



**Research Theme: Virology; Biophysics; Structural Biology; Drug discovery; Computational Biology**

**PhD Research Project Title: AI-facilitated *de novo* design antiviral fusion inhibitors**

**Scholarship category (Please indicate the source of funding for this project):**

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

**Principal Investigator/Supervisor: Xiao Tianshu**

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

**Project Description**

**a) Background:**

Infectious diseases caused by enveloped viruses, such as coronavirus and flavivirus, are critical threat to public health system, but mostly without effective antiviral drugs. Envelop protein located on the surface of viral particle is responsible for viral entry, the first step of infection cycle. Given the critical function, the envelop protein, such as S protein of coronavirus and E protein of dengue, is major target of immune responses and focus of antiviral research.

**b) Proposed work:**

In this project, we will de novo design inhibitors based on structure of the Envelop protein using AI-empowered methods. In combination of structural biology, biochemical and biophysical, the project aims to identify potent broadly effective inhibitors to block viral entry.

**c) Preferred skills: exposure to basic protein-related wet-lab skills, eg. Protein expression, purification and molecular cloning. Computation work on data analysis would be a big plus, but not indispensable**

**Supervisor contact:**

If you have questions regarding this project, please email the Principal Investigator: Xiao Tianshu, [tianshu.xiao@ntu.edu.sg](mailto:tianshu.xiao@ntu.edu.sg)

**SBS contact and how to apply:**

Associate Chair-Biological Sciences (Graduate Studies) : [AC-SBS-GS@ntu.edu.sg](mailto:AC-SBS-GS@ntu.edu.sg)

Please apply at the following:



**NANYANG  
TECHNOLOGICAL  
UNIVERSITY**  
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Reg. No. 200604393R

**Application portal:**

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