#### Keywords: Modelling, Biolab, Optimisation, Machine Learning

### Title:

Optimization Algorithm for Rapid Enzymatic Screening: A Fisher Information Matrix (FIM) and machine learning based Approach

# **Objective:**

To design, develop, and validate an optimization algorithm for efficient enzymatic screening. The algorithm will focus on suggesting new experimental setups while using the experimental data from the previous experiments. The parameters that the algorithm shall suggest include temperature patterns, substrate and buffer concentrations. Therefore, we want to compare different methods including Fisher Information based approaches and Bayesian Optimization.

# Tasks:

#### Literature Review:

a. Investigate the current state-of-the-art methods used in enzymatic screening, emphasizing optimization algorithms.

b. Dive into FIM-based approaches to understand their advantages and challenges in the context of enzymatic screening.

c. Look into Bayesian Optimization techniques.

#### **Parameter Estimation:**

a. Develop a robust method for parameter estimation essential for the FIM calculation.

b. Test and validate the estimation method using preliminary experimental datasets.

c. Fit a model that uses the Bayesian Optimization paradigm, i.e. a Gaussian process.

### **Algorithm Development:**

a. Implement an optimal experimental design-based Algorithm.

b. Ensure the developed algorithm can process experimental outputs efficiently to recommend new experiments within a one-hour window.

#### **Implementation and Integration:**

a. Integrate the developed algorithm with a platform that receives online experimental outputs.

b. Develop a interface to allow the automated experimental setup to read the experimental conditions and execute subsequent experiments.

# Validation and Testing:

a. Utilize real-world enzymatic screening datasets to test the efficiency and accuracy of the developed algorithm.

b. Compare the performance of the algorithm against existing methods in terms of speed, accuracy, and reliability of recommendations.

# **Optimization and Refinement:**

a. Analyze feedback and results from testing to identify areas of improvement.

b. Refine the algorithm based on identified challenges and retest using different datasets.

### **Documentation and Presentation:**

a. Document the development process, methods, and findings in a structured manner.

b. Prepare a presentation to showcase the developed algorithm, its advantages, and its potential impacts on the enzymatic screening process.

### **Conclusion and Future Recommendations:**

a. Summarize the research findings and the algorithm's performance in the context of enzymatic screening.

b. Provide recommendations for further enhancement or adaptation of the algorithm for other screening processes.