Lin Wang 王林

Postdoctoral Researcher | Computational Molecular Discovery

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I develop computational methods that integrate chemical priors into molecular representation learning and generative drug design. My research spans AI-driven drug discovery and protein–ligand and protein–protein interaction modeling, with emerging directions in phenotype-based and polypharmacology drug design. My latest work, Ouroboros, advances this broader program through a molecular foundation model that learns chemically informed representations from conformational-space and pharmacophore similarities for molecular property prediction and generation.

Research Focus

- Molecular representation and generation foundation models for medicinal chemistry
- Conformational-space- and pharmacophore-aware molecular representations
- Protein-ligand and protein-protein interaction modeling
- Phenotype-based and polypharmacology drug design

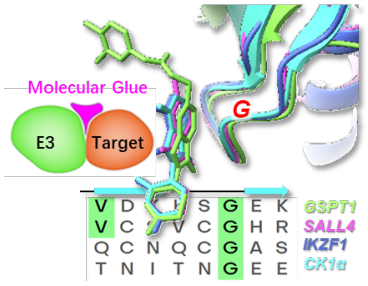
Education and Experience

Current	**Postdoctoral Researcher** Institute of Systems Medicine, Chinese Academy of Medical Sciences, Suzhou, China.
2019-2024	**Ph.D., ShanghaiTech University**
2019	**B.S. in Life Science, Northeast Agricultural University**

Funding

- National Natural Science Foundation of China, Young Scientists Fund (Category C), Grant No. T2600798
- Fundamental Research Funds for the Central Universities, Peking Union Medical College, Grant No. 3332025054

Selected Research



2022 | PPI and molecule glue

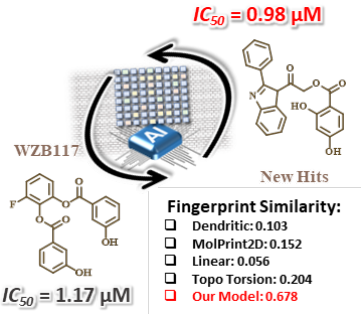
PPI-Miner

PPI-Miner searches receptor-compatible backbone motifs across sequence-divergent proteins, expanding interaction-partner discovery beyond sequence homology. Applied to CRBN, it produced a filtered G30 library of 1,739 candidate substrates.

Highlights

- Geometry-aware search recovered CRBN-compatible G-loops across unrelated protein families that sequence homology would miss
- At least 12 additional candidates in the released library were later supported by compound-dependent CRBN-recruitment assays, with signal lost upon mutation of the predicted G-loop glycine

JCIM | CRBN library | Code



2024 | Molecular representation

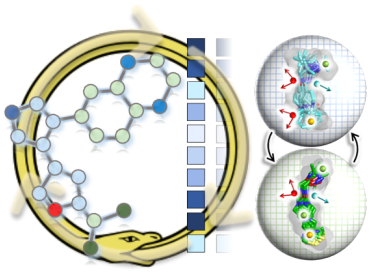
GeminiMol

GeminiMol addresses a central limitation of ligand-based discovery: functionally similar molecules can appear unrelated in two-dimensional structure. Learning from conformational-space and pharmacophore relationships supports cross-scaffold prediction, virtual screening, target identification, and scaffold hopping.

Highlights

- Screening 18 million compounds identified the scaffold-distinct GM-10, validated by whole-cell patch clamp against GluN1/GluN3A (IC_{50} = 0.98 ± 0.13 μM)
- First prize in the 2023 Shanghai International Computational Biology Innovation Competition

Advanced Science | Acta Pharmacol. Sin. | Code



2026 | Representation & generation

Ouroboros

Ouroboros connects molecular prediction and design within one chemically organized representation space. By preserving fingerprint, conformational-space, and pharmacophore relationships, it supports property prediction, similarity-based screening, targeted polypharmacology, and directed molecular optimization.

Highlights

- A shared chemical space closes the gap between predictive modeling and molecular generation, allowing property objectives to guide candidate design
- Conformational and pharmacophore organization supports scaffold-level exploration and multi-target design beyond fingerprint similarity alone

Advanced Science | Commun. Chem. | J. Med. Chem. | Code

Publications

= co-first author; * = co-corresponding author.

2026

CoCoBind: Consistency-Contrastive Multitask Learning for RNA–Ligand Interaction and Binding Site Prediction
Shihang Wang[#], **Lin Wang**[#*], Wei Zhao, Yuanlin He, Zhecheng Zhou, Jing Li, Yuxuan Jiang, Yuquan Li, Shaolong Lin, Silong Zhai, Daohong Gong, Yike Shen, Lingzhi Hu, Mutian He, Kai Xu, Lin Huang[*], Huanxiang Liu[*], Yang Zhang[*], Xiaojun Yao[*]
Journal of Medicinal Chemistry, 2026 - DOI

Integrating chemical priors and physical laws to mitigate hallucinations in structure-based drug design
Zhongyu Liu, Yadong Liu[*], Yihang Zhou, Zhiyuan Liu, Yuhang Yang, Zhiwen Wang, Tianyi Zang[*], **Lin Wang**[*], Yang Zhang[*]
Communications Chemistry, 2026 - DOI

Learned Conformational Space and Pharmacophore Into Molecular Foundational Model
Lin Wang, Yifan Wu, Hao Luo, Minglong Liang, Yihang Zhou, Cheng Chen, Chris Liu, Jun Zhang, Yang Zhang
Advanced Science, p. e13556, 2026 - DOI

Molecular glue degraders of HuR suppress BRAF-mutant colorectal cancer
Xiaocui Lu, Xiuyun Wang, Zheng Yang, Xusheng Wang, Lin Wang, Chunhui Xu, I Lo, Chenlu Geng, Yisheng Pu, Keyu Zhang, et al.
Nature, p. 1–10, 2026 - Google Scholar

ProteinConformers: Benchmark Dataset for Simulating Protein Conformational Landscape Diversity and Plausibility
Yihang Zhou[#], Chen Wei[#], Minghao Sun, Jin Song, Yang Li[*], **Lin Wang**[*], Yang Zhang[*]
Advances in Neural Information Processing Systems, vol. 38, 2026 - Google Scholar

Small Molecule Conformation Prediction
Lin Wang, Fang Bai
Artificial Intelligence for Drug Design, p. 527–546, book chapter, 2026 - Google Scholar

2025

DeepPSA: A Geometric Deep Learning Model for PROTAC Synthetic Accessibility Prediction
Ran Zhang, Shihang Wang, Lin Wang, Siyuan Tian, Yilin Tang, Fang Bai
Journal of Chemical Information and Modeling, vol. 65(13), p. 6861–6873, 2025 - Google Scholar

Discovery of novel GluN1/GluN3A NMDA receptor inhibitors using a deep learning-based method
Shi-hang Wang[#], Yue Zeng[#], Hao Yang[#], Si-yuan Tian[#], Yong-qi Zhou[#], **Lin Wang**[#], Xue-qin Chen, Hai-ying Wang, Zhao-bing Gao[*], Fang Bai[*]
Acta Pharmacologica Sinica, vol. 46(11), p. 3108–3115, 2025 - Google Scholar

Fitness costs of mobilised colistin resistance gene 3 (mcr-3): systematic review, epidemiological study, and functional analysis
Lujie Liang[#], Yaxin Li[#], **Lin Wang**[#], Wenli Wang, Yihao Zhang, Hui Zhao, Yaxuan Wang, Lingxuan Lyu, Jiachen Li, Dianrong Zhou, Zhe Hu, Lizhen Luo, Guanxiu Wang, Jia Wan, Lin Xu, Meisong Li, Min Dai, Meiting Yang, Shun Xiong, Lan-Lan Zhong, Fang Bai, Siyuan Feng, Guo-Bao Tian
EBioMedicine, vol. 120, p. 105923, 2025 - DOI

MAI-TargetFisher: A proteome-wide drug target prediction method synergetically enhanced by artificial intelligence and physical modeling
Shi-wei Li, Peng-xuan Ren, Lin Wang, Qi-lei Han, Feng-lei Li, Hong-lin Li, Fang Bai
Acta Pharmacologica Sinica, vol. 46(5), p. 1462–1475, 2025 - Google Scholar

NADPH-Independent Fluorescent Probe for Live-Cell Imaging of Heme Oxygenase-1
Liang Li, Xuanyi Lu, Qiyuan He, Chao Shu, Edward RH Walter[*], **Lin Wang**[*], Nicholas J Long[*], Lijun Jiang[*]
ACS sensors, vol. 10(1), p. 499–506, 2025 - Google Scholar

PhenoModel: A multimodal phenotypic drug design foundation model for discovering novel potential inhibitors of multiple cancer cells
Shihang Wang[#], Qilei Han[#], Weichen Qin[#], **Lin Wang**[#], Junhong Yuan, Fengyu Cai, Yiqun Zhao, Pengxuan Ren, Yunze Zhang, Yilin Tang, et al.
Acta Pharmaceutica Sinica B, 2025 - DOI

Recent advances in molecular representation methods and their applications in scaffold hopping
Shihang Wang, Ran Zhang, Xiangcheng Li, Fengyu Cai, Xinyue Ma, Yilin Tang, Chao Xu, Lin Wang, Pengxuan Ren, Lu Liu, et al.
Npj Drug Discovery, vol. 2(1), p. 14, 2025 - Google Scholar

2024

Conformational space profiling enhances generic molecular representation for AI-powered ligand-based drug discovery
Lin Wang, Shihang Wang, Hao Yang, Shiwei Li, Xinyu Wang, Yongqi Zhou, Siyuan Tian, Lu Liu, Fang Bai
Advanced Science, vol. 11(40), p. 2403998, 2024 - DOI

Salvianolic acid B attenuates liver fibrosis by targeting Ecm1 and inhibiting hepatocyte ferroptosis
Yadong Fu, Xiaoxi Zhou, Lin Wang, Weiguo Fan, Siqi Gao, Danyan Zhang, Zhiyang Ling, Yaguang Zhang, Liyan Ma, Fang Bai, et al.
Redox biology, vol. 69, p. 103029, 2024 - Google Scholar

2023

A new variant of the colistin resistance gene MCR-1 with co-resistance to β-lactam antibiotics reveals a potential novel antimicrobial peptide
Lujie Liang[#], Lan-Lan Zhong[#], **Lin Wang**[#], Dianrong Zhou, Yaxin Li, Jiachen Li, Yong Chen, Wanfei Liang, Wenjing Wei, Chenchen Zhang, et al.
PLoS Biology, vol. 21(12), p. e3002433, 2023 - Google Scholar

DeepSA: a deep-learning driven predictor of compound synthesis accessibility
Shihang Wang[#], **Lin Wang**[#], Fenglei Li, Fang Bai
Journal of Cheminformatics, vol. 15(1), p. 103, 2023 - DOI

Discovery, evaluation and mechanism study of WDR5-targeted small molecular inhibitors for neuroblastoma
Qi-lei Han, Xiang-lei Zhang, Peng-xuan Ren, Liang-he Mei, Wei-hong Lin, Lin Wang, Yu Cao, Kai Li[*], Fang Bai[*]
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Lianghe Mei, Lansong Xu, Sanan Wu, Yafang Wang, Chao Xu, Lin Wang, Xingyu Zhang*, Chengcheng Yu, Hualiang Jiang, Xianglei Zhang*, et al.
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Propofol exerts anti-anhedonia effects via inhibiting the dopamine transporter
Xiao-Na Zhu, Jie Li, Gao-Lin Qiu, Lin Wang, Chen Lu, Yi-Ge Guo, Ke-Xin Yang, Fang Cai, Tao Xu*, Ti-Fei Yuan*, et al.
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Jian Li, Jina Sun, Xianglei Zhang, Ruxue Zhang, Qian Wang, Lin Wang, Leike Zhang, Xiong Xie, Chunpu Li, Yu Zhou, et al.
Chemical Communications, vol. 59(7), p. 868–871, 2023 - Google Scholar

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A multi-targeting drug design strategy for identifying potent anti-SARS-CoV-2 inhibitors
Peng-xuan Ren, Wei-juan Shang, Wan-chao Yin, Huan Ge, Lin Wang, Xiang-lei Zhang, Bing-qian Li, Hong-lin Li, Ye-chun Xu, Eric H Xu, et al.
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Crystal structures of Wolbachia CidA and CidB reveal determinants of bacteria-induced cytoplasmic incompatibility and rescue
Haofeng Wang, Yunjie Xiao, Xia Chen, Mengwen Zhang, Guangxin Sun, Feng Wang, Lin Wang, Hanxiao Zhang, Xiaoyu Zhang, Xin Yang, et al.
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Discovery of potential small molecular SARS-CoV-2 entry blockers targeting the spike protein
Lin Wang#, Yan Wu#, Sheng Yao#, Huan Ge#, Ya Zhu, Kun Chen, Wen-zhang Chen, Yi Zhang, Wei Zhu*, Hong-yang Wang, et al.
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Xin Liu, Jiale Yu, Siyu Tao, Beiyuan Yang, Shike Wang, Lin Wang, Fang Bai, Jie Zheng
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PPI-Miner: a structure and sequence motif co-driven protein–protein interaction mining and modeling computational method
Lin Wang, Feng-lei Li, Xin-yue Ma, Yong Cang, Fang Bai
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Rapamycin targets STAT3 and impacts c-Myc to suppress tumor growth
Le Sun, Yu Yan, Heng Lv, Jianlong Li, Zhiyuan Wang, Kun Wang, Lin Wang, Yunxia Li, Hong Jiang, Yaoyang Zhang
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Recent advances in predicting protein–protein interactions with the aid of artificial intelligence algorithms
Shiwei Li, Sanan Wu, Lin Wang, Fenglei Li, Hualiang Jiang, Fang Bai
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Target-based virtual screening and LC/MS-guided isolation procedure for identifying phloroglucinol-terpenoid inhibitors of SARS-CoV-2
Bo Hou, Yu-Min Zhang, Han-Yi Liao, Li-Feng Fu, De-Dong Li, Xin Zhao, Jian-Xun Qi, Wei Yang, Geng-Fu Xiao, Lian Yang, et al.
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Zheng Wang, Mohit Hulsurkar, Lijuan Zhuo, Jinbang Xu, Han Yang, Samira Naderinezhad, Lin Wang, Guoliang Zhang, Nanping Ai, Linna Li, et al.
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Bingqian Li, Lin Wang, Huan Ge, Xianglei Zhang, Penxuan Ren, Yu Guo, Wuyan Chen, Jie Li, Wei Zhu, Wenzhang Chen, et al.
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Probing the allosteric inhibition mechanism of a spike protein using molecular dynamics simulations and active compound identifications
Qian Wang#*, **Lin Wang**#, Yumin Zhang#, XiangLei Zhang, Leike Zhang, Weijuan Shang, Fang Bai*
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2020

Antimicrobial resistance in clinical Ureaplasma spp. and Mycoplasma hominis and structural mechanisms underlying quinolone resistance
Ting Yang, Lianlian Pan, Ningning Wu, Lin Wang, Zhen Liu, Yingying Kong, Zhi Ruan, Xinyou Xie, Jun Zhang
Antimicrobial Agents and Chemotherapy, vol. 64(6), p. 10–1128, 2020 - Google Scholar

Structure of Mpro from SARS-CoV-2 and discovery of its inhibitors
Zhenming Jin, Xiaoyu Du, Yechun Xu, Yongqiang Deng, Meiqin Liu, Yao Zhao, Bing Zhang, Xiaofeng Li, Leike Zhang, Chao Peng, et al.
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The structural study of mutation-induced inactivation of human muscarinic receptor M4
Jingjing Wang, Meng Wu, Lijie Wu, Yueming Xu, Fei Li, Yiran Wu, Petr Popov, Lin Wang, Fang Bai, Suwen Zhao, et al.
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