创新教育模式
培养一流人才

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研究兴趣：

1)药物分子设计算法与应用
2)蛋白设计和三维结构预测
3)序列分析与功能预测

主要成果：

1)建立了CYSCORE、CB-Dock、FitDock、LigMate、CIS-RR等一系列分子模拟与设计算法与软件，获广泛使用，先后发现了针对MDM2、HSP70、 AchE、PB等药物靶点的活性化合物。

2)发展蛋白设计算法EvoDesign，成功设计出多个靶向HER2、EGFR等药物靶标的高稳定性、高亲和力、抗聚集的人工多肽、蛋白 。

3)建立AbRSA，AbAlign等抗体分析算法，成功完成新冠抗体R3P1-E4的亲和力优化、肿瘤靶标HMGB1、PrPc、 PD1抗体的人源化设计。

工作经历：

2014-今， 四川大学，生命科学学院，副教授
2011-2014，四川大学，生命科学学院，讲师

教育经历：

2020-2021，美国哈佛大学，生物信息，X. Shirley Liu Lab
2016-2017，美国密歇根大学，生物信息，Yang Zhang Lab
2004-2010，中科院生物物理所，生物信息，博士
2000-2004，西南交通大学，应用物理，学士

主要论著：

1. Y Liu, X Yang, J Gan, S Chen, ZX Xiao, **Y Cao***. CB-Dock2: improved protein–ligand blind docking by integrating cavity detection, docking and homologous template fitting. **Nucleic Acids Research**. In press, 2022.

2. X, Yang, Y Liu, J Gan, ZX Xiao, **Y Cao***. FitDock: protein–ligand docking by template fitting. **Briefings in Bioinformatics**. doi.org/10.1093/bib/bbac087, 2022

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10. Z Zhu, Y Fan, Y Liu, T Jiang, **Y Cao***, Y Peng*. Prediction of antiviral drugs against African swine fever viruses based on protein–protein interaction analysis. **PeerJ**, 8, e8855, 2020

11. Y Liu#, M Grimm#, W Dai, M Hou, ZX Xiao, **Y Cao***. CB-Dock: a web server for cavity detection-guided protein-ligand blind docking. **Acta Pharmacologica Sinica**. 41,138-144, 2020 (**ESI高被引论文**)

12. L Li#, S Chen#, Z Miao#, Y Liu, X Liu, ZX Xiao and **Y Cao***. AbRSA: a Robust Tool for Antibody Numbering. **Protein Science**. 28, 1524-1531, 2019

13. **Y Cao**, W Dai, Z Miao. Evaluation of Protein-Ligand Docking by Cyscore. **Methods in molecular biology** 1762, 233-243, 2018

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18. J Guo#, **Y Cao**#, K Qin, X Zhao, D Wang, Z Li, L Xin,Y Shu, J Zhou*. Limited effect of recombinant human mannose-binding lectin on the infection of novel influenza A (H7N9) virus in vitro. **Biochem Biophys Res Commun**. 458(1):77-81, 2015

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20. L Huang#, **Y Cao**#, J Zhou, K Qin, W Zhu, Y Zhu, L Yang, D Wang, H Wei*, Y Shu*., A conformational restriction in influenza A virus neuraminidase binding site by R152 caused the combinational effect of I222T with H274Y on oseltamivir resistance. **Antimicrob Agents Chemother**. 58(3), 1639-1645, 2014

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