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| **Research Theme: Computational Biology; Functional Genomics** |
| **PhD Research Project Title:**  Combining target and ligand- based tools for super-large molecular library virtual screening |
| **Principal Investigator/Supervisor: Mu Yuguang** |
| **Co-supervisor/ Collaborator(s) (if any):** |
| **Project Description**  **a) Background: In virtual screening millions of small molecules are needed to check their fitness to a certain protein/RNA/DNA target. Due to the large chemical space, the number of possible small molecules can be 10\*\*20. Usual structure-based docking tools are too slow to handle so many small molecules in a limited period. So much faster ligand-based searching algorithms are needed.**  **b) Proposed work: Develop ligand-based virtual screening tools based on graph representation of molecules in the frame of encoder-decoder which is combined with structure-based docking tools. In such a way 10 billion order of molecule library can be screened in a feasible short period.**  **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> |