

# CSCB Virtual Seminar Series

## Toward high-throughput activity prediction of protein mutants.

**Date:** 6<sup>th</sup> December 2021 (Monday)

**Time:** 12noon-1pm (SGT)

**Venue:** *via Zoom*

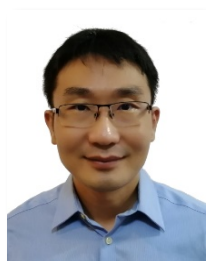
For details, please contact:

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### Abstract:

My group has been developing and applying computational methods to accurately predict 3D structures of protein mutants, and to evaluate the effects of these mutations on protein function and dynamics. Today I will present our recent studies on structure-function mechanism of human transporter Mfsd2a, cancer mutations and drug response of BRAF kinase, and catalysis engineering of bacteria enzymes with machine learning.

### Speaker:



### Dr. Hao Fan

Adjunct Associate Professor, Cancer and Stem Cell Biology (CSCB), Duke-NUS Medical School

Senior Principal investigator, Laboratory of Structure-based Ligand Discovery and Design, Bioinformatics institute, A\*STAR

**Dr. Hao Fan** received his B.A. from University of Science and Technology of China (USTC) in Biological Sciences. He obtained his Ph.D from University of Groningen (RUG) in Biophysical Chemistry supervised by Prof. Alan Mark. After PhD study, he did postdoctoral research at University of California, San Francisco (UCSF) supervised by both Prof. Andrej Sali and Prof. Brian Shoichet. Dr. Fan established his first independent laboratory at the Bioinformatics Institute, A\*STAR as Principal Investigator.

Dr. Fan has focused on developing computational methods to study protein-ligand interactions, including protein structure modelling, molecular docking, molecular dynamics simulations, chemoinformatics, and machine learning. The developed methods are used in basic research, to help understand and regulate biological processes, in particular, structure-function mechanisms of GPCRs, transporters, and kinases. Meanwhile, these methods were also employed in applied research, including preclinical drug development, enzyme engineering, and chemical toxicity identification.

### Host:

### Lisa Tucker-Kellogg

Assistant Professor  
Programme in Cancer & Stem Cell Biology  
Duke-NUS Medical School  
Singapore

**No registration is required.  
All are welcome.**