

Rui Li

Tel: +86 176 7142 2109; Email: lirui3@shanghaitech.edu.cn; Website: <https://drruili.github.io>
Address: School of Life Science and Technology, ShanghaiTech University, Shanghai, CN 201210

EDUCATION

- Sep. 2020 – **Shanghaitech University**, Shanghai, CN. **Ph.D.** in Biology
- Jun. 2025 (Expected) **Shanghai Institute of Nutrition and Health of the Chinese Academy of Sciences**, Shanghai, CN. **Joint** doctoral training
- Research Interests: Metabolomics methodology, Metabolic flux, Mass spectrometry algorithm, Multi-omics, Bioinformation
 - Dissertation title: “*Mass spectrometry-based metabolite isotopomer analysis algorithm and application of metabolomics*”
 - Supervisor: Professor Huiyong Yin
- Sep. 2016 – **Wuhan University of Technology**, Wuhan, China
- Jun. 2020 **B.Sc.** in Biotechnology
- Research Interests: Neuron science, Biological modeling
 - Thesis title: “*Observation and Simulation of neural activity in mouse visual cortex by two-photon calcium imaging*”
 - Supervisor: Professor Jing Li

PROFESSIONAL EXPERIENCES

- Oct. 2024 – **City University of Hong Kong**, Hong Kong, HK
- Oct. 2025 (Expected) **Research Assistant**
- Research field: Metabolomics methodology, Mass spectrometry algorithm, Bioinformation.
 - Supervisor: Professor Huiyong Yin

RESEARCH INTERESTS

- Development of metabolomic methodologies
- Metabolic flux analysis based on isotopomer
- Quantitatively modeling for kinetic metabolic processes

RESEARCH EXPERIENCE

- **Mass Spectrometry based Isotopomer Parsing (MSIP)**

Project website: <https://drruili.github.io/MSIP>

Current stable isotope-labeled metabolic flux analysis is mostly based on isotopologues rather than isotopomers. Although isotopomers can provide more detailed metabolic dynamics and support more accurate quantitative modeling, their application is limited due to the lack of appropriate analytical methods. We developed an algorithm, MSIP, to analyze isotopomers. It constructs an

atom-tracing model, acquires and parses informative MS2 spectra, and then determines the proportion of possible isotopomers. This method first achieves high-throughput and comprehensive isotopomer analysis based on mass spectrometry.

- **Metabolic flux network analysis (MFNA)**

Project Website: <https://drruili.github.io/MSIP/articles/MFNA>

The information of isotopomers is too complicated for human-understanding and biological interpretation. Therefore, advanced modeling becomes necessary to process the isotopomers data from MSIP. Here we build an atom-transfer-based metabolic flux network model using KEGG reaction database. This model encodes reactions as atom-transfer processes between molecular graphs and performs network diffusion to simulate isotope flux in metabolic processes. This project is still under development.

- **Metabolomics data analysis and methodology development platform**

The lack of a universal analytical platform is one of the key factors limiting the biological application and development of metabolomics methodologies. We developed a metabolomics data analysis and method development platform, MSdev. MSdev integrates and develops various core tools and databases, including mass spectrometry data analysis, chemical computations, metabolomics databases, and molecular graph structures. This platform not only facilitates our routine metabolomics and metabolic flux analysis but also supports the development of advanced methods such as MSIP and MFNA.

- **Biomarkers in metabolic disease**

Metabolomics has become a powerful tool for identifying metabolite biomarkers for disease diagnosis and prediction. We screened biomarkers for predicting hyperuricemia and gout in a cohort of 330 patients and validated them in four independent cohorts, with a total of 1,247 patients. The related product has been applied in clinical practice. We also identified biomarkers for predicting frequent gout flares and hypothyroidism. In these project, we developed untargeted metabolomics method for more accurate identification and pseudotargeted/targeted metabolomics for precise and stable quantification.

- **Multi-omics analysis of ESCC immunoresistance**

Immunotherapy has significantly improved the prognosis of Esophageal Squamous Cell Carcinoma (ESCC), but immunoresistance still limits its clinical application, and early prediction of immunotherapy resistance remains challenging. We perform multi-omics analysis, including transcriptomics, proteomics, metabolomics, and lipidomics, on patient samples before and after immunotherapy to comprehensively investigate the mechanisms underlying ESCC immunotherapy resistance and identify potential biomarkers for early prediction.

SKILLS

- Proficient in metabolic data analysis and algorithm development, including tools such as XCMS, EI-MAVEN, MS-DIAL, etc. and self-developed MSdev, MSIP.
- Extensive experience in mass spectrometry operation, including Thermo Fisher instruments (Astral, QE, TSQ, LTQ), Sciex (6600, 6500, 5500), and Bruker rapifleX.
- Skilled in multiple programming languages, including R, Python, MATLAB.
- Trained in biological laboratory techniques, including cell culture, animal experimentation and

basial biological experiments.

PUBLICATIONS

Wang M*, **Li R***, Qi H, et al. Metabolomics and Machine Learning Identify Metabolic Differences and Potential Biomarkers for Frequent versus Infrequent Gout Flares[J]. Arthritis Rheumatol, 2023.

Shao F*, **Li R***, Guo Q, et al. Plasma Metabolomics Reveals Systemic Metabolic Alterations of Subclinical and Clinical Hypothyroidism[J]. The Journal of Clinical Endocrinology & Metabolism, 2022.

Li R*, Liang N*, Tao Y, et al. Metabolomics in Hyperuricemia and Gout[J]. Gout, Urate, and Crystal Deposition Disease, 2023, 1(1): 49-61.

Xin C*, Cai M*, Jia Q*, Huang R, **Li R**, et al. Dietary sulfur amino acid restriction improves metabolic health by reducing fat mass[J]. Life Metabolism, 2025.

Liang N*, Yuan X*, Zhang L, Shen X, Zhong S, Li L, **Li R**, et al. Fatty acid oxidation-induced HIF-1 α activation facilitates hepatic urate synthesis through upregulating NT5C2 and XDH[J]. Life Metabolism, 2024.

Li L*, Zhong S, **Li R**, et al. Aldehyde dehydrogenase 2 and PARP1 interaction modulates hepatic HDL biogenesis by LXR α -mediated ABCA1 expression[J]. JCI Insight, 2022, 7(7).

Unpublished work:

Sun W*, **Li R***, Dalbeth N, et al. Metabolomic profiles underlying gout flares: a prospective study of people with gout[J]. RMD Open, 2025. (Under revision).

Li R*, Xie Z*, et al. MSIP: A Novel Algorithm for Detailed Isotopomer Parsing in Mass Spectrometry-Based Metabolomics. (Manuscript in preparation)

Guo X*, **Li R***, Ma H*, et al. Multi-Omics Reveals that ITGB6 Regulates Lipid Metabolism and Immunotherapy Resistance in ESCC through the MAPK Pathway. (In preparation)

FELLOWSHIPS AND AWARDS

Academic Scholarship, Shanghaitech University, 2020-2024

Excellent Student, Shanghaitech University, 2023

Outstanding Student, Shanghaitech University, 2022

Volunteer Certificate, 2021 World Artificial Intelligence Conference, 2021

Outstanding Graduate, Wuhan University of Technology, 2020

Recommendation for Direct Admission to Master's-Ph.D. Program, 2019

First Prize in the Independent Innovation Research Fund Undergraduate Project, 2019

Third Prize in the 2nd China Undergraduate Life Sciences Contest, 2018

Third Prize in the 18th "Innovation Cup" Student Academic and Technological Works Competition of Wuhan University of Technology, 2018

First Prize in the 5th Undergraduate Biological Experiment Skills Competition of Hubei Province, 2018

Third Prize in the 3rd National Undergraduate Life Science Innovation and Entrepreneurship Competition, 2018

National Encouragement Scholarship, 2017

Outstanding Student, Wuhan University of Technology, 2017

REFERENCES

Professor Huiyong Yin

Department of Biomedical Sciences

City University of Hong Kong

Tat Chee Avenue, Kowloon

Hong Kong, HK 02138

+852-3442-2812

huiyoyin@cityu.edu.hk

Professor Lifeng Yang

Shanghai Institute of Nutrition and Health

Chinese Academy of Sciences

320, Yueyang Road

Shanghai, CN 200000

+86-21-54920241

llyang@sinh.ac.cn