

## Intro To Systems Biology - Project

Pranay Gupta (20161088)

Ayush Deva (201501098)

**Project Topic:** Using system-based methodologies to analyze the mycolic acid pathways (MAP).

**Project Overview:** During drug discovery, it is common to identify biological agents/pathways that are crucial for the growth and survival of the pathogen. By identifying and inhibiting certain important reactions in these pathways, we can inhibit the growth of the disease, helping in its cure.

In this project, we aim to look at one such pathway for identifying targets for anti-Tuberculosis drugs. *Mycobacterium tuberculosis*, the pathogen responsible for TB, is closely linked with mycolic acids for its growth and survival. Hence, we shall understand the mycolic acid pathways (MAP), as thoroughly studied in [1], and try to understand how flux balance analysis helps us identify these targets.

### Methodologies

1. **Literature Review:** Study and understand the existing literature concerning flux balance analysis, stochastic modeling, and drug target identification.
2. **Model Building:** Through [1], we wish to build a model for the MAP using the set of reactions already given on the project page.
3. **FBA:** Constructing the stoichiometric matrix and performing Flux Balance Analysis of the model. We have 219 reactions, 28 proteins, and 197 metabolites.
4. **Effect of Removing Reactions:** We wish to analyze how the removal of certain reactions affect the pathways. This hasn't been currently talked about in [1].

### References :

[1] Raman, Karthik, Preethi Rajagopalan, and Nagasuma Chandra. "Flux balance analysis of mycolic acid pathway: targets for anti-tubercular drugs." *PLoS computational biology* 1.5 (2005).

[2] Raman, Karthik, and Nagasuma Chandra. "Flux balance analysis of biological systems: applications and challenges." *Briefings in bioinformatics* 10.4 (2009): 435-449.

[3] Colijn, Caroline, et al. "Interpreting expression data with metabolic flux models: predicting *Mycobacterium tuberculosis* mycolic acid production." *PLoS computational biology* 5.8 (2009).

[4] Chen, Liang-Chun, et al. "Identifying co-targets to fight drug resistance based on a random walk model." *BMC systems biology* 6.1 (2012): 5.