

1. THE PROBLEM

- UK clinical trials cost up to £1.3 million per study.
- ~90% clinical trial drug failure rate.
- Drug Toxicity ~30% of failures.
- Traditional toxicity testing slow and expensive.

HARNESSING ARTIFICIAL INTELLIGENCE FOR DRUG TOXICITY PREDICTION

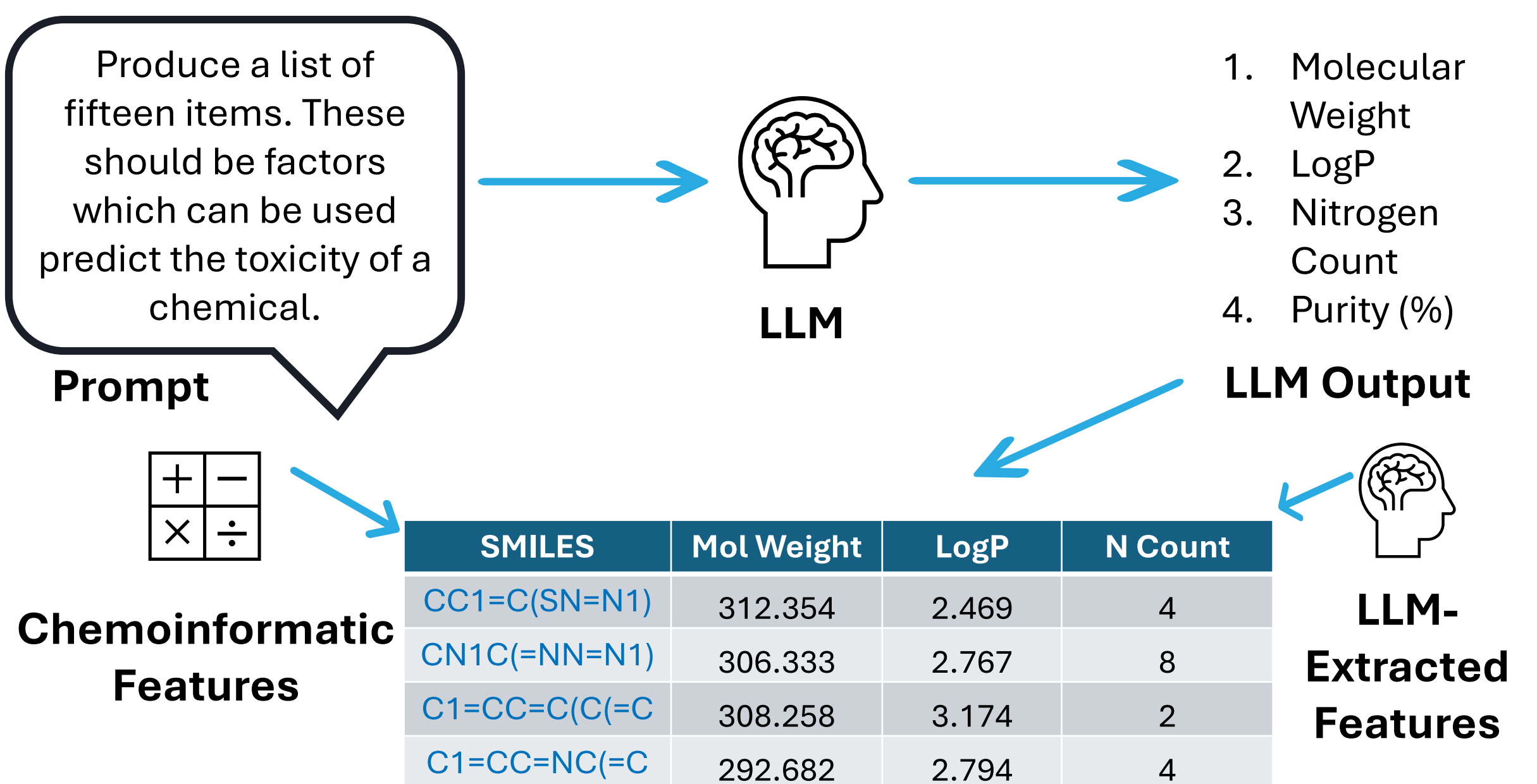
MIA MACGREGOR, AAKASH WELGAMAGE DON & MARK BARTLETT

2. PROJECT AIMS

The aim of this research is to utilize AI for drug toxicity prediction using **machine learning, LLMs, XAI**, and **counterfactual explanations**, while **considering scientists** as the primary target users to ensure practical **end-user applicability**.

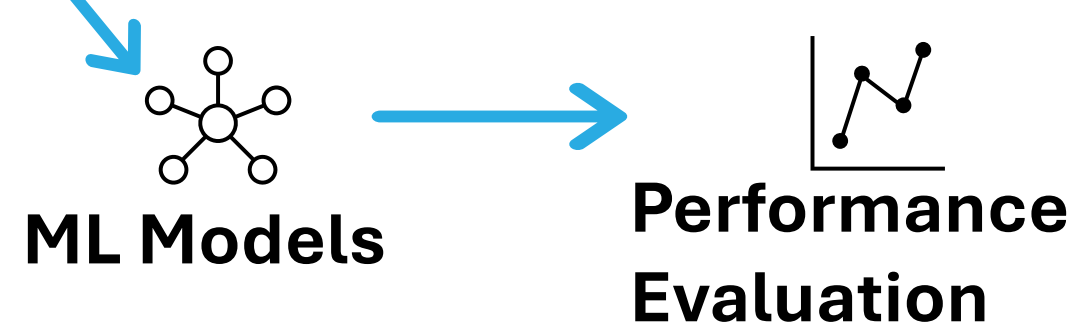
The research focuses on the following areas:

- Analysis of **Prompt Engineering** for Drug Toxicity Prediction
- **Presenting an Explanation** of Drug Toxicity Prediction
- **Counterfactual Explanations** of Drug Toxicity Prediction

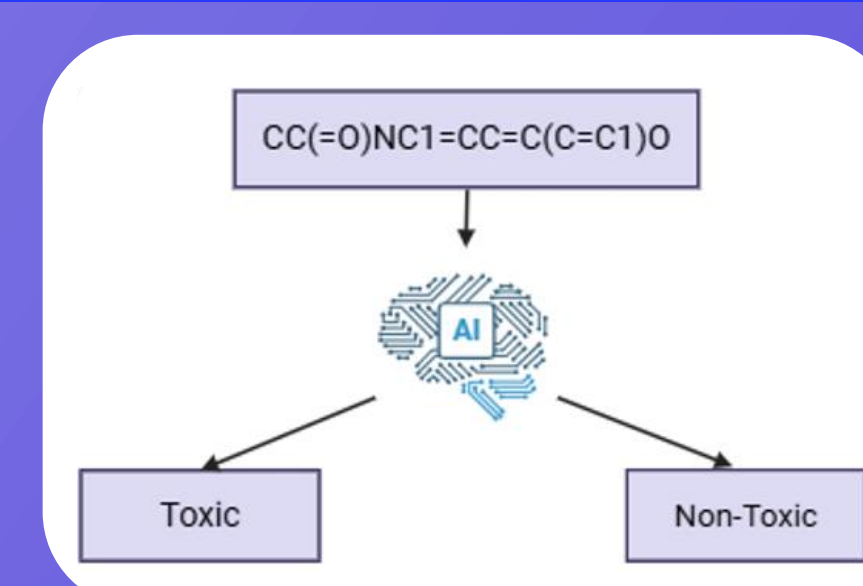


3. PROMPT ENGINEERING

Tailored prompts can be provided to LLMs (e.g., ChatGPT) to elicit specific outputs.



4. PRESENTING AN EXPLANATION

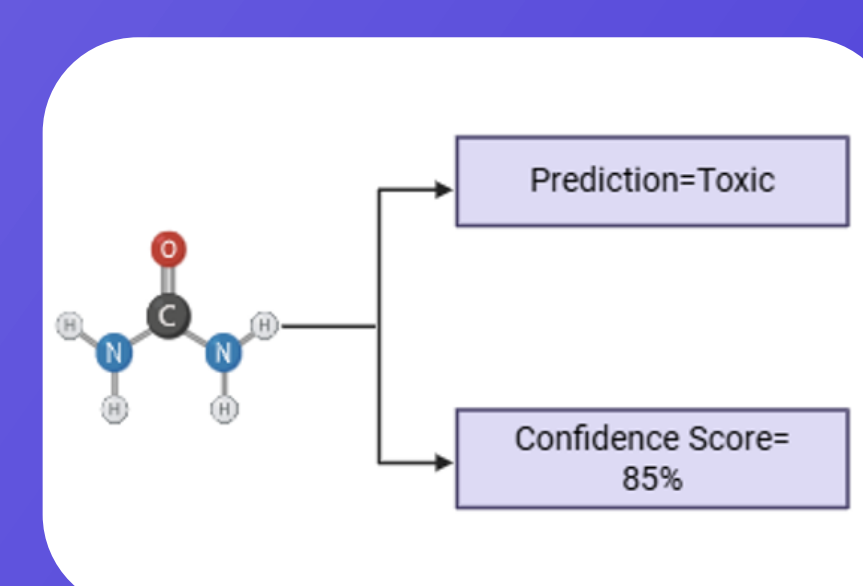


BINARY CLASSIFICATION

The features of most significance for toxicity prediction;

1. Molecular Weight
2. LogP
3. Hydrogen Bond Donors
4. Total Polar Surface Area
5. Solubility

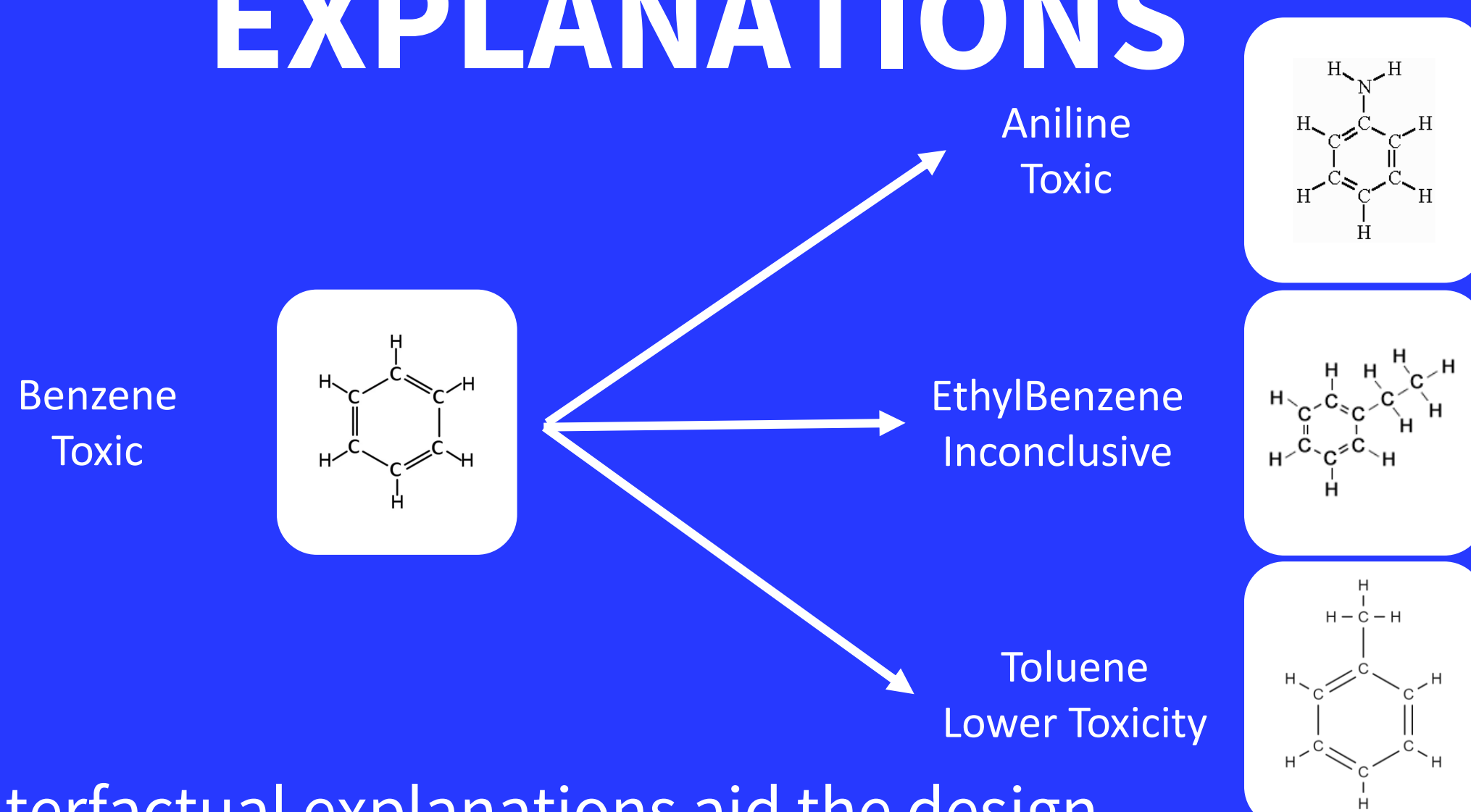
FEATURE IMPORTANCE



CONFIDENCE SCORING

A survey will assess formats and pipeline use in drug toxicity prediction.

5. COUNTERFACTUAL EXPLANATIONS



Counterfactual explanations aid the design of compounds with lower predicted toxicity.

