

# H.E.P.A.R: A Hepatic Ensemble Predictive Resource

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# What is the Problem?

01

Drug-induced liver injury (DILI) accounts for 13% of all acute liver toxicity<sup>1</sup>

02

Developing nations are hit especially hard because of reduced access to modern technologies<sup>2</sup>

03

DILI can cause fatality rates from 10%, up to 50%

# Current Approaches



LAB-BASED AND CLINICAL LIVER  
BIOPSY IS THE GOLDEN  
STANDARD<sup>3</sup>



COMPUTATIONAL METHODS  
FOCUS ON CHEMICAL  
STRUCTURE ANALYSIS



USES EXTREME COMPUTING TO  
SIMULATE CHEMICAL AND  
BIOLOGICAL DOCKING



# Research Question

**Can we implement a stratified bimodal approach to improve accuracy of accessible DILI models and reduce overall costs?**

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# Materials and Methodology



## DATA COLLECTION:

USED A PUBLICLY AVAILABLE FDA DATASET TO CURATE A LIST OF 1,199 DIFFERENT DRUGS

01



## CHEMICAL ANALYSIS:

ORGANIZE AND COMPILE SMILES STRINGS FOR EACH COMPOUND

02



## FEATURE EXTRACTION:

2,600+ BIOLOGICAL AND CHEMICAL FEATURES WERE EXTRACTED, 1,855 WERE USED FOR MODEL TRAINING

03



## ENSEMBLE DEVELOPMENT:

COMBINE INDIVIDUAL LEARNING MODELS INTO A VOTING ENSEMBLE

04



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## Novel Metabolic Analysis

- Developed a novel combination algorithm using Graph Neural Networks (GNNs), and Genetic Algorithms (GA)
- Accurately filtered out the most important metabolic features involved in drug-induced liver toxicity

# Results and Findings

Accurately  
predicted DILI  
76% of the time

Maintained  
high AUC-ROC  
of 0.77



# References and Citations

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