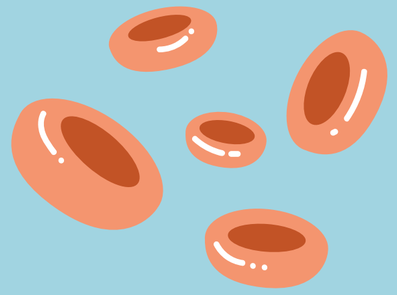
DRUG TARGET INTERACTION PREDICTION

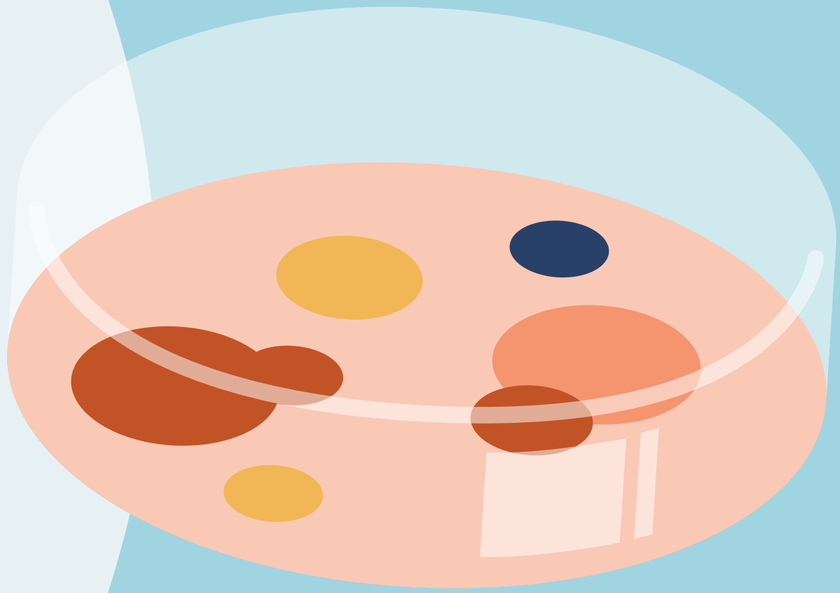


Computational Biology

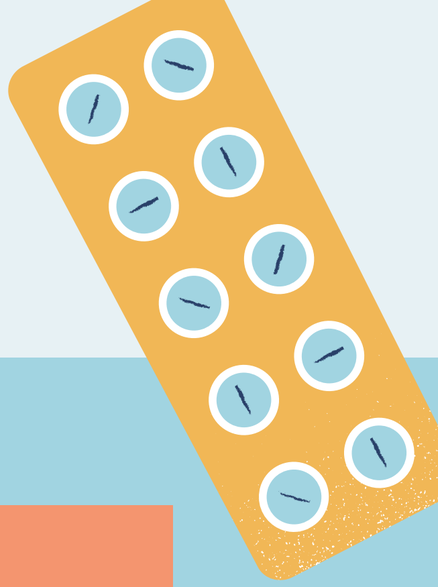
MEMBERS

Jason Andrew Harjawidjaja
(2702350781)

Azka Dwi Putra Azhad
(2702357926)



FINAL PROJECT PRESENTATION



Overview

What is it?

Drug-target interaction is the binding of a drug molecule to a biological target, such as a protein, which causes a change in the target's function and produces a physiological effect.

The idea is to predict the binding relationships between drug compounds and biological targets. Our goal is to choose a single drug (Aspirin) and interact it with the other drugs to obtain a unique result. e.g. acetylsalicylic acid and nictone.

Gantt Chart

Drug Interaction Prediction Progress

Task	Week 2-7	Week 8	Week 9	Week 10	Week 11	Week 12	Week 13
Topic							
Research & PPT							
Finding Datasets							
Code Implementation							
Training Models							
Fine-Tuning & Debugging							
Documentation & Final Report							

Code & Dataset

```
print("Loading data...")
df = pd.read_csv(CSV_PATH)
print("Rows loaded:", len(df))
# check expected column names (adjust if different)
# Many DDI datasets call columns drug1_name / drug2_name or drug1 / drug2
# We'll try to detect common names:
if "drug1_name" in df.columns and "drug2_name" in df.columns:
    drug1_col = "drug1_name"
    drug2_col = "drug2_name"
elif "drug1" in df.columns and "drug2" in df.columns:
    drug1_col = "drug1"
    drug2_col = "drug2"
else:
    # fallback to first two columns that look like names
    drug1_col = df.columns[0]
    drug2_col = df.columns[1]
print("Using columns:", drug1_col, drug2_col)

# load types if present
if os.path.exists(XLSX_PATH):
    types_df = pd.read_excel(XLSX_PATH)
    print("Loaded types xlsx:", types_df.shape)
else:
    types_df = pd.DataFrame()

# Standardize drug name columns
df[drug1_col] = df[drug1_col].astype(str).str.strip()
df[drug2_col] = df[drug2_col].astype(str).str.strip()
df["interaction_type"] = df["interaction_type"].astype(str).str.strip()

# lowercase names for consistency
df[drug1_col] = df[drug1_col].str.lower()
df[drug2_col] = df[drug2_col].str.lower()
df["interaction_type"] = df["interaction_type"].str.lower()

# remove exact duplicates (optional)
df = df.drop_duplicates(subset=[drug1_col, drug2_col, "interaction_type"]).reset_index(drop=True)
print("After dedup:", len(df))
```

DDI_data

drug1_id	drug2_id	drug1_name	drug2_name	interaction_type
DB00006	DB00346	Bivalirudin	Alfuzosin	serum concentration
DB00006	DB13783	Bivalirudin	Acemetacin	risk or severity of bleeding
DB00006	DB06605	Bivalirudin	Apixaban	anticoagulant activities
DB00006	DB06695	Bivalirudin	Dabigatran etexilate	anticoagulant activities
DB00006	DB09075	Bivalirudin	Edoxaban	anticoagulant activities
DB00006	DB06228	Bivalirudin	Rivaroxaban	anticoagulant activities
DB00006	DB00227	Bivalirudin	Lovastatin	serum concentration
DB00006	DB09030	Bivalirudin	Vorapaxar	risk or severity of adverse effects
DB00006	DB00683	Bivalirudin	Midazolam	serum concentration
DB00006	DB00641	Bivalirudin	Simvastatin	serum concentration
DB00006	DB00932	Bivalirudin	Tipranavir	serum concentration
DB00006	DB00248	Bivalirudin	Cabergoline	serum concentration
DB00006	DB01200	Bivalirudin	Bromocriptine	serum concentration
DB00006	DB00320	Bivalirudin	Dihydroergotamine	serum concentration
DB00006	DB00696	Bivalirudin	Ergotamine	serum concentration
DB00006	DB01253	Bivalirudin	Ergonovine	serum concentration
DB00006	DB00353	Bivalirudin	Methylergometrine	serum concentration
DB00006	DB00897	Bivalirudin	Triazolam	serum concentration

Dataset

Mendeley Data

data of multiple-type drug-drug interactions

Published: 6 July 2020 | Version 1 | DOI: 10.17632/md5czfsfnd.1
Contributor: Hui Yu

Description

DDI_data.csv file is we extracted from drug bank v5.1, it includes the five items: Drug1_id, Drug2_id, Drug1_name, Drug2_name, and the interaction types between Drug1 and Drug2.
DDI_types.xlsx file includes 114 types of DDI and the class index after merged them.
DDI_types_merged.xlsx includes the type name of interactions and their corresponding ID.

Download All 2.18 MB

Files

DDI_data.csv	14.3 MB
DDI_types_merged.xlsx	11 KB
DDI_types.xlsx	12.1 KB

Dataset metrics

Views	2432
Downloads	831
Citations	2

Latest version

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Cite this dataset

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Outcome

```
Loading DDI dataset...
Loaded 222646 interactions
Unique drugs: 1868
Computing latent features with SVD (dim=30)...
Creating training dataset...
Training pairs: 222271 positive + 222271 negative
Total interaction types: 77
Building feature vectors...
  Processed 5000/20000 pairs...
  Processed 10000/20000 pairs...
  Processed 15000/20000 pairs...
Filtered out 12 samples from rare classes
Training samples: 19988, Classes: 65
Train: 14991 | Test: 4997
Training models...
  SVM training on 10000 samples...
  Neural Network training on 14991 samples...
```

Model Training

```
================================================================================
MODEL EVALUATION
================================================================================

SVM:
--------------------------------------------------
Precision: 0.3653 | Recall: 0.1927 | F1: 0.2340

Neural Network:
--------------------------------------------------
Precision: 0.5276 | Recall: 0.4285 | F1: 0.4524

Confusion matrix has 61 classes - showing simplified version
Accuracy on valid samples: 0.8393

Generating interaction predictions for: ACETYLSALICYLIC ACID
```

Evaluation

Outcome

```
Choose how many drugs to display:
1) Top 5
2) Top 10
3) Top 15
0) Exit
Select option: 1

================================================================================
TOP 5 ASPIRIN INTERACTIONS (MIXED)
================================================================================
              Drug                    Interaction_Type  Severity Confidence
0  Dimethyl Fumarate                         Metabolism     Major     100.0%
1        Dicoumarol          Anticholinergic Activities     Major     100.0%
2        Nimesulide          Neuroexcitatory Activities     Major     100.0%
3        Omeprazole              Hypokalemic Activities     Major      99.9%
4     Etacrynic Acid  Risk Or Severity Of Qtc Prolongation  Moderate      99.8%
```

Top 5

```
Choose how many drugs to display:
1) Top 5
2) Top 10
3) Top 15
0) Exit
Select option: 2

================================================================================
TOP 10 ASPIRIN INTERACTIONS (MIXED)
================================================================================
              Drug                                    Interaction_Type  Severity Confidence
0   Dimethyl Fumarate                                         Metabolism     Major     100.0%
1         Dicoumarol                          Anticholinergic Activities     Major     100.0%
2         Nimesulide                          Neuroexcitatory Activities     Major     100.0%
3         Omeprazole                              Hypokalemic Activities     Major      99.9%
4      Etacrynic Acid                  Risk Or Severity Of Qtc Prolongation  Moderate      99.8%
5        Nateglinide                              Hyperkalemic Activities     Major      99.3%
6    Sodium Phosphate                               Hypotensive Activities     Major      99.2%
7          Betaxolol                             Anticoagulant Activities     Major      97.9%
8  Estradiol Valerate  Risk Or Severity Of Renal Failure And Rhabdomyolysis  Moderate      97.7%
9       Valproic Acid                        Myelosuppressive Activities     Major      95.3%
```

Top 10

```
Choose how many drugs to display:
1) Top 5
2) Top 10
3) Top 15
0) Exit
Select option: 3

================================================================
TOP 15 ASPIRIN INTERACTIONS (MIXED)
================================================================
                Drug                                    Interaction_Type  Severity Confidence
0    Dimethyl Fumarate                                         Metabolism     Major     100.0%
1          Dicoumarol                          Anticholinergic Activities     Major     100.0%
2          Nimesulide                          Neuroexcitatory Activities     Major     100.0%
3          Omeprazole                              Hypokalemic Activities     Major      99.9%
4       Etacrynic Acid                  Risk Or Severity Of Qtc Prolongation  Moderate      99.8%
5         Nateglinide                              Hyperkalemic Activities     Major      99.3%
6     Sodium Phosphate                               Hypotensive Activities     Major      99.2%
7           Betaxolol                             Anticoagulant Activities     Major      97.9%
8   Estradiol Valerate  Risk Or Severity Of Renal Failure And Rhabdomyolysis  Moderate      97.7%
9        Valproic Acid                        Myelosuppressive Activities     Major      95.3%
10         Osimertinib                    Risk Or Severity Of Hyperkalemia  Moderate      91.7%
11       Moxifloxacin  Hypotensive, Nephrotoxic, And Hyperkalemic Activities     Major      88.6%
12       Streptomycin                                Constipating Activities     Major      82.7%
13         Duloxetine                          Antihypertensive Activities     Major      79.2%
14            Digoxin                              Hypoglycemic Activities  Moderate      63.8%
```

Top 15

REFERENCES

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https://www.mdpi.com/1422-0067/25/14/7753

https://www.nature.com/articles/s41467-025-62235-6

https://www.nature.com/articles/s44385-024-00003-9

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