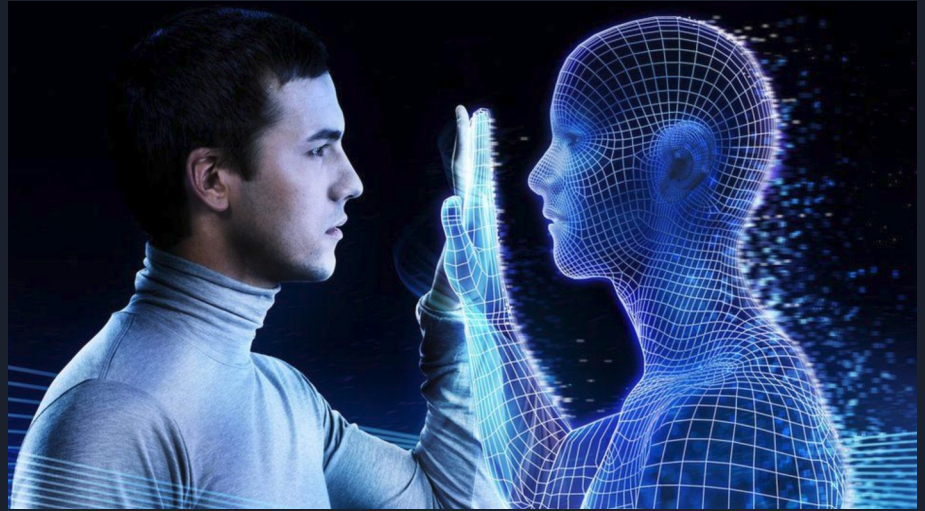


# PharmaPros



Team Members: Taha Abdullah, Triyaksh Mathur, Tanvi Dhamdhere,  
Michael Rizzo, Omnya Mohamed Izzeldin, Daniel

# Problem statement

- Use of animal models
  - Time-consuming
  - Expensive
  - Inaccurate
  - Raises Ethical Concerns
- Nine out of ten drug trials that work with animals fail in human clinical trials
- We will focus on Alzheimer's Disease

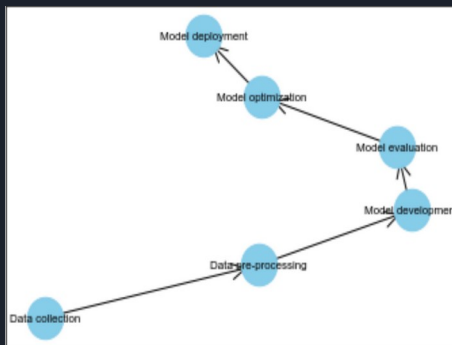
Animal trials



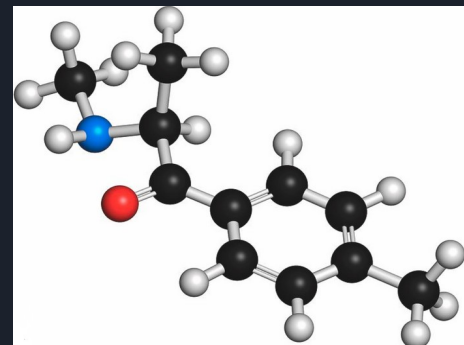
Human trials



Method

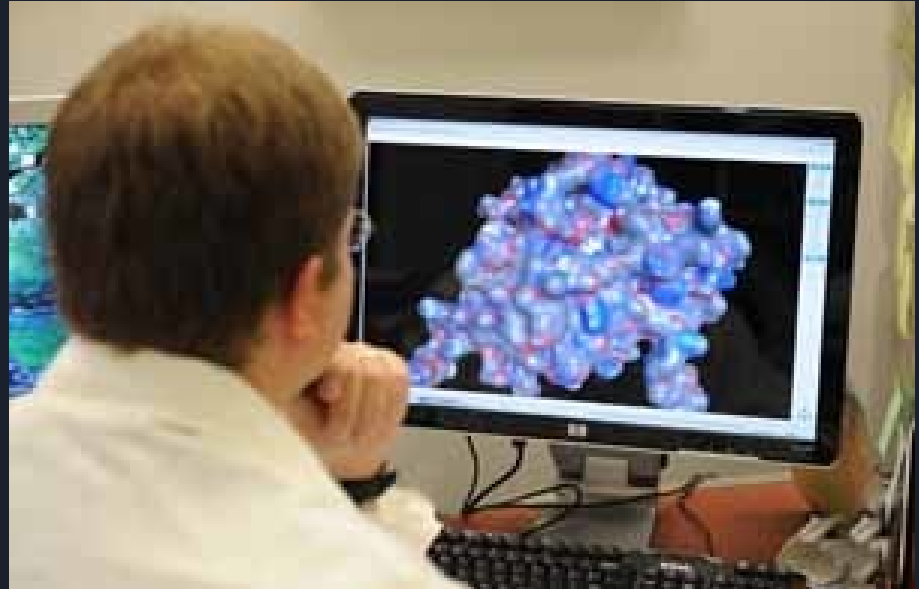


Expected Outcome



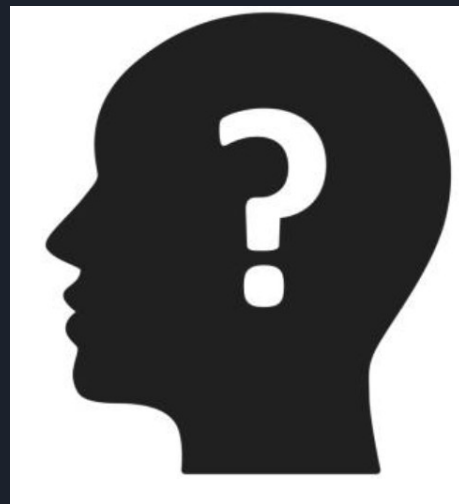
## Goal:

- Improved drug discovery process
- Incorporation of in-silico modelling for target identification
- Validation to enhance drug efficacy and accuracy



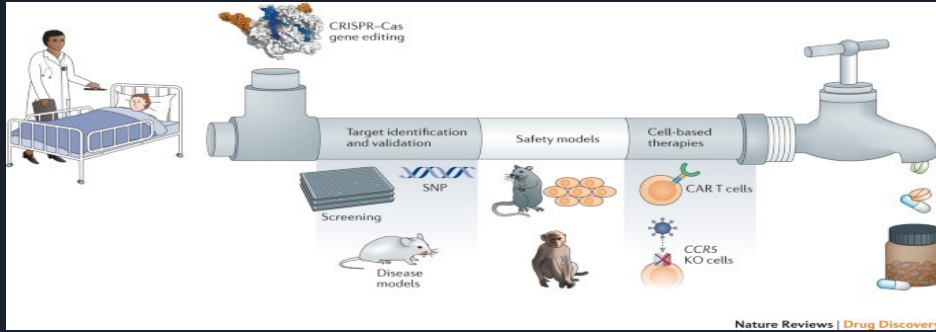
# The Need for In Silico Models in Alzheimer's Disease Research

|   |      |
|---|------|
| People affected by Alzheimer's worldwide (millions) | 50   |
| Costs of Alzheimer's (trillions)                    | 1.1  |
| Failure rate of clinical trials (%)                 | 99.6 |

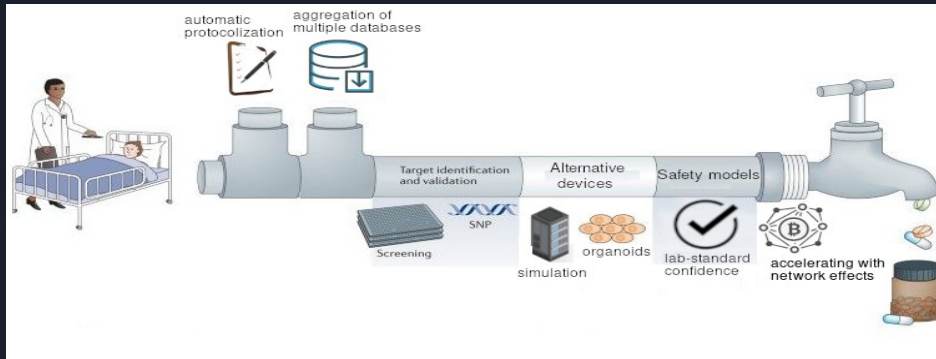


Call to action: Invest in in-silico models to improve the chances of developing effective drugs for Alzheimer's disease

# The Solution

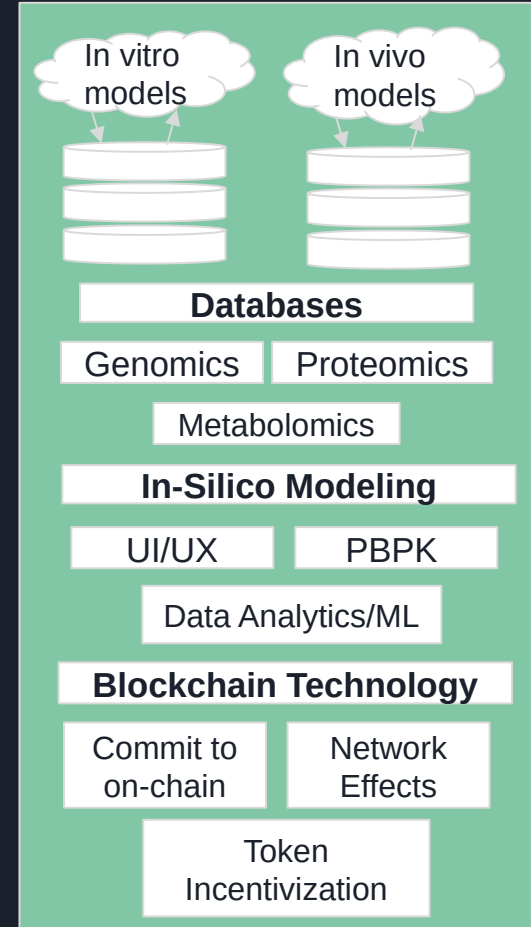


Existing  
Approach



Our  
approach

Building a Computational Model MVP



## Application Snippets:

The screenshot shows the first step of the application: "1. Upload your CSV data". It includes a file input area with a "Browse files" button and a "Predict" button at the bottom. A large graphic overlay reads "BIOACTIVITY PREDICTION APP" and illustrates the workflow: an "Input Molecule" (chemical structure) is processed by an "ML" (Machine Learning) model to predict a "Target Protein" (labeled as "plc<sub>50</sub> = 6.5") and a "Predicted Bioactivity".

This app allows you to predict the bioactivity towards inhibiting the [Acetylcholinesterase enzyme](#). [Acetylcholinesterase](#) is a drug target for Alzheimer's disease.

**Credits**

- App built in `python` + `streamlit` by [Chanin Nantasenamat \(aka Data Professor\)](#)
- Descriptor calculated using [PaDEL-Descriptor \(Read the Paper\)](#).

---

## Original input data

|   | 0   | 1            |
|---|---|--------------|
| 0 | CCOC1=NC=COC(=O)C=C(C)C1=O                | CHEMBL133897 |
| 1 | O=C(NC(=O)C1=NC=C(C=C1)N(C)C(=O)C1=O)C1=O | CHEMBL336398 |
| 2 | CN(C)C1=NC=C(C=C1)C(=O)N(C)C(=O)C1=O      | CHEMBL133598 |
| 3 | O=C(NC(=O)C1=NC=C(C=C1)N(C)C(=O)C1=O)C1=O | CHEMBL336398 |
| 4 | C=C(C)C1=NC=C(C=C1)C(=O)N(C)C(=O)C1=O     | CHEMBL133478 |

## Calculated molecular descriptors

| Name           | PubChemFP0 | PubChemFP1 | PubChemFP2 | PubChemFP3 | PubChemFP4 | PubChemFP5 |
|----------------|------------|------------|------------|------------|------------|------------|
| 0 CHEMBL133628 | 1          | 1          | 1          | 0          | 0          | 0          |
| 1 CHEMBL336398 | 1          | 1          | 1          | 0          | 0          | 0          |

## Calculated molecular descriptors

|   | Name         | PubchemP0 | PubchemP1 | PubchemP2 | PubchemP3 | PubchemP4 | PubchemP5 |
|---|--------------|-----------|-----------|-----------|-----------|-----------|-----------|
| 0 | CHEMBL130628 | 1         | 1         | 1         | 0         | 0         | 0         |
| 1 | CHEMBL336386 | 1         | 1         | 1         | 0         | 0         | 0         |
| 2 | CHEMBL33897  | 1         | 1         | 1         | 0         | 0         | 0         |
| 3 | CHEMBL13188  | 1         | 1         | 0         | 0         | 0         | 0         |
| 4 | CHEMBL130678 | 1         | 1         | 0         | 0         | 0         | 0         |

(5, 862)

## Subset of descriptors from previously built models

|   | PubchemP5 | PubchemP12 | PubchemP13 | PubchemP15 | PubchemP16 | PubchemP18 | PubchemP1 |
|---|-----------|------------|------------|------------|------------|------------|-----------|
| 0 | 0         | 1          | 0          | 1          | 1          | 1          | 1         |
| 1 | 0         | 1          | 0          | 1          | 1          | 1          | 1         |
| 2 | 0         | 1          | 0          | 1          | 0          | 1          | 1         |
| 3 | 0         | 1          | 0          | 1          | 1          | 1          | 1         |
| 4 | 0         | 0          | 0          | 1          | 1          | 1          | 1         |

(5, 218)

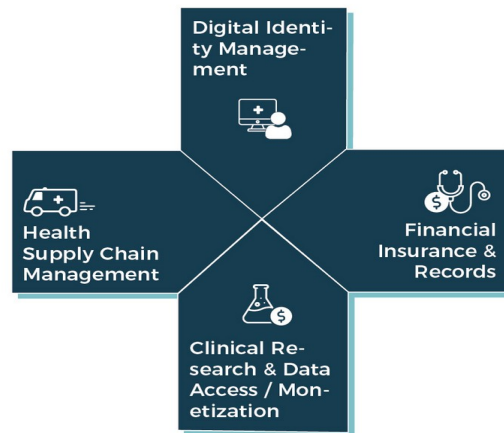
[illegible]

# Underlying Technology

## Techniques, Tools and Infrastructure

- A platform for building and running in-silico models
  - PBPK Modeling
  - Integrated with Molecular dynamics suites
  - Machine learning and statistical analysis
  - Visualization software and web-based interfaces
- Data integration and management tools for Big Data
  - API's, cloud-based solutions, etc
  - HPC Clusters
- Blockchain-based Integrations
  - On-chain metadata, smart contracts, decentralized storage
- IT Support for building, deploying and maintaining
- Highly available network for our business

## BLOCKCHAIN Use case categories in Healthcare



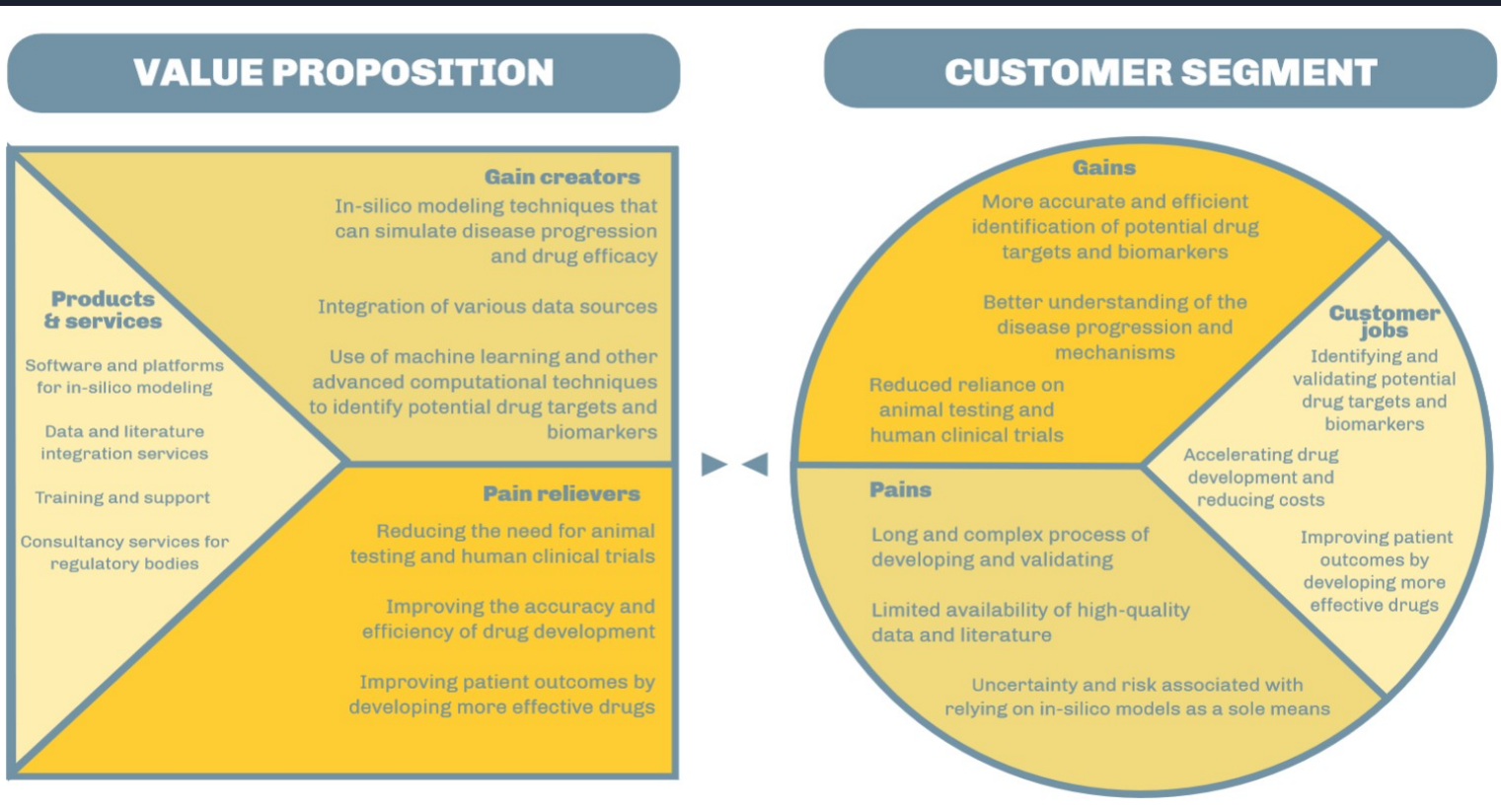
Web3 technologies, such as blockchain, can be used in healthcare to improve

- Data Storage


In our case we intend to

- Generate a confidence factor
- Improve credibility by putting metadata on-chain for verification

# Value proposition and Longevity Challenge







**We aim at improving transferability of research results from animal to human trials and eventually replace parts of animal trials with in silico models.**

**Our current aim is to present a PoC around detecting toxicity of drugs for humans that are developed using animal trials (e.g. Alzheimer's).**

**Incorporated as a part of our aim is recent research that focuses a lot on not only longevity, but also "Healthy Longevity", which includes knowing about long-time toxicity of a drug but also patient conditions and life-quality.**

# Audience and IP Strategy

## IP Strategy:

- Patents for simulation algorithms and data integration methods
- Open-source data storage and blockchain integration
- Exclusive licensing agreements for certain technology and simulation methods with clear terms for sharing and collaboration
  - Dual-licensing model
  - Commercial vs Open-source licensing
- Option for individual patients to own and control their own data

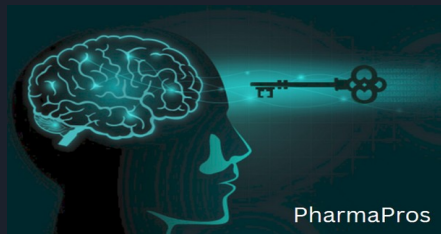
## Target Audience:

- Pharmaceutical companies
- Biotechnology companies
- Medical Device Manufacturers
- Research Institutions



# Competition

Our Niche:



- Stronger emphasis on integrating data from various sources
- Incorporating blockchain technology to secure data and improve traceability and verifiability of results
- Providing a digital twin for improved visualization and intuition in drug discovery and real-time information for more up-to-date insights
- Combining in silico modeling with in vivo testing to provide a more comprehensive approach to drug discovery

## The Landscape

Artificial Intelligence and Machine Learning for Drug Discovery:



Pharmacokinetic and Pharmacodynamic Modeling:



Computational Tools for Drug Discovery:



# Validation and Feasibility

## Validation:

- We will need to test and validate the simulation and data integration methods
  - Leverage partnerships
- Compare simulation results to in vivo and in vitro experimental data



## Feasibility:

- Proof-of-concept studies with industry partners
  - Demonstrate utility
  - Examine cost-effectiveness
- Scalability analysis to ensure the platform can handle large amounts of data and multiple simultaneous users

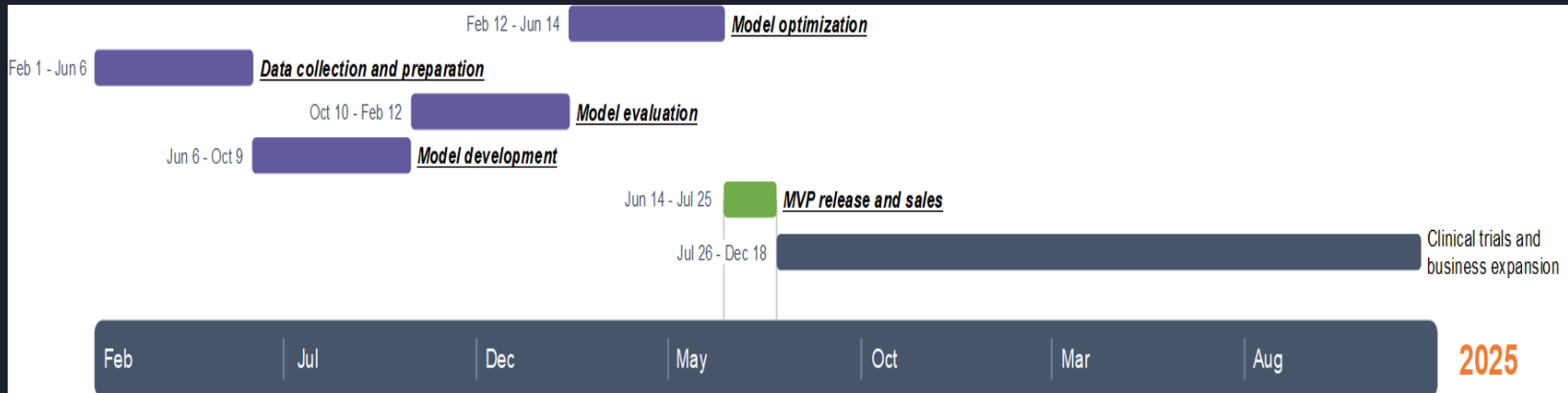
# Novelty

- Increasing the traction of alternative drug-discovery methods
  - Reduce need for specific types of animal trials out of the box
- Use of advanced modeling techniques
- Integration with other in silico platforms
- Personalized predictions on how to modernise your workflow
- Examine a much broader range of “What-if” scenarios
- Interoperability with existing scientific tools



# Timeline and Revenue Model

## Gantt Chart for Development Timeline

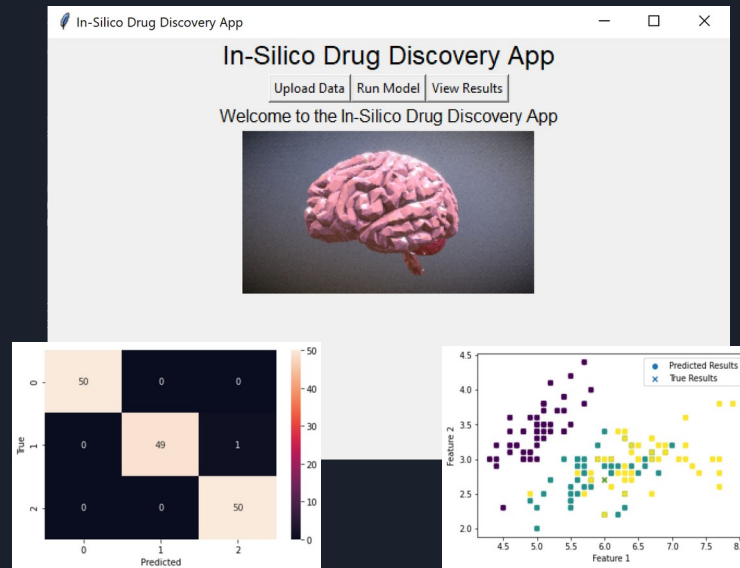


## Ways we could make money at onset

- Subscription-based model
  - Charging a medium fee to use our plugin for a popular software suite
  - One time fees for utilization of tool
- Consulting services
  - Fee for helping customers use the tool better
  - Fee for insights generated by our experts

# Conclusion

- Develop an accurate and reliable method for predicting drug efficacy and toxicity in Alzheimer's disease  
(reduces the reliance on animal models)
- Blockchain technology to improve confidentiality and open access
- Plan to continue to test and validate our MVP, seek funding and partnerships
  - Develop a plugin and web interface



PharmaPros: *Unlocking the secrets of Alzheimer's one in-silico model at a time*

# PharmaPros Team



Triyaksh Mathur  
VR developer and  
bioengineer



Tanvi Dhamdhare  
T.Y Student B.tech



Taha Abdullah  
Android & IoT



Michael Rizzo  
Engineer (ECE)



Omnya Mohamed  
Izzeldin  
Bioengineer and Data  
Science