School of Biological Sciences College of Science

Reg. No. 200604393R

Research Theme: Computational Biology; Microbial Genomics; Al

PhD Research Project Title: LLM-Guided Knowledge Graph to Identify Druggable Microbiome Targets

Scholarship category (Please indicate the type of scholarship for this project):

(a) SBS Research Student Scholarship (for SBS faculty only)

Principal Investigator/Supervisor: Dr. Anni Zhang (AnniZ Lab https://genomiverse.net/)

Co-supervisor/ Collaborator(s) (if any):

Project Description

a) Background:

The gut microbiome plays a key role in neurological diseases, especially through the gut-brain axis. However, the expanding volume and heterogeneity of microbiome literature make it difficult to identify consistent, druggable targets for intervention. Existing literature mining tools mostly summarize known relationships and rarely propose new hypotheses. This highlights a critical need for an efficient and systematic approach that integrates the literature to discover previously unrecognized therapeutic targets.

b) Proposed work:

We propose to use large language models (LLMs) to extract entities and relationships—such as bacterial genes, species, pathways, metabolites, host organs, and disease states—from one million gut microbiome publications. These will be used to construct a comprehensive knowledge graph. We will then apply AI models, including graph neural networks, to generate new hypotheses by predicting novel associations between bacterial genes and neurological diseases.

- Aim 1: Build the knowledge graph. We will develop an LLM-based pipeline to extract structured information from full-text publications. Accuracy will be evaluated against benchmark datasets. An AI model will be trained on the graph to predict novel associations.
- Aim 2: Prioritize targets. We will design a ranking algorithm to identify microbiomederived genes most strongly associated with neurological diseases, based on network connectivity, strength of evidence, and study consistency. We will validate findings using public metagenomic datasets.

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c) Preferred skills:

- A curiosity about microbes
- An interest in coding
- A dedication to research

Coding or data analysis experiences would be a big plus, but not necessary.

Supervisor contact:

If you have questions regarding this project, please email the Principal Investigator: anni.zhang@ntu.edu.sg

SBS contact and how to apply:

Associate Chair-Biological Sciences (Graduate Studies): <u>AC-SBS-GS@ntu.edu.sg</u>
Please apply at the following:

Application portal:

https://venus.wis.ntu.edu.sg/GOAL/OnlineApplicationModule/frmOnlineApplication.ASPX