



UQ - B³i Drug Di Chall

Wednesday, May 31 -

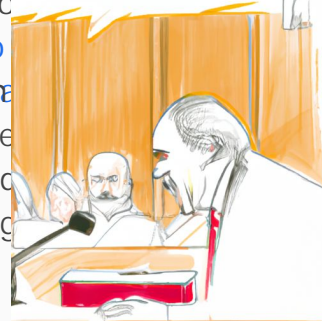
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The following exercise is provided solely for informational purposes and should not be considered real or implemented in any practical application. The information provided are intended for training purposes only and do not have any resemblance to real-world applications. It is essential to exercise caution and seek appropriate advice when dealing with real-life situations or making decisions. No liability is taken based on the content of this exercise and it should not be applied to monetary transactions, rewards, or financial decisions. It should not be misconstrued as real or applicable.

ELM-THERAPEUTICS CEO INDICTED

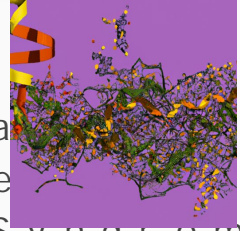
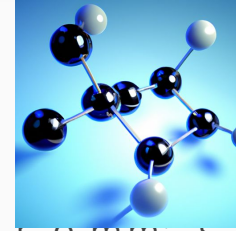
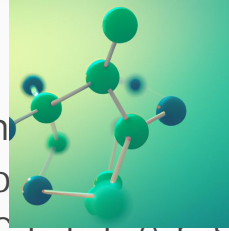


Pharmaceutical company Elm-Therapeutics finds itself in dire straits. The company's stock price has plummeted since the previous year's series of drug candidates that incurred substantial losses. The CEO has been forced into retirement. The company's shoddy statistical analyses led to the discovery that it had been falsifying data and hiding losses from shareholders.



ELM-THERAPEUTICS THROWS HAT THE HUNT TO CURE GIFFERSTROM'S

Taking their last bit of funding, ELM-THERAPEUTICS has
attempt the creation of a novel treatment for a previously
described genetic disease, Gifferstrom's Syndrome.
The disease is characterized by a malfunctioning
cytoplasmic protein that eventually
and causes damage across various organs.



ELM-THERAPEUTICS USES ML FOR

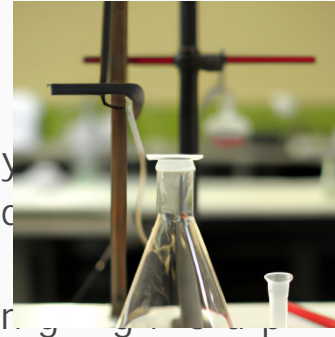
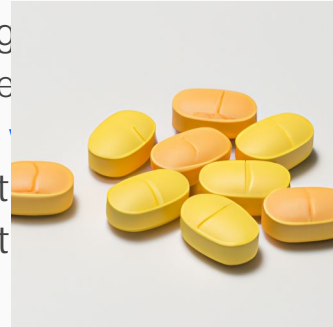
Using advanced LLM-based machine learning for chemical discovery, the company has discovered 6 candidates. The company performs human derived cell studies in house with these drug candidates and automation microscopy.

Compound	Tested efficiency	Mechanism of action
TDZ1098	Unknown	Unknown
ABT1564	Unknown	Unknown
ANX5511	Unknown	Unknown
KOS1273	Unknown	Unknown
OGX1900	Unknown	Unknown
TMCA187	Unknown	Unknown

ELM-THERAPEUTICS CONTRACTS UQ-BIO SUMMER SCHOOL IN FIM

Oh no! ELM-Therapeutics cut the 2022 to save money (thus causing reputational damage) but they have to work on their data that the most promising.

ELM-Therapeutics CTO, Sam Jimmerson, was a participant. Having build strong participation in the UQ-Bio Care out and transferred the summer school company and offer to hire the best board of this struggling multi-t included).



UQ-B³ Drug Discovery Challenge

The challenge requires the diverse and skilled teams, expertise from various sciences, their collective knowledge and their enthusiasm for collaboration. Teams will embark on an intense journey to unravel the mysteries surrounding the target. The **ultimate objective is to decipher the underlying mechanisms** of the drug's impact on the genetic safety of the drug for potential



Rules of the challenge

Teams: teams consisting of 5-6 scientists and one co

Tasks: Each team will participate in five tasks: experim
learning, model generation, and model parametrizat

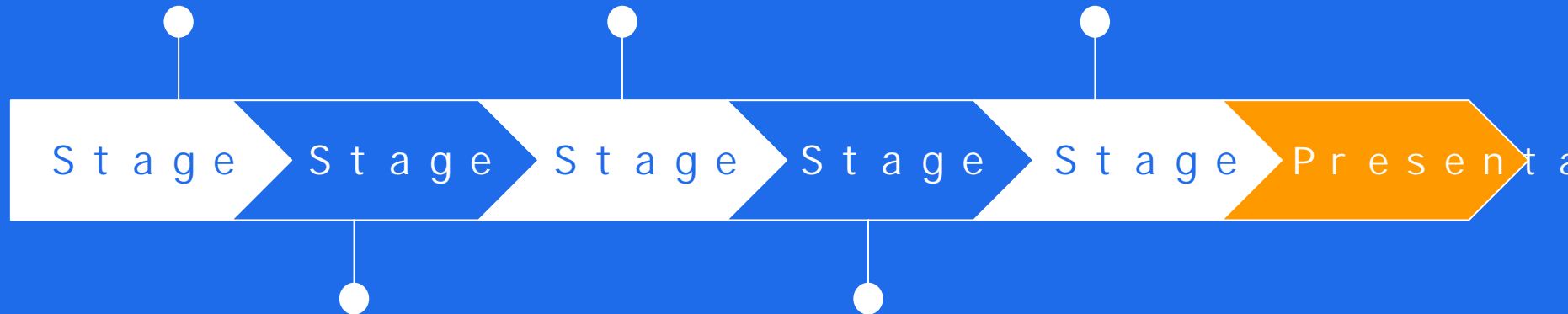
Time: The challenge last 2 weeks, with final presentati

Expected Results: Teams will present their final results for
selection of the final drug, and their efforts to d

Final Evaluation: that gives the clearest and most c
reproducible codes and clear statistical analyses)

Challenge Stages

Experimental (Luis / Will) Quantification (Will / Zach) Linear Model (Michael / Kaan) Parametrization



Statistical Analysis (Brian / Ania) Model Generation (Joshua / Michael / Keisha)

Stage 1: Experimental

Instructional/Will

Materials: related microscopy images

Task: Create a streamlined image processing pipeline to quantify protein and RNA expression in simulated

Expected (output) CSVs: file with processed data and generate these data from image sets. Data will include protein concentration (AU), number of mRNA in nuclei, and transcription sites.

The team that produces the fastest and most accurate results will be awarded the title of "Image Analysis Expert" and will be responsible for subsequent tasks.

Stage 2: Statistical Analysis

Instructor: Britton / Ania

Material: CSV dataset from image processing for all drugs

Task (1): Visualize and analyze statistics for cell death rate using bar plots, histograms, and summary statistics. Calculate correlations between features. Determine statistical significance of drug treatment effects. Perform similar analyses on any appropriately formatted data.

Expected Output: Presentation of data and comparison of assigned drugs in terms of their efficacy (fraction of deaths). Based on all teams' analyses, the entire team will continue testing in the next stage.

The team that produces the clearest and most statistically significant results will be awarded the title of "Community Favorite" and will be available to all other teams.

Stage 3: Machine Learn

Instructions: Each

Material: A pre-trained image analysis pipeline (stage 1) that generates and processed CSV files) for drug titration experiment (training concentrations (testing data)).

Task (1) Perform regression analysis and machine learning to predict cell vitality, and other cell response features as functions of drug concentration on held out data sets with unlabeled drug concentrations. (3) The model maximizes the reward metric for efficacy and minimizes toxicity (expression).

Expected Output: (1) A statistical model to relate cell features to drug concentrations in the three held out samples. (3) Predicted Reward. (4) A streamlined notebook performing all regression

The team that produces the most accurate estimates of the drug concentration, the title of "Artificial Intelligence Experts", and their

Stage 4: Model Generation

Instructor: Michael / Keisha

Material: Various hypotheses for the mechanism of the

Task (1) Propose stoichiometry vectors and propensities that could reproduce the observed statistics of the data. Simulate the dynamics of these models before and after the intervention. (3) Tune parameters by hand to reproduce the data.

Expected Output: A clear presentation of different candidate mechanisms, and direct comparison of statistics and model responses for each model. (2) A streamlined notation for the models.

The team that produces the most efficient and clear "Cell Simulation Experts", and their codes and models.

Stage 5: Model Parameter

Instruction: Mitchell / Kaan

Material Chosen Model Hypothesis (Stage 3) + Dataset (Stages 0-2).

Task(1) Propose a simplified model to capture the gene expression and drug effect and solve this maximum likelihood of data given the model and an arbitrary adjust parameters to maximize the FSP MLE analysis available data. (4-optional) Quantify parameter sweeps or MCMC. (5) Use model to predict responses have not previously been tested (provided by control)

Expected(1) Output Parametrized model and FSP analysis Streamlined notebook to analyze model and search response and cell vitality versus time for required

The Stage 5 Challenge will be evaluated along

Final Stage: Project P

On Tuesday, June 13, 2023 at 2:00pm, ,
and explain your team's approach. to a
winner team, based on the following factors

Presentation quality

Reproducibility of approach

Statistical rigour

Team's ability to respond to technical que



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