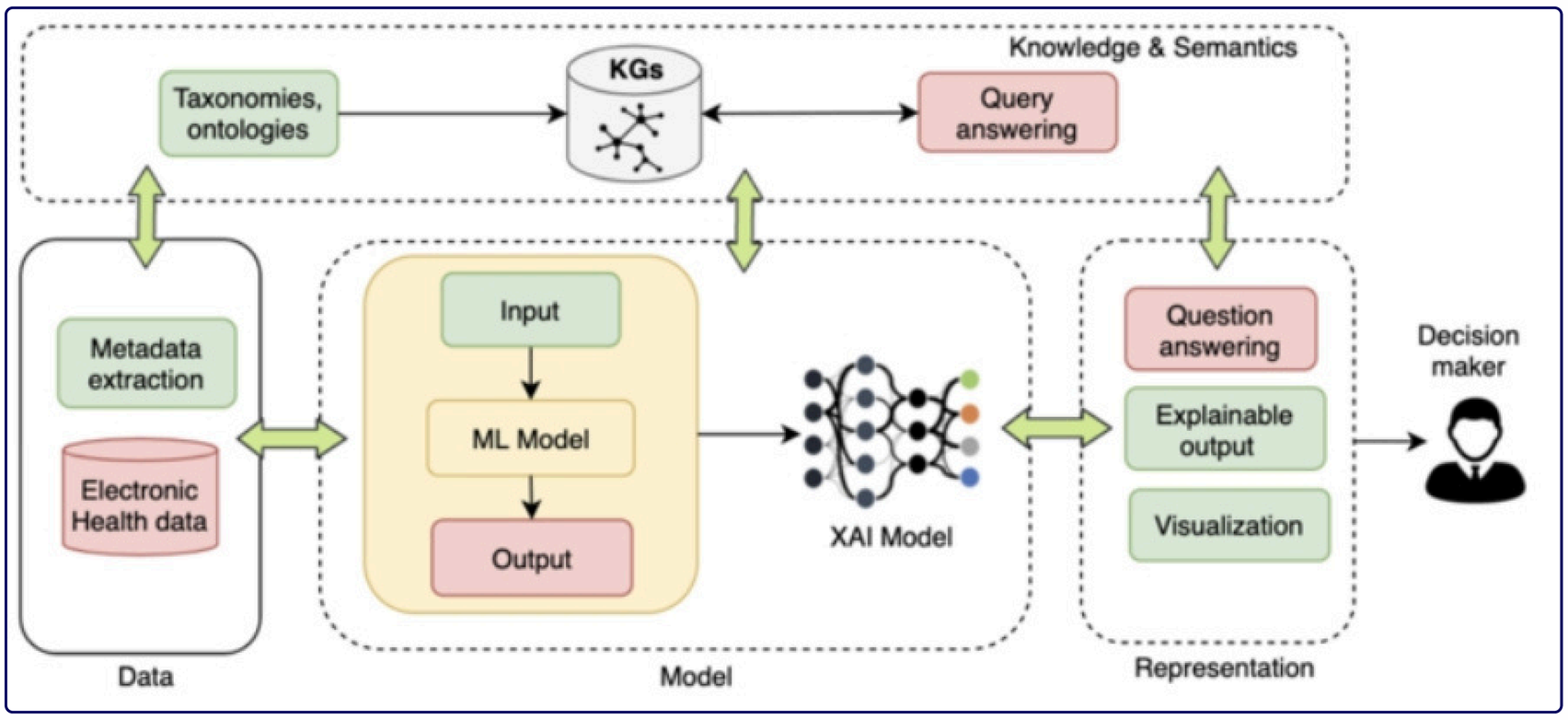
CASE STUDY 4: Accelerating Drug Target Identification with Knowledge Graph Platform

- **Context:** Target enzymes involved in specific bacterial reproduction and metabolic pathways were to be identified and prioritized for in silico repurposing efforts
- **Objective:** To leverage the capabilities of a knowledge graph-based platform, enhanced by large language models (**LLMs**), for efficient discovery and validation of novel drug targets in complex biological systems and emloy Medvolt's drug repurposing module

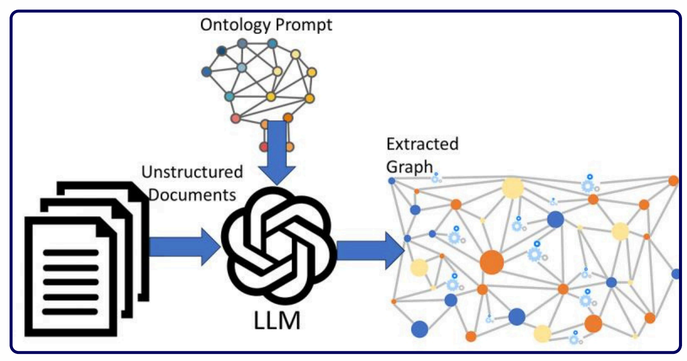
Method + Flow

Graph Analytics Implementation: Deploy graph analytics to pinpoint potential targets through their connectivity and influence within disease-relevant networks

LLM Enhancement: Employ LLMs to enrich the knowledge graph with the latest biomedical research findings and to refine predictive models for target identification



- Data Compilation
- Knowledge Graph Construction
- Network Analytics
- Predictive Modelling
- Target Prioritization
- In silico Studies



Results

- Combining knowledge graphs and LLMs identified key targets within disease networks
- Refined by LLM insights, machine learning models revealed targets with new disease links, offering novel therapeutic avenues for in silico studies
- Targets prioritized this way showed greater validation success, proving the effectiveness of integrating knowledge graphs and LLMs in drug target discovery