Shihang Wang

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EDUCATION

09/2022-06/2025	M.S., Biology, ShanghaiTech University
	Overall GPA: 3.58/4.0
09/2018−06/2022	B.S.A., Aquaculture, Shanghai Ocean University
	Overall GPA: 3.6/4.0

RESEARCH INTERESTS

➢ AI4Science; Computer-aided Drug Design; Molecular Properties Prediction; Generative Model;

PUBLISHED PAPER

[1] **Shihang Wang**[#], Qilei Han[#], Weichen Qin[#], Lin Wang[#], Junhong Yuan, Yiqun Zhao, Pengxuan Ren, Yunze Zhang, Yilin Tang, Ruifeng Li, Zongquan Li, Wenchao Zhang, Shenghua Gao*, Fang Bai*. PhenoScreen: A Dual-Space Contrastive Learning Framework-based Phenotypic Screening Method by Linking Chemical Perturbations to Cellular Morphology. *BioRxiv, 2024*.

[2] **Shihang Wang**[#], Lin Wang[#], Fenglei Li, Fang Bai*. DeepSA: a deep-learning driven predictor of compound synthesis accessibility. *Journal of Cheminformatics,* **2023**, 15, 103. (IF: 8.6)

[3] **Shihang Wang**[#], Zhehan Shen[#], Taigang Liu, Wei Long, Linhua Jiang*, Sihua Peng*. DeepmRNALoc: a novel predictor of eukaryotic mRNA subcellular localization based on deep learning. *Molecules,* **2023**, 28, 2284. (IF: 4.6)

[4] **Shihang Wang**, Xuanyu Xu, Cai Wei, Sicong Li, Jingying Zhao, Yin Zheng, Xiaoyu Liu, Xiaomin Zeng, Wenliang Yuan, Sihua Peng*. Molecular evolutionary characteristics of SARS-CoV-2 emerging in the United States. *Journal of Medical Virology,* **2022**, 94, 310-317. (IF: 12.7)

[5] **Shihang Wang**[#], Yue Zeng[#], Hao Yang[#], Siyuan Tian[#], Yongqi Zhou[#], Lin Wang[#], Xueqin Chen, Haiying Wang, Zhaobing Gao, and Fang Bai*. Discovery of Novel GluN1/GluN3A NMDA Receptor Inhibitors Using a Deep Learning-based Method. *Acta Pharmacologica Sinica,* Peer Review

[6] **Shihang Wang**, Ran Zhang, Xiangcheng Li, Fengyu Cai, Xinyue Ma, Yilin Tang, Chao Xu, Lin Wang, Pengxuan Ren, Lu Liu, Sanan Wu, Qiyang Qian, and Fang Bai*. Recent Advances in Molecular Representation Methods and Their Applications in Scaffold Hopping. *npj drug discovery,* Peer Review

[7] Mengmeng Lin[#], **Shihang Wang**[#], Xudong Zeng[#], *et al.* AI and protein structures facilitate discovering specific antivirals against Coronavirus. Submitted to *Cell*.

[8] Lin Wang, **Shihang Wang**, Hao Yang, Shiwei Li, Xinyu Wang, Yongqi Zhou, Siyuan Tian, Lu Liu, Fang Bai*. Conformational Space Profile Enhances Generic Molecular Representation Learning. *Advanced Science,* **2024**, 11, 2403998. (IF: 14.4)

[9] Bo Li, Bob Zhang, Chengyang Zhang, Weiliang Huang, **Shihang Wang**, Qing Wang, Mengran Li, Yong Zhang, Qianqian Song*. PhenoProfiler: Advancing Phenotypic Learning for Image-based Drug Discovery. Submitted to *Nature Computational Science*.

[10] Pengxuan Ren, Shiwei Li, **Shihang Wang**, Xianglei Zhang, Fang Bai*. Computer-Aided

Prediction of the Interactions of Viral Proteases with Antiviral Drugs: Antiviral Potential of Broad-Spectrum Drugs. *Molecules*, **2023**, 29, 225. (IF: 4.6)

[11] Cai Wei, Dan Sun, Wenliang Yuan, Lei Li, Chaoxu Dai, Zuozhou Chen, Xiaomin Zeng, **Shihang Wang**, Yuyang Zhang, Shouwen Jiang, Zhichao Wu, Dong Liu, Linhua Jiang*, Sihua Peng*. Metagenomics revealing molecular profiles of microbial community structure and metabolic capacity in Bamucuo lake, Tibet. *Environmental Research*, **2023**, 217, 114847. (IF: 8.3)

[12] Xiaoyu Liu, Jingying Zhao, Sicong Li, Cai Wei, **Shihang Wang**, Xuanyu Xu, Yin Zheng, Xiangyu Deng, Wenliang Yuan*, Xiaomin Zeng*, Sihua Peng*. Clarifying real receptor binding site between coronavirus HCoV-HKU1 and 9-O-Ac-Sia based on molecular docking. *Journal of Bioinformatics and Computational Biology*, 2022, 20.

INTERNSHIP EXPERIENCE

➢ 09/2021-06/2022   BGI Research
➢ 09/2020-09/2021   Shanghai Institute of Nutrition and Health, Chinese Academy of Sciences

AWARDS

➢ 2022-2023   National Scholarships, ShanghaiTech University
➢ 2023-2024   National Scholarships, ShanghaiTech University
➢ 2024.9 The first prize in the 2023 Shanghai International Computational Biology Innovation Competition