Computational modeling of protein-ligand interactions

Hao FAN
https://web.bii.a-star.edu.sg/~fanh
https://www.a-star.edu.sg/bii/research/bsmd/sldd
Structure and function (basic research)  

Outside: BELGIUM, CHINA, USA  
Local: NCCS, DUKE-NUS

Krishna Deepak, Ravi Verma, Shreyas Supekar, Xu Qisong  
Enzyme engineering (applied research 1)

Shreyas Supekar, Zhao Lina, Yossa Hartono, Ho Wei Chin

Structure 2020, DMM 2020

Outside: UK, HUNGARY
Local: Sebastian, ICES, SIFBI, IHPC, NUS SynCTI
Food and chemical safety (applied research 2)

Local: Lit-Hsin, Sebastian, Hwee Kuan, IMCB, NUS Pharmacy

Chaitanya Jaladanki, Ravi Verma, Lin Fu

Arch. Tox. 2020, Mol. Pharm. 2021, JPET 2020
Ligand discovery (applied research 3)

Local: SIFBI, GIS, NCCS, NUS microbiology

Zhao Lina, Du Weina, Srdan Masirevic, Chaitanya Jaladanki

IJMS 2020, iScience 2021, Patent 2020, TD 2021