Kairós

Predicting Drug Interactions

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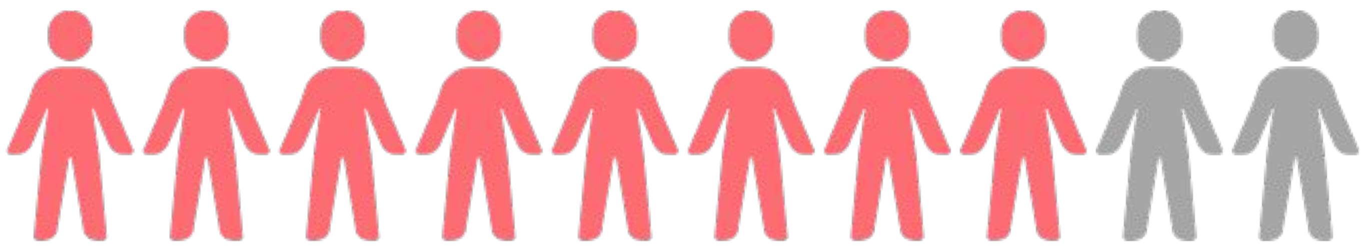
Our Solution

Kairós is a web app that uses machine learning to predict adverse drug interactions, providing real-time insights to prevent harmful side effects and enhance safety.

Why?

The FDA estimates **2 million serious adverse drug events** and 100,000 deaths annually in the U.S. due to drug interactions.

MVP Demo



Target Users

Individuals taking prescription or over-the-counter medications

A diabetic person seeks to understand if their current prescription will interact with a new supplement they are considering.

A person wants to determine if a new metabolism booster could adversely affect their health while using a specific antibiotic.

Market Research

Competitors	Target Users	Uses ML	User Data	OCR
WebMD	Consumers	✖	♥	✖
Drugs.com	Consumers	✖	♥	✖
Medscape	Consumers / Medical Pros	✖	♥	✖
AlphaFold3	Scientists	♥	✖	✖
Kairos	Consumers	♥	♥	♥

Kairós is the only tool that integrates ML modeling, User Data, and OCR into one simple to use platform.

DATA SOURCES & EDA

Size: 192,347 drug-to-drug interaction pairs
Split: Train (70%), Validation (15%), Test (15%)

Target Variable: Boolean for:

- Acetylation
- Amidation
- Hydrolysis of Amide

DrugBank

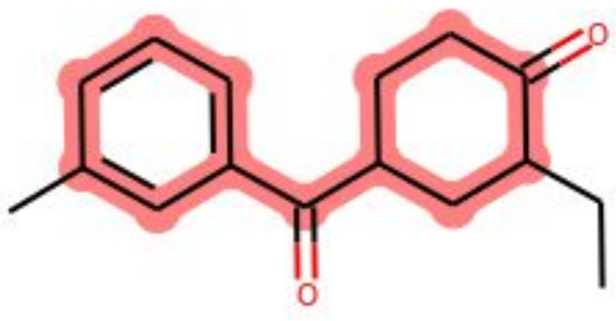
ChEMBL

NIH Dietary Supplements

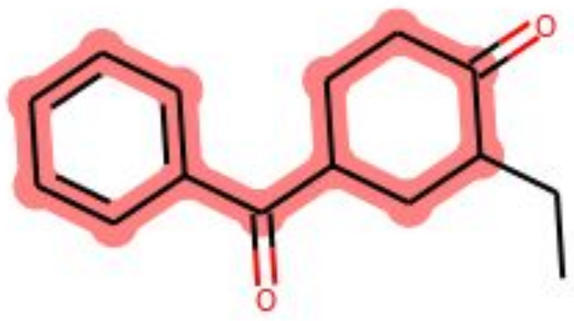
Reaction Modeling

	Drug1_ID	Drug1 (Canonical Smiles)	drug1_name	Drug2_ID	Drug2 (Canonical Smiles)	drug2_name	acetylation_reaction_flag (RDKit Reaction)
0	DB00855	NCC(=O)CCC(O)=O	Aminolevulinic acid	DB00460	COC(=O)CCC1=C2NC(\C=C3/N=C(/C=C4\N\C(=C/C5=N/C...	Verteporfin	1
1	DB09536	O=[Ti]=O	Titanium dioxide	DB00460	COC(=O)CCC1=C2NC(\C=C3/N=C(/C=C4\N\C(=C/C5=N/C...	Verteporfin	0
2	DB09536	O=[Ti]=O	Titanium dioxide	DB00460	COC(=O)CCC1=C2NC(\C=C3/N=C(/C=C4\N\C(=C/C5=N/C...	Verteporfin	0
3	DB01600	CC(C(O)=O)C1=CC=C(S1)C(=O)C1=CC=CC=C1	Tiaprofenic acid	DB00460	COC(=O)CCC1=C2NC(\C=C3/N=C(/C=C4\N\C(=C/C5=N/C...	Verteporfin	1
4	DB09000	CC(CN(C)C)CN1C2=CC=CC=C2SC2=C1C=C(C=C2)C#N	Cyamemazine	DB00460	COC(=O)CCC1=C2NC(\C=C3/N=C(/C=C4\N\C(=C/C5=N/C...	Verteporfin	0
...	...	...	...	...	...	...	...
185402	DB00281	CCN(CC)CC(=O)NC1=C(C)C=CC=C1C	Lidocaine	DB06708	CCCCN(CCCC)CC(O)C1=C2C(=CC(Cl)=C1)\C(=C/C1=CC=...	Lumefantrine	1
185403	DB01088	[H][C@]12C[C@@H](O)[C@H](\C=C\[C@@H](O)C(C)CC#...	Iloprost	DB01235	N[C@@H](CC1=CC(O)=C(O)C=C1)C(O)=O	Levodopa	1
185404	DB00857	CN(C\C=C\C#CC(C)(C)C)CC1=CC=CC2=CC=CC=C12	Terbinafine	DB00196	OC(CN1C=NC=N1)(CN1C=NC=N1)C1=C(F)C=C(F)C=C1	Fluconazole	0
185405	DB00734	CC1=C(CCN2CCC(CC2)C2=NOC3=C2C=CC(F)=C3)C(=O)N2...	Risperidone	DB02703	[H][C@@]12C[C@@H](O)[C@@]3([H])[C@@]4(C)CC[C@@...	Fusidic acid	0
185406	DB00356	ClC1=CC2=C(OC(=O)N2)C=C1	Chlorzoxazone	DB00934	CNCCCC12CCC(C3=CC=CC=C13)C1=CC=CC=C21	Maprotiline	0

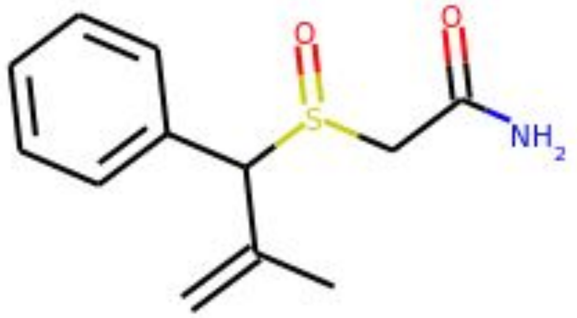
Open-Source Cheminformatics and Machine Learning



c1ccc(CC2CCCCC2)cc1



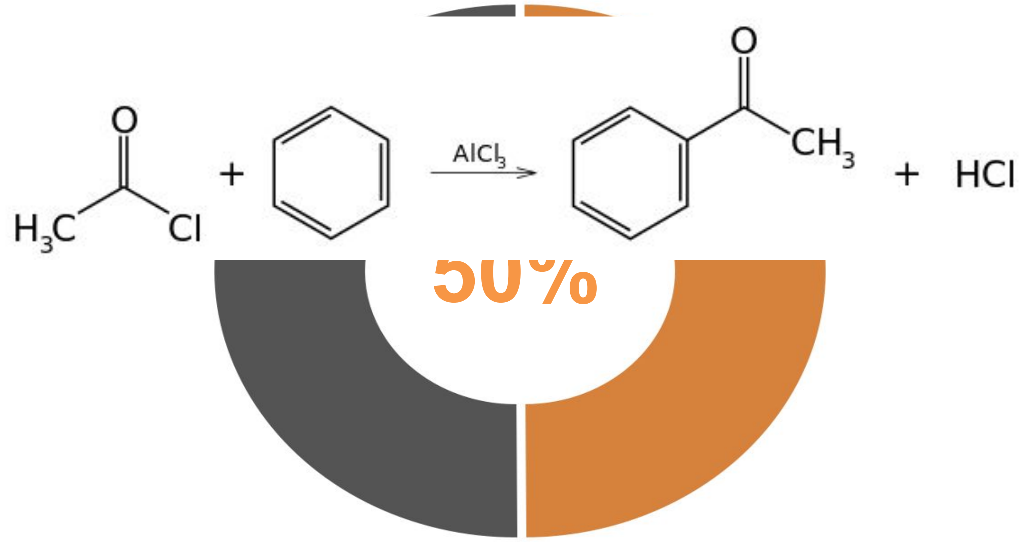
c1ccc(CC2CCCCC2)cc1



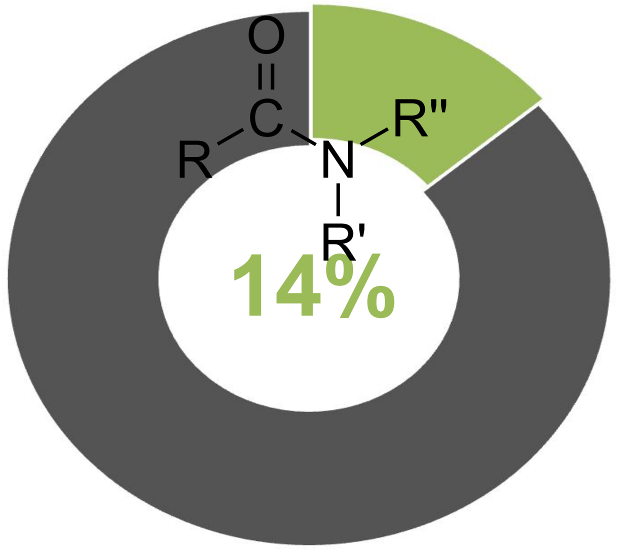
c1ccccc1

Type of Reactions

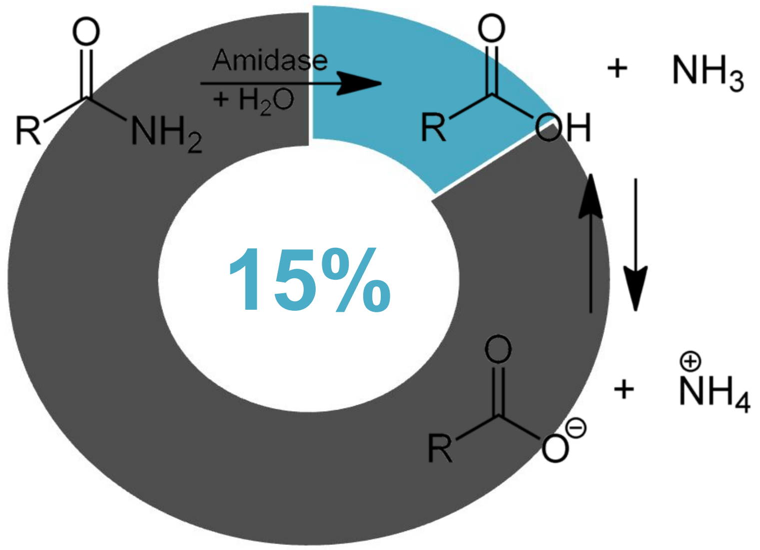
Acetylation



Amidation



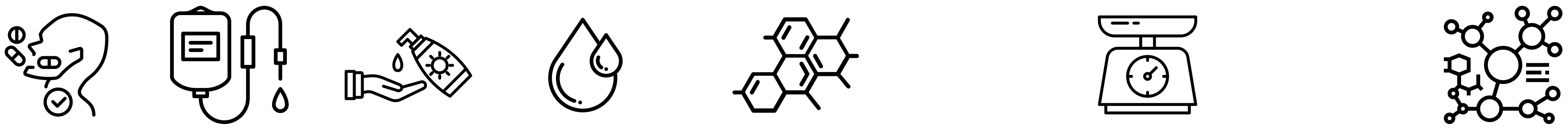
Hydrolysis of Amide



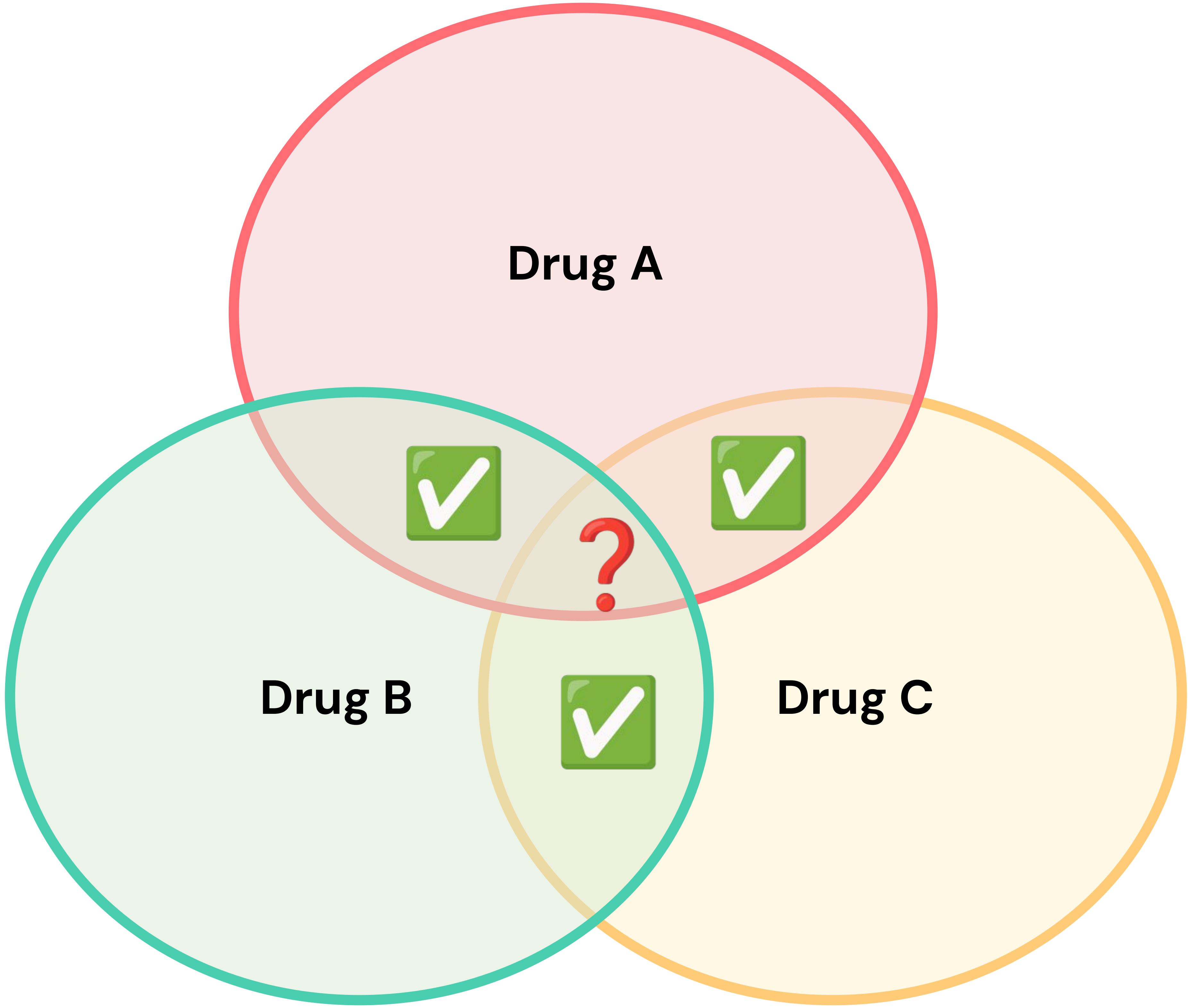
Each reaction is generated with a different reaction template, resulting in 3 sets of target variables with different class distributions

Feature Selection

		Route of Administration			Molecular Properties			Hydrogen Bond Acceptor / Donor	
	name	oral	parenteral	topical	alogp	aromatic_rings	full_molecular_weight	hba	hbd
0	LISINOPRIL ANHYDROUS	☑	☐	☐	1.24	1	405.5	5	4
1	NAPROXEN	☑	☐	☐	3.04	2	230.26	2	1



Model Limitation: Multiple Drug Interactions



Guided screen for synergistic three-drug combinations:https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7347197/
Design of high-order antibiotic combinations against M. tuberculosis by ranking and exclusion:https://www.nature.com/articles/s41598-019-48410-y
Systematic exploration of synergistic drug pairs:https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3261710/

ML PIPELINE

DATA PREP

- Dataset Ingestion
- Data Preprocessing
- Feature Engineering / Selection

ML MODELING

- Model Selection
- Model Training
- Hyperparameter Tuning

MODEL TESTING

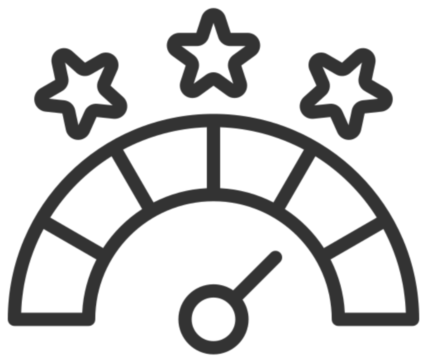
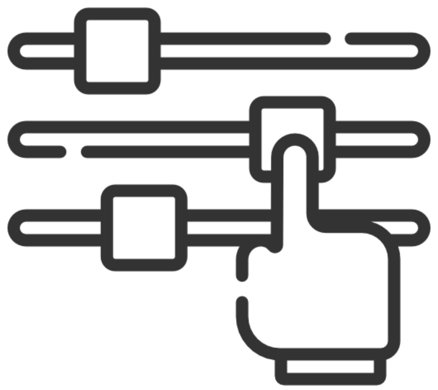
- Model Evaluation
- Model Selection
- Addl. Training & Data Acquisition

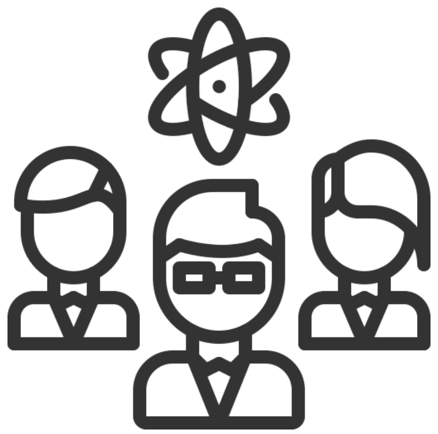
Model Results

Reaction	Model	Mean F2 Score		Mean F1 Score		Mean PR AUC	
		Val	Train	Val	Train	Val	Train
Acetylation	**XGBoost**	0.995	0.996	0.996	0.997	0.997	0.999
	Random Forest	0.973	0.999	0.965	0.999	0.971	0.999
	SVM	0.799	0.803	0.789	0.793	0.839	0.842
	Logistic Regression	0.620	0.611	0.643	0.633	0.747	0.738
Amidation	**XGBoost**	0.988	0.990	0.983	0.990	0.989	0.998
	Random Forest	0.954	0.949	0.939	0.935	0.982	0.980
Hydrolysis of Amide	**XGBoost**	0.993	0.989	0.993	0.990	0.993	0.997
	Random Forest	0.853	0.827	0.88	0.862	0.903	0.951

Best Models vs Test Data

Reaction	Model	Mean F2 Score			Mean F1 Score			Mean PR AUC		
		Test	Val	Train	Test	Val	Train	Test	Val	Train
Acetylation	**XGBoost**	0.996	0.995	0.996	0.996	0.996	0.997	0.997	0.997	0.999
Amidation	**XGBoost**	0.990	0.988	0.990	0.991	0.983	0.990	0.992	0.989	0.998
Hydrolysis of Amide	**XGBoost**	0.992	0.993	0.989	0.992	0.993	0.990	0.993	0.993	0.997



Future Enhancements & Goals

User Data Management & Security

- Expand User Profile Information
- Personalized User Experience
- Use strict user data privacy & protocols

Chatbot & OCR Improvements

- Improve Chatbot experience
- Include other languages for chatbot and OCR

Reaction Severity Score

- Integrate more datasets in order to predict severity score
- Add High / Medium / Low Score
- Update the ML models

Kairós

Multiple Drug Interactions

ML Modeling Integrated

User Input / Login

OCR Integrated

3 Types of Reactions

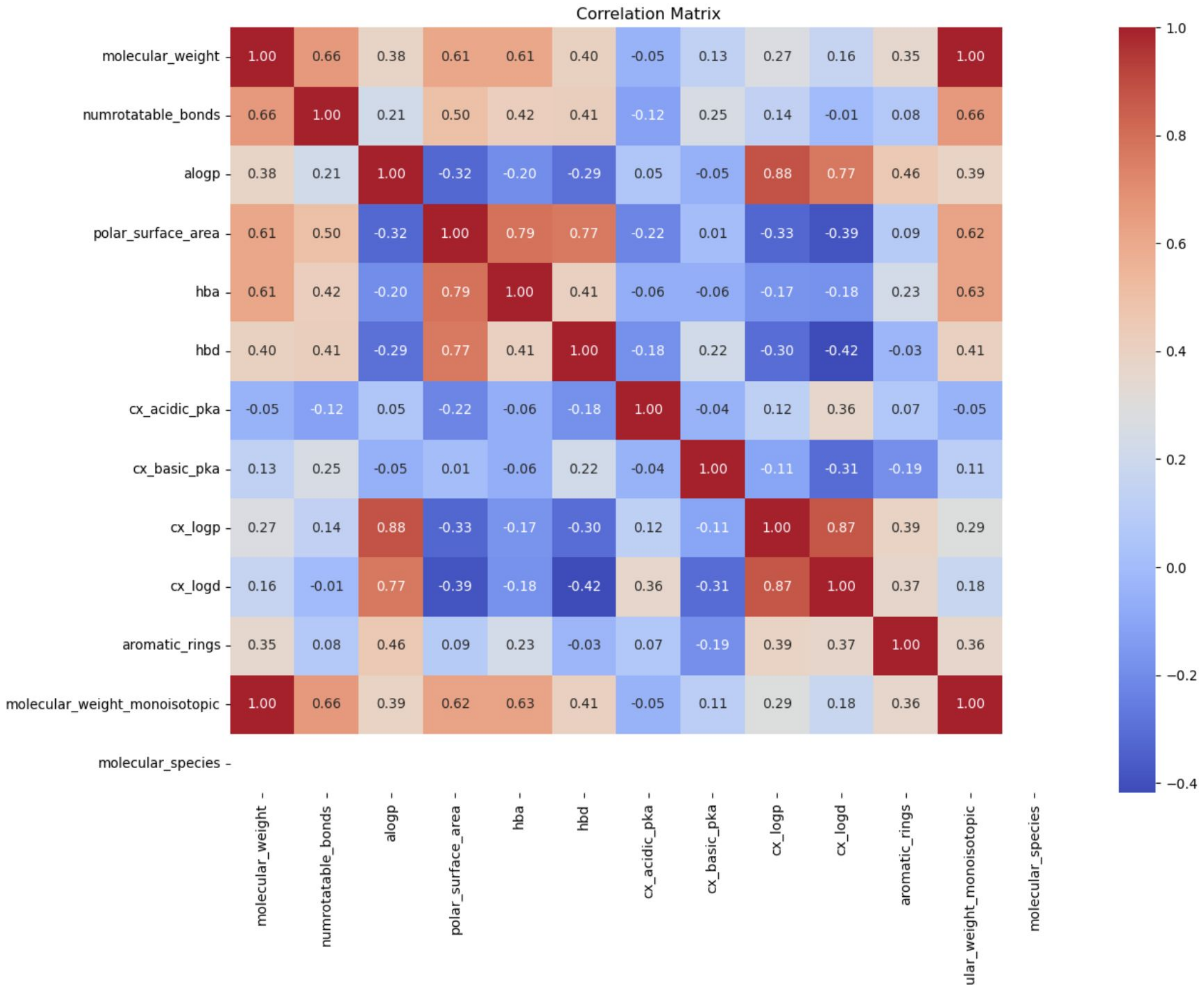
THANK YOU

Kairós team

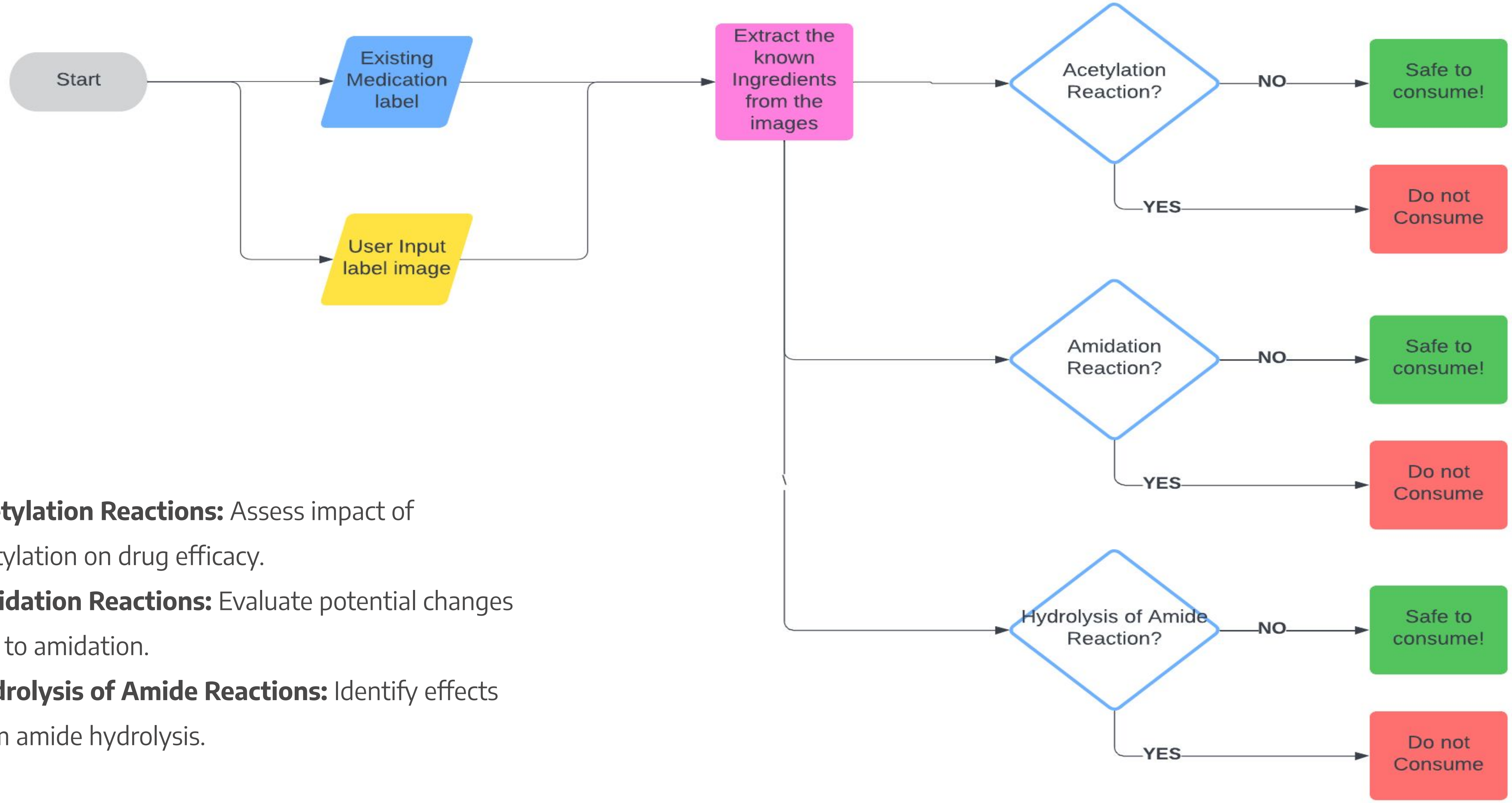
SUMMARY

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Etiam mattis, nunc vitae eleifend posuere, turpis mauris vestibulum purus, in pellentesque tellus elit vel nisl. Nam elementum nunc quis sapien pretium, at tincidunt mauris dignissim.

Appendix


Correlation Matrix
molecular_weight
numrotatable_bonds
alogp
polar_surface_area
hba
hbd
cx_acidic_pka
cx_basic_pka
cx_logp
cx_logd
aromatic_rings
molecular_weight_monoisotopic
molecular_species
1.00 0.66 0.38 0.61 0.61 0.40 -0.05 0.13 0.27 0.16 0.35 1.00
0.66 1.00 0.21 0.50 0.42 0.41 -0.12 0.25 0.14 -0.01 0.08 0.66
0.38 0.21 1.00 -0.32 -0.20 -0.29 0.05 -0.05 0.88 0.77 0.46 0.39
0.61 0.50 -0.32 1.00 0.79 0.77 -0.22 0.01 -0.33 -0.39 0.09 0.62
0.61 0.42 -0.20 0.79 1.00 0.41 -0.06 -0.06 -0.17 -0.18 0.23 0.63
0.40 0.41 -0.29 0.77 0.41 1.00 -0.18 0.22 -0.30 -0.42 -0.03 0.41
-0.05 -0.12 0.05 -0.22 -0.06 -0.18 1.00 -0.04 0.12 0.36 0.07 -0.05
0.13 0.25 -0.05 0.01 -0.06 0.22 -0.04 1.00 -0.11 -0.31 -0.19 0.11
0.27 0.14 0.88 -0.33 -0.17 -0.30 0.12 -0.11 1.00 0.87 0.39 0.29
0.16 -0.01 0.77 -0.39 -0.18 -0.42 0.36 -0.31 0.87 1.00 0.37 0.18
0.35 0.08 0.46 0.09 0.23 -0.03 0.07 -0.19 0.39 0.37 1.00 0.36
1.00 0.66 0.39 0.62 0.63 0.41 -0.05 0.11 0.29 0.18 0.36 1.00
molecular_weight
numrotatable_bonds
alogp
polar_surface_area
hba
hbd
cx_acidic_pka
cx_basic_pka
cx_logp
cx_logd
aromatic_rings
ular_weight_monoisotopic
molecular_species
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4

MVP Flow

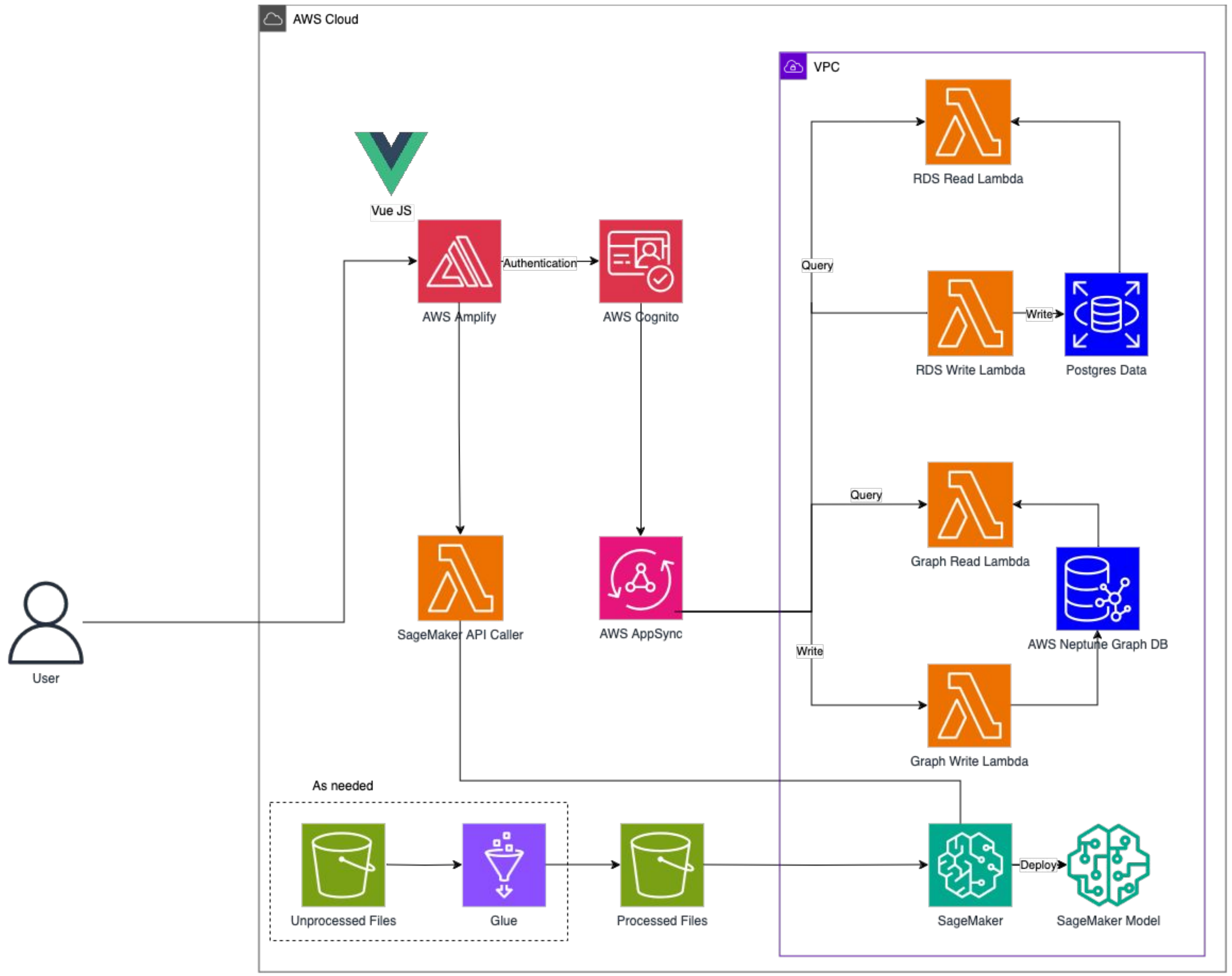


Acetylation Reactions: Assess impact of acetylation on drug efficacy.

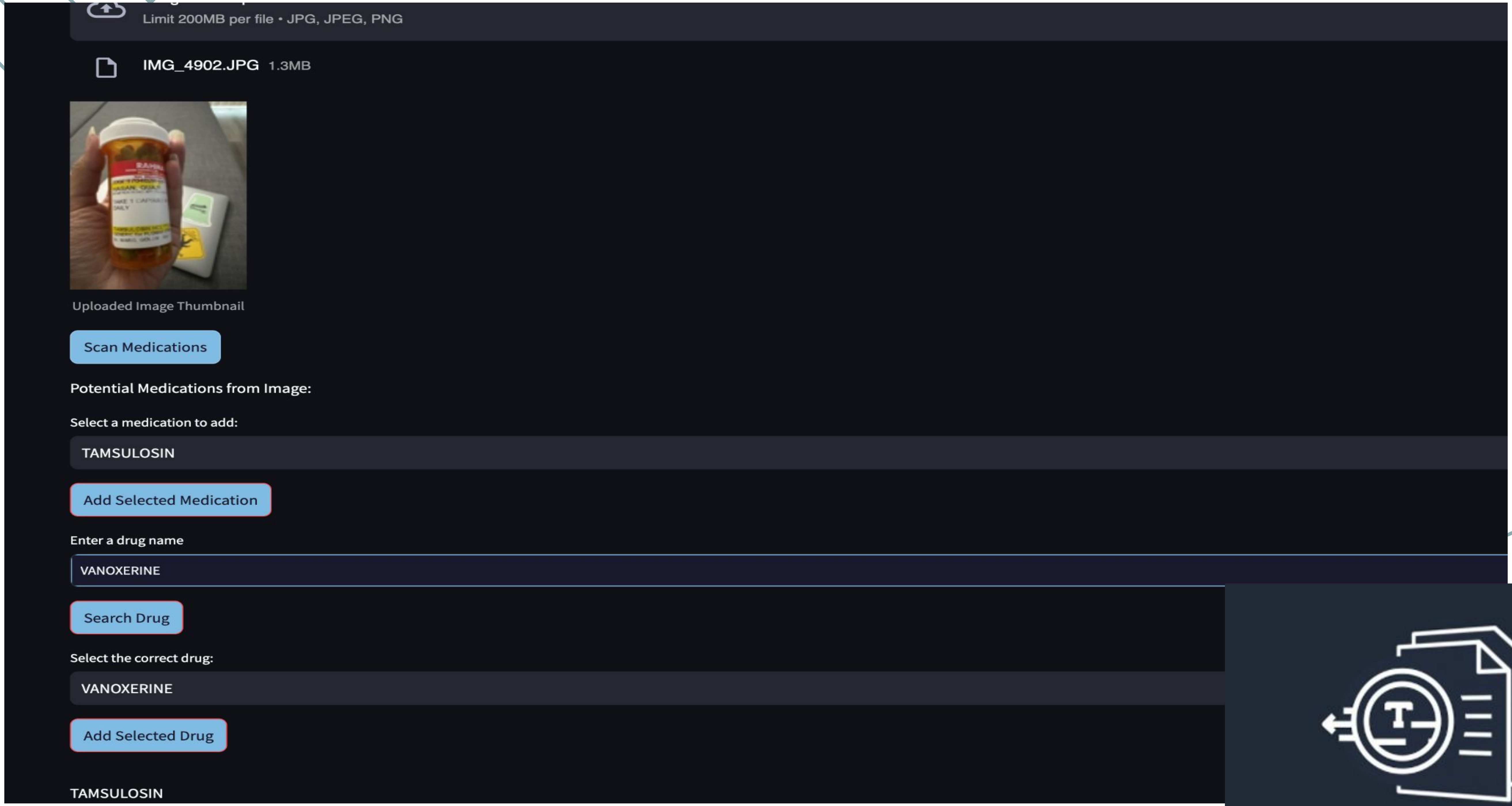
Amidation Reactions: Evaluate potential changes due to amidation.

Hydrolysis of Amide Reactions: Identify effects from amide hydrolysis.

Data Architecture



OCR Integration



Amazon Textract

Type of Reactions

Acetylation

Many drugs are processed in the body through the acetylation reaction, either by biotransformation into an effective compound or to be metabolized into substances that the body can excrete in a more simpler manner.

Amidation

Amides are polar, meaning they have regions of high positive and negative electrical charge density, which allows them to interact with biological receptors and enzymes. Amides are also stable and can help drugs resist rapid metabolic degradation in the human body.

Hydrolysis of Amide

Amide hydrolysis is important in drug discovery and development because it can make drugs active