Indian Institute of Technology Delhi

School of Interdisciplinary Research (SIRe)

SIRe Project Number

2022-01-01

(will be assigned by SIRe)

PhD Project

Project Details	
Project Title	Deep learning-based prediction of metabolite concentration class and reaction class prediction in synthesis pathways.
Project Summary	Measuring metabolite concentrations in biological samples is a non-trivial task, and this often involves elaborate and time-consuming methods of extraction, biochemistry, and analyses. Additionally, the process requires the use of sophisticated and expensive analytical equipment and a skilled workforce. Plants are an excellent source of metabolites with proven agrochemical, pharmaceutical, cosmetic and medicinal value. An easy-to-use solution to select plants bearing a higher concentration class of metabolites in its organs will provide a powerful solution to the industry. It shall bring the final price of metabolite lower. The proposal aims to collect plant organs, measure specific intracellular metabolites, and design and use sophisticated deep learning tools to measure metabolite class prediction using the morphology of images. Pathway tools and databases are valuable repositories that allow us to infer and understand the order of reaction events leading up to the synthesis of plant-derived secondary metabolites of industrial importance. Pathway engineering and synthetic biology rely on this information to engineer components of key pathways in heterologous host organisms. However, the information on many pathways leading upto the synthesis of secondary metabolites is at best patchy and only partially available. The gaps in those pathways are a severe impediment in inferring the correct sequence of events leading to the synthesis of secondary metabolites. The proposal aims to learn and build deep learning-based models from known and predicted structures, and use the models to learn and build models from the known structures, and use the models to predict the potential reaction class resulting in a specific reactant-to-product transformation. Doing so further helps in narrowing down the set of potential enzymes catalyzing unassigned reactions.

PhD Supervisors

Role	Faculty	Academic Unit in IITD/Others	Email ID
Supervisor 1	Professor Aditya Mittal	Kusuma School of Biological Sciences	amittal@bioschool.iitd.ac.in
Supervisor 2	Professor Binay Panda	School of Biotechnology, JNU	binaypanda@jnu.ac.in

Project requirements (Student qualifications, experience required, etc.)

- First class UG/PG degree in Computer Science, Chemical/Biochemical Engineering, Biotechnology, Chemistry or related fields from a reputed institution.
- Experience in using image-based deep learning tools, preferably with biological data.

Source of funding (IRD/FITT Project details, if any)

DBT (extramural funding), Full time

Role of Faculty Members involved:

- Binay Panda: Metabolite concentration measurement, Deep learning tools design and optimization for metabolite concentration class determination.
- Aditya Mittal: Structure-based design of deep learning tools for reaction class determination.