

### Research Interests

Al Al for biomedicine, multi-omics, structure biology and drug discovery

Bioinformatics Multi-omics disease mechanism research, drug mechanism discovery and network pharmacology

### Education

2024.5- Visiting scholar, National University of Singapore, Singapore, Singapore

2024.11 Bioinformatics & AI, Structure biology

2020.9- PhD Student, Tsinghua University, Beijing, China

present Bioinformatics & Al

2018.3- Exchange Student, Shanghai Jiao Tong University, Shanghai, China

2018.8 Automation

2016.9- Bachelor's Degree, Harbin Institute of Technology, Harbin, China

2020.8 Automation

## Selected Publications

2025 Transfer Learning and Permutation-Invariance improving Predicting Genome-wide, Cell-Specific and Directional Interventions Effects of Complex Systems

Wang B, Pan B, Zhang T, Liu Q, Li S\*.

Advanced Science, 2025. (IF=14.1, published)

2025 Revealing the Mechanisms of Compound Kushen Injection on Oxidative Stress Regulation in the Treatment of Radiation-Induced Lung Injury

**Wang B**, Kong D, Yang Z, Kang J, Sun D, Duan X, Zhang T, Liu Q, Yin H\*, Li K\*, Li S\*. *Engineering*, 2025. (IF=11.7, published)

2025 Revolutionizing Drug Discovery from Natural Products: The Roles of Artificial Intelligence and Multi-Omics in Accelerating Innovation

**Wang B**#, Liu Q#, Zhang T, Zhao W, Zhang D, Sutcharitchan C, Li S\*. *Acta Pharm Sin B*, 2025. (IF=14.6, accepted)

2025 Leveraging Network Target Theory for Efficient Prediction of Drug-Disease Interactions:
A Transfer Learning Approach

Liu Q#, Chen Z#, **Wang** B#, Pan B#, Zhang Z, Shen M, Zhao W, Zhang T, Li S\*, Liu L\*. *Advanced Science*, 2025. (IF=14.1, published)

A computational based new treatment strategy with randomized, double-blind, threearmed, parallel-controlled, multicenter clinical trials on Mycoplasma pneumoniae pneumonia in children

Zhong C#, Guo S#, Liu Q#, Sun D#, **Wang B**#, Hu S, Li X, Zhao W, Ding Y, Yuan B, Liu J, Xiang L, Li N, Xue Z, Li Y, Teng Y, Yi R, Li S\*, Ma R\* *Chinese Medicine*, 2025. (IF=5.7, published)

2025 A computational based new treatment strategy with randomized, double-blind, threearmed, parallel-controlled, multicenter clinical trials on Mycoplasma pneumoniae pneumonia in children

Liu Q#, Zhang D#, **Wang B**#, Zhao W, Zhang T, Sutcharitchan C, Li S\* *Science of Traditional Chinese Medicine*, 2025. (published)

2024 Comparison of Jinzhen Oral Liquid and Ambroxol Hydrochloride and Clenbuterol Hydrochloride Oral Solution in the Treatment of Acute Bronchitis in Children: A Multicenter, Non-inferiority, Prospective, Randomized Controlled trial

Fan Q#, Wu C#, Du Y#, **Wang B**#, Xie Y, Zhang Z, Su W, Wang Z, Xu C, Li X, Ding Y, An X, Chen J, Xiao Y, Yu R, Li N, Wang J, Teng Y, Lv H, Yang N, Wen Y, Huang X, Pan W, Liu Y, Xi X, Zhao Q, Liu C, Xu J, Zhang H, Zhuo L, Rong Q, Xia Y, Shen Q, Li S\*, Wang J\*, Wu S\*. *Acta Pharm Sin B*, 2024 Dec;14(12):5186-5200. (IF=14.6, published)

2024 Elucidating the role of artificial intelligence in drug development from the perspective of drug-target interactions

**Wang B**#, Zhang T#, Liu Q#, Sutcharitchan C, Zhou Z, Zhang D, Li S\*. *Journal of Pharmaceutical Analysis*, 2024. (IF=8.9, published)

- Uncovering the role of traditional Chinese medicine in immune-metabolic balance of gastritis from the perspective of Cold and Hot: Jin Hong Tablets as a case study Wang B#, Zhang T#, Liu Q#, Sutcharitchan C, Zhou Z, Zhang D, Li S\*.

  Chinese Medicine, 2024 Oct 4;19(1):134. (IF=5.7, published)
- Biological mechanism of Traditional Chinese Medicine Formula and Herbs in Treating Diseases from the perspective of Cold and Hot
   Wang B, Chen P, Zhang P, Li S\*.
   World Journal of Traditional Chinese Medicine, February 29, 2024. 10(3):p 274-283. (IF=4.4,
- 2023 Exploring the effect of Weifuchun capsule on the toll-like receptor pathway mediated HES6 and immune regulation against chronic atrophic gastritis

Wang B#, Zhou W#, Zhang H#, Wang W, Zhang B, Li S\*. Journal of Ethnopharmacology, 2023 Mar 1; 303:115930. (IF=5.4, published)

2023 Uncovering the mechanisms of Yi Qi Tong Qiao Pill in the treatment of allergic rhinitis based on Network target analysis

**Wang B**, Zhang D, Zhang T, Sutcharitchan C, Hua J, Hua D\*, Zhang B\*, Li S\*. *Chinese Medicine*, 2023 Jul 24; 18(1):88. (IF=5.7, published)

# Works In Progress

published)

#### Bioinformatics and Algorithm Developing

Gao Z#, Wang B#, et al. Uncovering the metabolic reprogramming of macrophages for Gegen Qinlian Decoction in alleviating meta-inflammation of T2DM.

(Signal Transduction and Targeted Therapy, in revision)

Wang B#, Zhao W#, Chen P#, et al. ARegulation of Cell Cycle by Pien Tze Huang in preventing Hepatocellular carcinoma progression.

(Phytomedicine, in revision)

Zhang T#, Wang B#, Qu J#, et al. Screening the Homologous Food-Medicine Kelp as a Dietary Intervention for Fructose-accelerated colitis-associated colorectal cancer tumorigenesis.

(Genome Medicine, under review)

Pan B#, Wang B#, et al. Systematic Development of Multi-Component Drug from Traditional Medicine: Targeting EGFR-PCNA Axis through Synergistic Danggui Sini Decoction-derived Compounds in Gastric Cancer.

(Chemical Engineering Journal, in revision)

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③ wby20.github.io/paul.github.io/ • ⑤ Boyang Wang • ☐ WBY20

Zhang T#, Wang B#, Zhang D, et al. A Phenotype-Molecule Transfer Learning Model: Clinical Analysis and Mechanistic Insights of Yinqiao Qingre Pill in Wind-Heat Syndrome Common Cold Intervention.

(Chinese Herbal Medicine, in revision)

Structure Biology and Algorithm Developing

Hu T#, Wang B#, et al. A Rapid Al-driven mutation screening method for enhancing protein functionality.

(Science China-Life Science, in revision)

# Research Projects Involved

Multidisciplinary and Interdisciplinary Innovation Team Program on Traditional Chinese Medicine (TCM), National Administration of Traditional Chinese Medicine (2024)

Special Program for the Interpretation of Foundational Principles in Traditional Chinese Medicine (Toyota Joint Research Fund) Intelligent and Precision Research of Traditional Chinese Medicine for Spleen-Stomach Diseases

Mechanistic Study of Modified Gegen Qinlian Decoction in Treating Intestinal Damp-Heat Syndrome-type T2DM by Regulating Macrophage Metabolic Reprogramming

Mechanistic Study of Tuo Min Zhi Ti Tang in Preventing and Treating Allergic Rhinitis based on Network Target Technology

Mechanistic Study of Xiao Chai Hu Granules in Treating Pediatric Gastroenteric Cold based on the UNIQ System

### Awards and Honors

- 2025 He Meiying and Li Yanda Scholarship for Academic Endeavor in Tsinghua University
- 2024 Highest prize in 49th International Exhibition of Inventions Geneva (**Gold with congratulations of the Jury**, the 3rd author)
- 2024 Wuhai Talent Scholarship 2nd Prize in Tsinghua University
- 2023 Jiukun Scholarship 2nd Prize in Tsinghua University
- 2020 National Scholarship in HIT
- 2020 Outstanding Graduate in HIT
- 2020 Merit Student in HIT
- 2020 Outstanding Youth League Cadre in Automation Department in HIT
- 2018–2020 People's Scholarship 1st Prize in HIT (4 times)
  - 2019 "AVIC" 2nd Class Scholarship in HIT
  - 2017 College Student Science and Technology Innovation Project 1st Prize in HIT