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| **Research Theme: Computational Biology; Functional Genomics** |
| **PhD Research Project Title:**  Develop reverse docking techniques for drugs repurposing |
| **Principal Investigator/Supervisor: Mu Yuguang** |
| **Co-supervisor/ Collaborator(s) (if any):** |
| **Project Description**  **a) Background With the fast development of AI methods for protein structure prediction, the 3D structures of all proteins in human genome are available. This gives us a chance to exam possible protein targets for FDA drugs.**  **b) Proposed work: Develop benchmark dataset to test the accuracy of applying the current docking tools in the exercises of reverse docking. Improve docking and scoring functions to achieve better accuracy. Apply these functions to search protein targets for biologically important molecules, e.g., the main components of traditional Chinese medicines.**  **c) Preferred skills: 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:** |
| **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:  **Application portal:** <https://venus.wis.ntu.edu.sg/GOAL/OnlineApplicationModule/frmOnlineApplication.ASPX> |