

Graduate Student

- 1. Foundations
- 2. Pharmacometrics
- 3. Computational Medicinal Chemistry

- 1. Foundations
- 2. Neurology / Psychiatry
- 3. Pharmacometrics (course coordinator)



Graduate Student



Nan Wu (UOI-PhD)



Graduate Student



Tianjian Liang (UOP-PhD)



Chih-Jung Chen (UOM-PhD)
Jiayi Yuan (UOP-PhD)
Chen Jiang (UOP-PhD)
Yixuan Hao (Res. Assi.)



Graduate student



Siyi Wang (UCSF-PhD)
Mingzhe Shen(UM-PhD)



- 1. Foundations
- 2. Systems Pharmacology
- 3. Computational Medicinal Chemistry

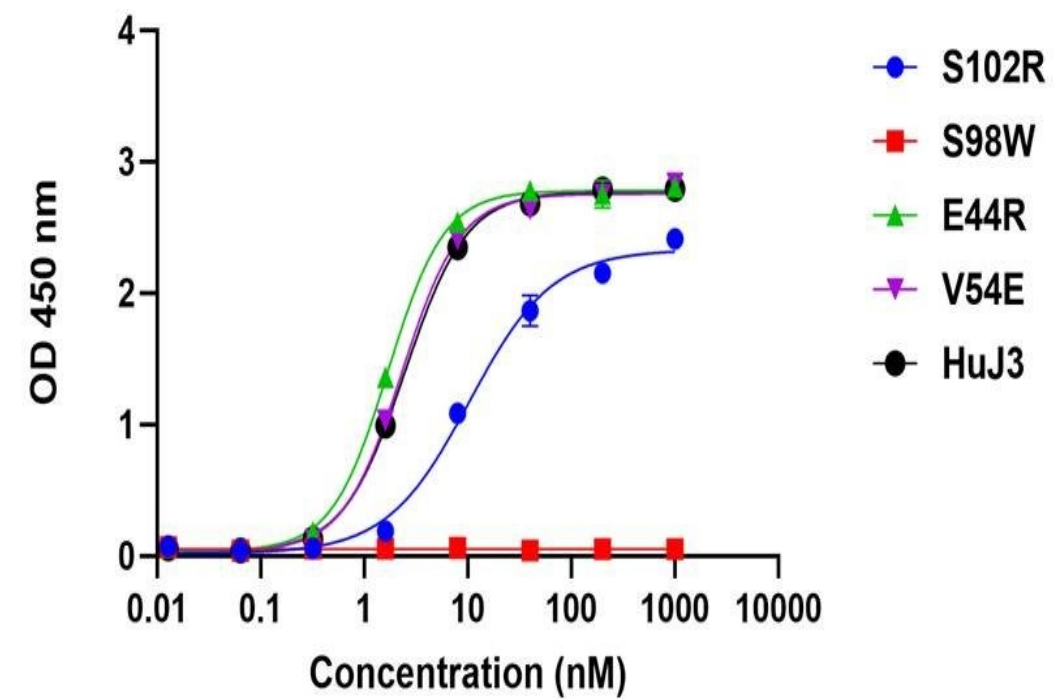
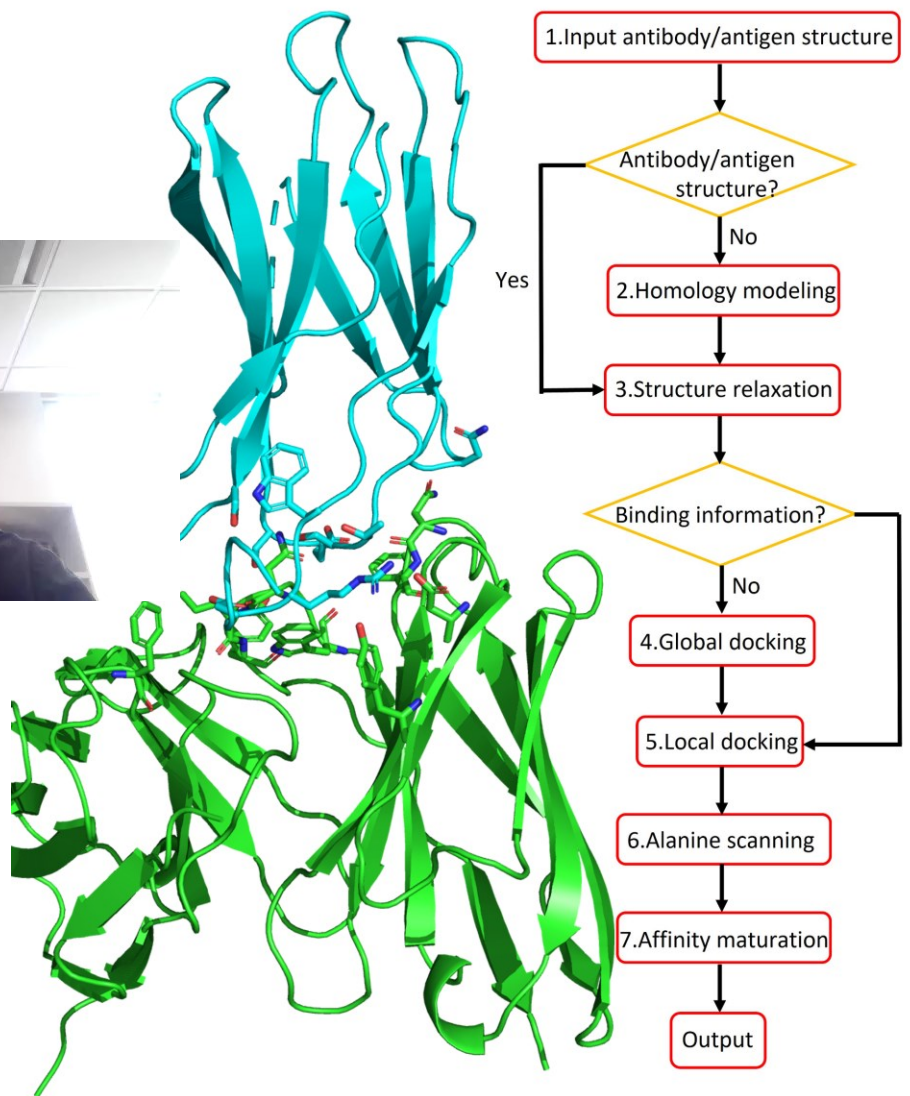
- 1. Foundations
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1 Antibody discovery

Briefings in bioinformatics, 22(5), bbab143.

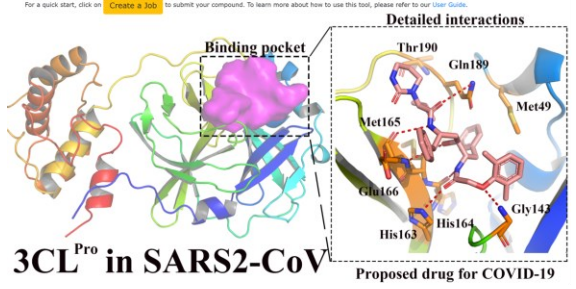
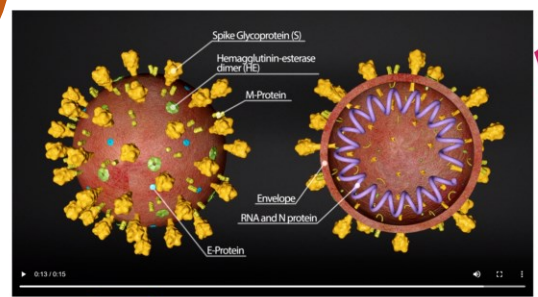


Affinity determination of HuJ3 variants predicted by the in silico (*Flex ddG*) affinity maturation. The binding affinity was tested by ELISA. The HIV B clade gp140 antigen was coated in immunosorbent plates followed by addition of gradient concentrations of HuJ3 variants. After washing, the binding was detected by the HRP conjugated anti-FLAG tag antibody. Colomeric development was achieved by the TMB substrate. HuJ3 harboring the E44R mutation shows enhanced binding affinity compared to the prototype HuJ3.



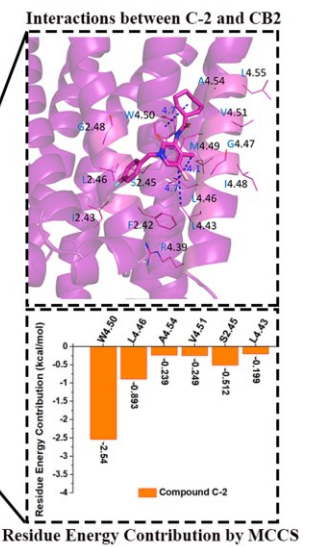
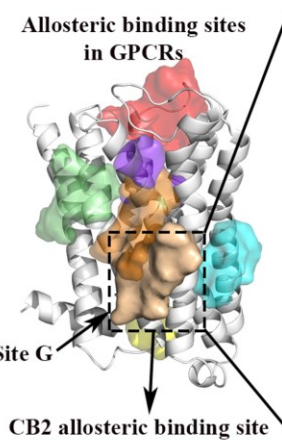
2 Algorithms & Application

Molecular Complex Characterizing System



Approved drug for OVID-19

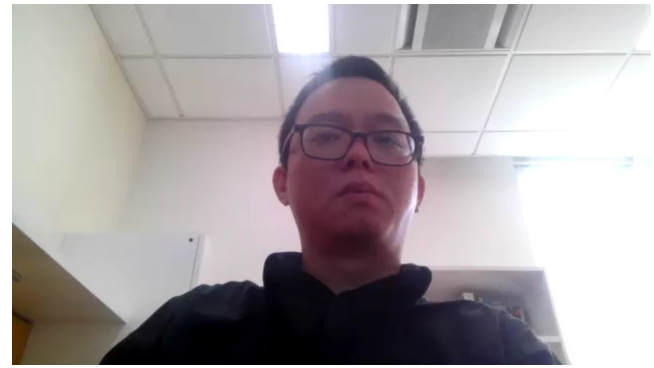
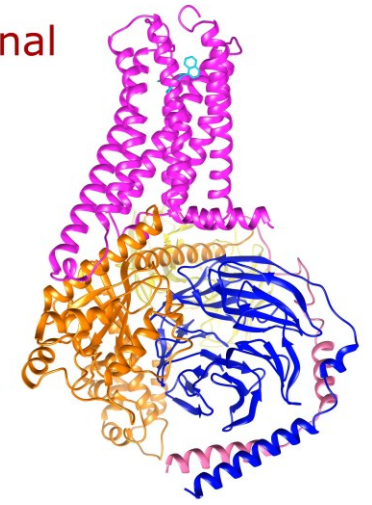
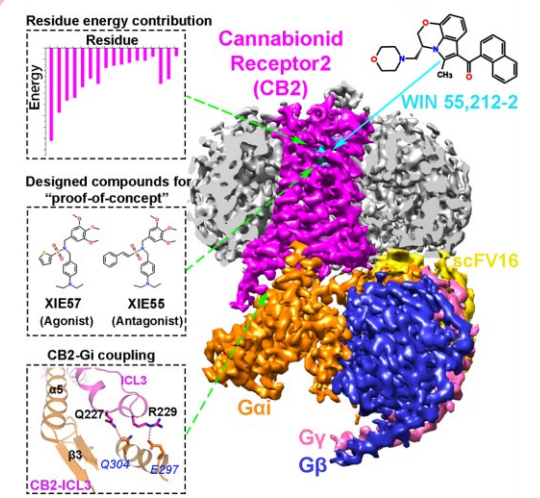
MCCS



MCCS-Cryo-EM

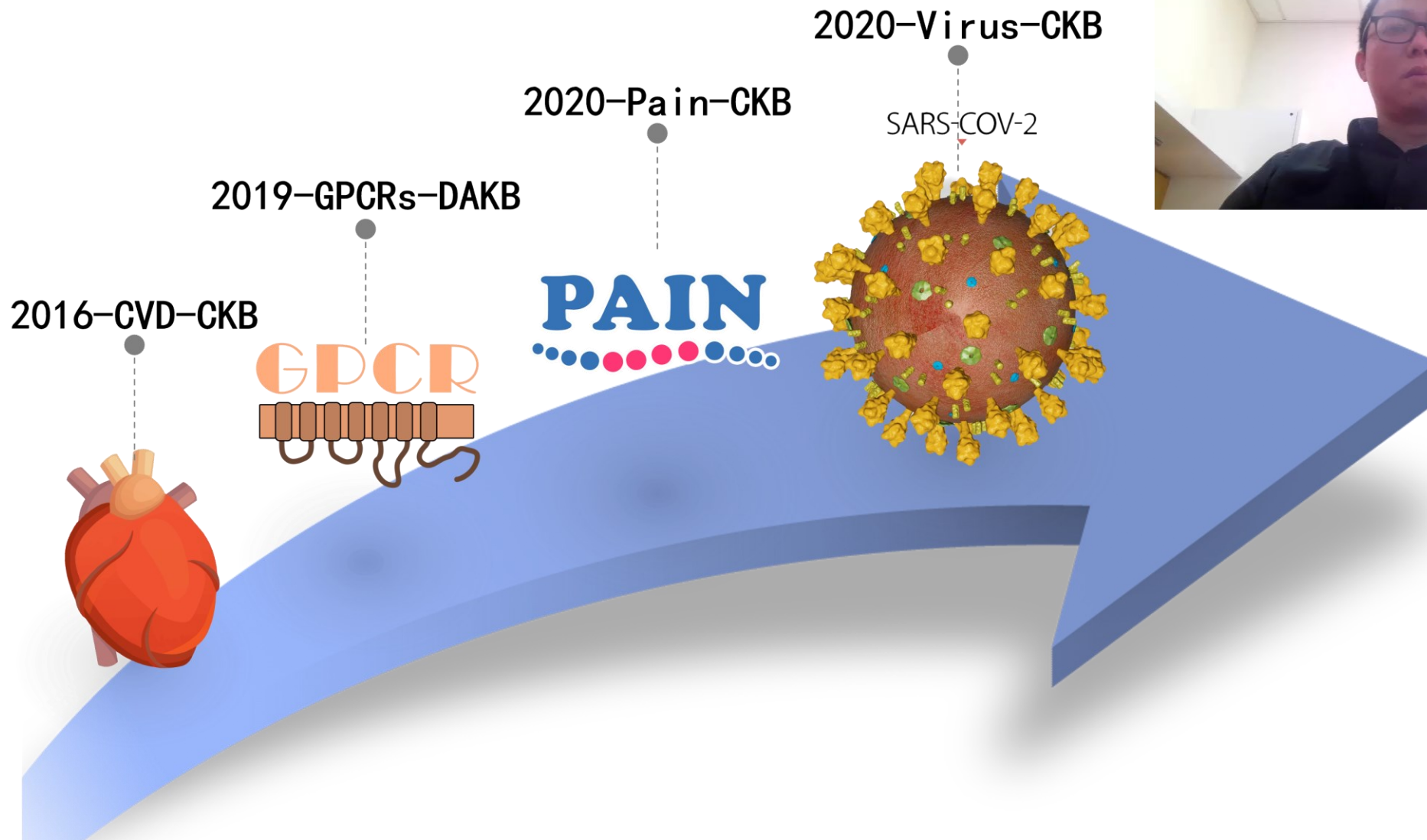
GPCRS Binding Feature

2020 CELL journal





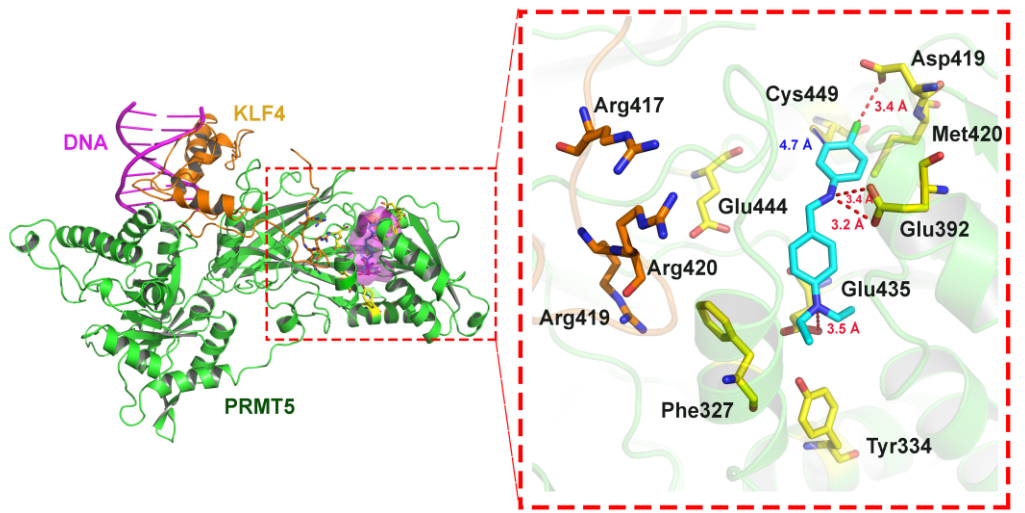
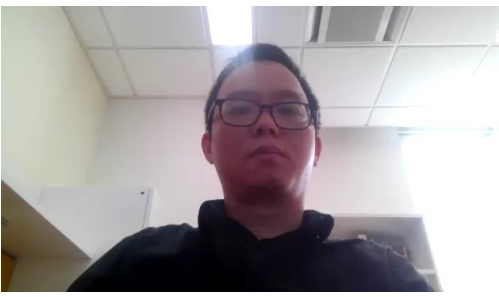
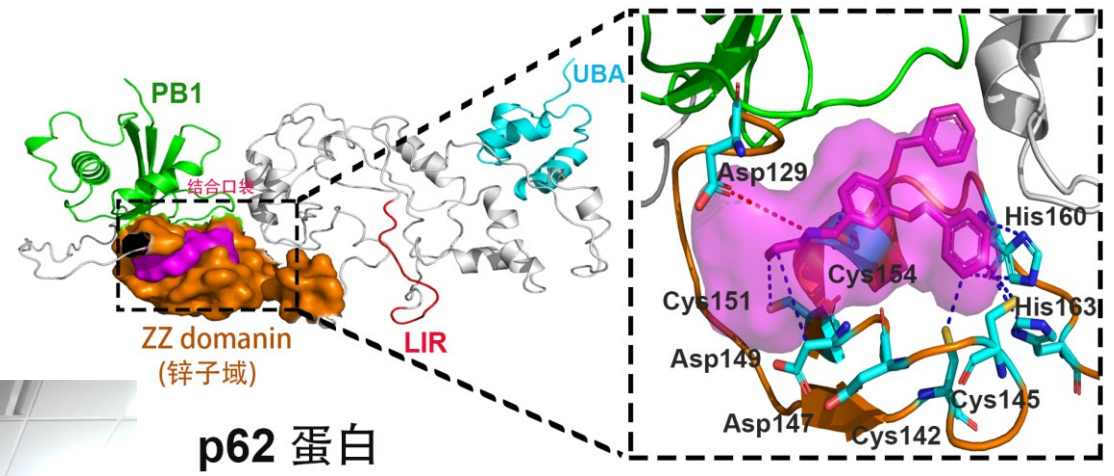
3 Knowledgebase



CVD-CKB ([Sci. Rep. 2016,\(1\), 1-14](#));DAKB-GPCRs ([J. Chem. Inf. Model., 2019, 59, 1283](#));Pain-CKB ([J. Chem. Inf. Model., 2020, 60, 4429](#)) and Virus-CKB ([Brief. Bioinform., 2021, bbaa155](#)).



4 Lead Discovery & Optimization



p62(SQSTM1) first-in-class drug candidate([Nat. Commun., 2017, 8, 1](#)); novel WX2-43 for PRMT5 ([EBioMedicine, 2019, 44, 98](#)); Novel TRPV1 compounds([J. Chem. Inf. Model., 2015, 55, 572](#); [AAPS J., 2016, 18, 898](#)); Novel CB2 agonists-antagonists ([Cell, 2020, 180, 645](#); [Kidney Int., 2018, 94, 756](#)).