

# Xiaotao Shen, Ph.D.

Nanyang Assistant Professor

Lee Kong Chian School of Medicine, Nanyang Technological University, Singapore

959 Nanyang Dr., Singapore, 636921.

#### **Research Interests**

- Multi-omics Data Integration Methods Development
- Host-Microbe Interaction
- Aging and Neurodegenerative Diseases
- Maternal and Child Health
- Wearable Data and Precision Medicine
- **Environmental Health**

## **Education & Research Experiences**

Director

Adjunct Principle Investigator

**Nanyang Assistant Professor** 

**Postdoctoral Research Fellow** 

Ph.D. in Bioinformatics and Metabolomics

2025/2-present, Singapore Phenome Center

2024/10-present, KK Women's and Children's Hospital, Singapore

2024/5-present, Nanyang Technological University, Singapore

2019/4-2024/4, Stanford University

(Advisor: Prof. Michael Snyder)

2013/9-2018/12, Chinese Academy of Sciences

(Advisor: Prof. Zheng-Jiang Zhu)

2009/9-2013/6, Inner Mongolia University

#### **Honors & Awards**

Young Investigator Award

**B.S. in Biotechnology** 

The 3<sup>rd</sup> Chinese American Society For Mass Spectrometry Conference (2023)

SPORR 2023 Rigor and Reproducibility Award

**Stanford Program on Research Rigor and Reproducibility** (2023)

Winner Selected by the Event Committee

Student Travel Award for Oral Presentation

International Conference Travel Award

China National Scholarship

Award for Outstanding Youth Report

Merit Student

Award for Outstanding Youth Report

Inner Mongolia Outstanding Graduate

National Encouragement Scholarship

**Exposome Data Challenge Event** (2021)

The International Metabolomics Society (2018)

The Metabolites Journal (2018)

Ministry of Education of the People's Republic of China (2017)

The 3<sup>rd</sup> China MS Analysis Conference (2017)

**University of Chinese Academy of Sciences** (2016)

The 34th China MS Society Conference (2016)

**Inner Mongolia Autonomous Region** (2013)

Inner Mongolia University (2011)

# **First/Co-first Author Publications**

- +: Co-first Author. \*: Co-Corresponding Author
- 1. X. Shen+, S. Chen+, L. Liang+, M. Avina, H. Zackriah, L. Jelliffe-Pawlowski, L. Rand, M. P. Snyder\*, Longitudinal Urine Metabolic Profiling and Gestational Age Prediction in Pregnancy. *Briefing in Bioinformatics*, 2025, 26 (1). *♂*
- 2. X. Shen+, C. Wang+, X. Zhou, W. Zhou, D. Hornburg, S. Wu, and M.P. Snyder\*, Nonlinear dynamics of multi-omics profiles during human aging. *Nature Aging*, 2024, 4, 1619-1634
- 3. X. Zhou+, X. Shen+, J. Johnson, D. Spakowicz, M. Agnello, W. Zhou, M. Avina, A. Honkala, F. Chleilat, S. Chen, K. Cha, S. Leopold, C. Zhu, L. Chen, L. Lyu, D. Hornburg, S. Wu, X. Zhang, C. Jiang, L. Jiang, L. Jiang, R. Jian, A. Brooks, M. Wang, K. Contrepois, P. Gao, S. Rose, T. Tran, H. Nguyen, A. Celli, B. Hong, E. Bautista, Y. Dorsett, P. Kavathas, Y. Zhou, E. Sodergren, G.M. Weinstock, M.P. Snyder\*. Longitudinal Profiling of the Microbiome at Four Body Sites Reveals Core Stability and Individualized Dynamics During Health and Disease. *Cell Host&Microbe*, 2024
- 4. X. Shen<sup>+</sup>, R. Kellogg<sup>+</sup>, D. Panyard<sup>+</sup>, N. Bararpour<sup>+</sup>, K. Castillo, B. Lee-McMullen, A. Delfarah, J. Ubellecker, S. Ahadi, Y. Rosenberg-Hasson, A. Ganz, K. Contrepois, B. Michael, I. Simms, C. Wang, D. Hornburg, M.P. Snyder<sup>\*</sup>, Multi-omic Microsampling Captures Health Perturbations in A Lifestyle Context. *Nature Biomedical Engineering*, 2023.
- 5. X. Shen+\*, C. Wang+, M.P. Snyder\*, massDatabase: Utilities for the Operation of the Public Compound and Pathway Database, *Bioinformatics*, 2022, btac546.
- 6. X. Shen+, W. Shao+, C. Wang+, L. Liang, S. Chen, S. Zhang, M. Rusu\*, M.P. Snyder\*, **Deep Learning-based Pseudo-Mass**Spectrometry Imaging Analysis for Precision Medicine, *Briefing in Bioinformatics*, 2022, bbac331.
- 7. X. Shen+, H. Yan+, C. Wang+, P. Gao, C.H. Johnson\*, M.P. Snyder\*, **TidyMass an Object-oriented Reproducible**Analysis Framework for LC-MS Data, *Nature Communications*, 2022, 4365.
- 8. P. Gao+, X. Shen+, X. Zhang, C. Jiang, M. P. Snyder\*, Precision Environmental Health Monitoring by Longitudinal Exposome and Multi-omics Profiling, *Genome Research*, 2022, **32**, 1199-1214.
- 9. X. Shen+, S. Wu+, L. Liang, S. Chen, K. Contrepois, Z.-J. Zhu\* and M.J. Snyder\*, metID: an R Package for Automatable Compound Annotation for LC-MS-based Data, *Bioinformatics*, 2021, 1, 1-2.
- 10. X. Shen, R. Wang, X. Xiong, Y. Yin, Y. Cai, J. Ma, N. Liu, Z.-J. Zhu\*, Large-scale Metabolite Identification for Untargeted Metabolomics Using Metabolic Reaction Network, *Nature Communications*, 2019, 10:1516.
- 11. X. Shen and Z.-J. Zhu\*, MetFlow: An Interactive and Integrated Workflow For Metabolomics Data Cleaning and Differential Metabolite Discovery, *Bioinformatics*, 2019, 35, 16.
- 12. H. Jia+, X. Shen+, Y. Guan, M. Xu, M. Mo, J. Zhu\* and Z.-J. Zhu\*, Predicting the Pathological Response to Neoadjuvant Chemoradiation Using Untargeted Metabolomics in Locally Advanced Rectal Cancer, *Radiotherapy and Oncology*, 2018, 128, 548-556.
- 13. J. Wang+, T. Zhang+, X. Shen+, J. Liu, D. Zhao, Y. Sun, L. Wang, Y. Liu, X. Gong, Y. Liu, Z.-J. Zhu\*, F. Xue\*, Serum Metabolomics for Early Diagnosis of Esophageal Squamous Cell Carcinoma by UHPLC-QTOF/MS, *Metabolomics*, 2016, 12: 116.
- 14. X. Shen, X. Gong, Y. Cai, Y. Guo, J. Tu, T. Zhang, J. Wang, F. Xue, Z.-J. Zhu\*, Normalization and Integration of Large-Scale Metabolomics Data Using Support Vector Regression, *Metabolomics*, 2016, 12: 89.

## **Collaborative Publications**

- 1. M. Gladding, X. Shen, M. Snyder, P. Havel, S. Adams. Interindividual Variability in Postprandial Plasma Fructose Patterns in Adults. *Nutrients*, 2024, 16 (18), 3079.
- 2. E. Xie, X. Shen, Y. Yeo, Z. Xing, J. Ebinger, Y. Duan, Y. Zhang, S. Cheng, F. Ji, J. Deng. Exploring the underlying molecular mechanisms of acute myocardial infarction after SARS-CoV-2 infection. *American Heart Journal Plus: Cardiology Research and Practice*, 2024, 44, 100417.
- 3. C. Peng, Q. Chen, S. Tan, X. Shen, C. Jiang. Generalized Reporter Score-based Enrichment Analysis for Omics Data, *Briefings in Bioinformatics*, Volume 25, Issue 3, May 2024, bbae116. *♂*
- 4. D. Ding, X. Shen, M.P. Snyder, R. Tibshirani, Semi-supervised Cooperative Learning for Multiomics Data Fusion, Machine Learning for Multimodal Healthcare Data. ML4MHD 2023. *Lecture Notes in Computer Science*, vol 14315. Springer, Cham.
- S. Jain, L. Pei, J. Spraggins, M. Angelo, J. Carson, N. Gehlenborg, F. Ginty, J. Gonçalves, J. Hagood, J. Hickey, N. Kelleher, L. Laurent, S. Lin, Y. Lin, H. Liu, A. Naba, E. Nakayasu, W. Qian, A. Radtke, P. Robson, B. Stockwell, R. Plas, I. Vlachos, M. Zhou, HuBMAP Consortium, K. Borner, M. Snyder, HuBMAP Consortium, Advances and Perspectives for the Human BioMolecular Atlas Program (HuBMAP), Nature Cell Biology, 2023.
- 6. W. Wei, N. Riley, X. Lyu, X. Shen, J. Guo, S. Raun, M. Zhao, M. Moya-Garzon, H. Basu, A. Tung, V. Li, W. Huang, A. Wiggenhorn, K. Svensson, M. Snyder, C. Bertozzi, J. Long, Organism-wide, Cell-type-specific Secretome Mapping of Exercise Training in Mice, *Cell Metabolism*, 35: 1-19, 2023.
- S. Zhang, J. Cooper-Knock, A. Weimer, M. Shi, L. Kozhaya, D. Unutmaz, C. Harvey, T. Julian, S. Furini, E. Frullanti, F. Fava, A. Renieri, P. Gao, X. Shen, I. Timpanaro, K. Kenna, J. Baillie, M. Davis, P. Tsao, M.P. Snyder, Multiomic Analysis Reveals Cell-type-specific Molecular Determinants of COVID-19 Severity, Cell Systems, 13(8):598-614, 2022.
- 8. L. Maitre, J. Guimbaud, C. Warembourg, N. Güil-Oumrait, P. Petrone, M. Chadeau-Hyam, M. Vrijheid, X. Basagaña, J. Gonzalez, Exposome Data Challenge Participant Consortium, State-of-the-art methods for exposure-health studies: Results from the exposome data challenge event, *Environment International*, 168: 107422, 2022.
- 9. M. Wei, L. Zhao, J. Lv, X. Li, G. Zhou, B. Fan, X. Shen, D. Zhao, F. Xue, J. Wang, T. Zhang, The Mediation Effect of Serum Metabolites On The Relationship Between Long-Term Smoking Exposure and Esophageal Squamous Cell Carcinoma, *BMC cancer*, 21, 415.
- 10. J. Lv, J. Wang, X. Shen, J. Liu, D. Zhao, X. Li, B. Fan, Y. Sun, F. Xue, Z.-J. Zhu, T. Zhang, A Serum Metabolomics Analysis Reveals A Panel of Screening Metabolic Biomarkers for Esophageal Squamous Cell Carcinoma, *Clinical and Translational Medicine*, 2021, 11, 5.
- 11. X. Li, L. Zhao, M. Wei, J. Lv, Y. Sun, X. Shen, D. Zhao, F. Xue, T. Zhang, J. Wang, Serum Metabolomics Analysis for The Progression of Esophageal Squamous Cell Carcinoma, *Journal of Cancer*, 2021, 12, 3190–3197.
- 12. L. Liang, M. Rasmussen, B. Piening, X. Shen, S. Chen, H. Rost, J. Snyder, R. Tibshirani, L. Skotte, N. Lee, K. Contrepois, B. Feenstra, H. Zackriah, M.J. Snyder, M. Melbye, Metabolic Dynamics and Prediction of Gestational Age and Time to Delivery in Pregnant Women, *Cell*, 2020, 181, 7, 1680-1692.
- 13. Z. Wang, B. Cui, F. Zhang, Y. Yang, X. Shen, Z. Li, W. Zhao, Y. Zhang, K. Deng, Z. Rong, K. Yang, X. Yu, K. Li, P. Han, and Z.-J. Zhu, Development of A Correlative Strategy to Discover Colorectal Tumor Tissue Derived Metabolite Biomarkers in Plasma Using Untargeted Metabolomics, *Analytical Chemistry*, 2019, 91, 3, 2401-2408.

- 14. Z. Zhou, X. Shen, X. Chen, J. Tu, X. Xiong, and Z.-J. Zhu, LipidIMMS Analyzer: Integrating Multi-dimensional Information to Support Lipid Identification in Ion Mobility–Mass Spectrometry based Lipidomics, *Bioinformatics*, 2018, 35, 4, 698-700. *♂*
- 15. Z. Zhou, J. Tu, X. Xiong, X. Shen, and Z.-J. Zhu, LipidCCS: Prediction of Collision Cross-Section Values for Lipids with High Precision to Support Ion Mobility-Mass Spectrometry based Lipidomics, *Analytical Chemistry*, 2017, 89, 9559–9566. *⊘*
- 16. Z. Zhou, X. Shen, J. Tu, and Z.-J. Zhu, Large-Scale Prediction of Collision Cross-Section Values for Metabolites in Ion Mobility-Mass Spectrometry, *Analytical Chemistry*, 2016, 88, 11084-11091. *♂*

## **Submitted Manuscripts**

- 1. X. Shen+,\*, P. Gao, X. Zhang, Decoding Links Between the Exposome and Health Outcomes by Multi-omics Analysis. Submitted.
- 2. X. Shen<sup>+\*</sup>, M.P. Snyder<sup>\*</sup>, microbiomeDataset: A Tidyverse-style Framework for Organizing and Processing Microbiome Data. Submitted.
- 3. S. Chen+, G. Wang+, X. Shen+, D. Hornburg, S. Rego, R. Hoffman, S. Nevins, X. Cheng, M.P. Snyder\*, Integration and Comparison of Multi-omics Profiles of NGLY1 Deficiency Plasma and Cellular Models to Identify Clinically Relevant Molecular Phenotypes. Submitted to *Clinical and Translational Medicine*.

#### **Patents**

- 1. M.P. Snyder, R. Kellogg, X. Shen, Multi-Omic Sample Analysis Methods, 2022, USA.
- 2. L. Liang, M.P. Snyder, X. Shen, S. Chen, Systems and Methods for Evaluating Gestational Progress and Applications Thereof, 2023, 18251702, USA.
- 3. Z-J. Zhu, X. Shen, A Method for Metabolite Annotation and Dysregulated Pathway Analysis, 2019, China.

#### **Invited Talks**

- 1. Dynamic Changes During Human Aging Revealed in Multi-omics Profiles. 2024 Chinese Biophysics Congress, 2024/7, Lanzhou, China.
- 2. Multi-omics For Precision Medicine. Hong Kong Baptist University, 2024/7, Hong Kong, China.
- 3. **Multi-omics For Precision Medicine. Metabolomics in Human Health,** 2024/5, Lee Kong Chian School of Medicine, Nanyang Technological University, Singapore.
- 4. R for Mass Spectrometry Data Processing. CAS Center for Excellence in Molecular Plant Sciences. 2024/5, Shanghai, China.
- 5. Multi-omics For Precision Medicine. Interdisciplinary Research Center on Biology and Chemistry, 2024/3, Shanghai, China.
- Remote and Flexible Microsampling Multi-omics for Precision Medicine. The iPOP Summit 2023. 2023/4, Stanford University, USA.
- 7. Bioinformatics Algorithm Development for Mass Spectrometry Data and its Application to Precision Medicine. University of Colorado. 2023/4, Denver, Colorado, USA.

- 8. Bioinformatics Algorithm Development for Mass Spectrometry Data and its Application to Precision Medicine.

  University of Minnesota. 2023/4, Twin Cities, Minnesota, USA.
- 9. Bioinformatics Algorithm Development for Mass Spectrometry Data and its Application to Precision Medicine.

  University of Connecticut. 2023/3, Storrs, Connecticut, USA.
- 10. Bioinformatics Algorithm Development for Mass Spectrometry Data and its Application to Precision Medicine. Altos Labs. 2023/3, Redwood City, USA.
- 11. Bioinformatics Algorithm Development for Mass Spectrometry Data and its Application to Precision Medicine.

  Ohio State University. 2023/2, Columbus, USA.
- 12. Bioinformatics Method Development for Mass Spectrometry and its Application to Precision Medicine. Stanford CVI Early Career Research Roundtable, 2022/11, Stanford, USA.

#### **Oral Presentations**

- 1. Nonlinear Dynamic Changes During Human Aging Revealed in Multi-omics Profiles. Bay Area Metabolism Meeting (BAMM) 2023, 2023/9, Palo Alto, USA.
- 2. Multi-omics Microsampling for The Profiling of Lifestyle-Associate Changes in Health. The 3<sup>rd</sup> Chinese American Society for Mass Spectrometry Conference, 2023/8, Virtual meeting.
- 3. Multi-omics Microsampling for The Profiling of Lifestyle-Associate Changes in Health. The 71<sup>th</sup> American Society for Mass Spectrometry Conference, 2023/6, Houston, USA.
- 4. Multi-omics Microsampling for The Profiling of Lifestyle-Associate Changes in Health. Invited presentation, 2023/2, Huazhong University of Science and Technology, China.
- Multi-omics Microsampling for The Profiling of Lifestyle-Associate Changes in Health. Stanford Postdoc Symposium, 2023/2, Stanford, USA.
- 6. Deep Learning-based Pseudo-Mass Spectrometry Imaging Analysis for Precision Medicine. CASMS Virtual Conference, 2022/10, Virtual meeting.
- 7. TidyMass: An Object-oriented Reproducible Analysis Framework for LC-MS Data. ACS Fall 2022, 2022/8, Virtual meeting.
- 8. metID: an R Package for Automatable Compound Annotation for LC-MS-based Data. The 69<sup>th</sup> American Society for Mass Spectrometry Conference, 2021/11, Philadelphia, USA.
- 9. Decoding Links Between the Exposome and Health Outcomes by Multi-omics Analysis. Exposome Data Challenge Event, 2021/4, Virtual meeting.
- 10. Metabolic Reaction Network-based Recursive Metabolite Identification for Untargeted Metabolomics. The 14<sup>th</sup> International Conference of the Metabolomics Society, 2018/6, Seattle, USA.
- 11. Assessment of the Response to Neoadjuvant Chemo-Radiation in Rectal Cancer Patients based on a Metabolomics Approach. The 3<sup>rd</sup> China Mass Spectrometry Analysis Conference, 2017/12, Xiamen, China.
- 12. Normalization and Integration of Large-Scale Mass Spectrometry-based Metabolomics Data Using Support Vector Regression. The 34<sup>th</sup> China Mass Spectrometry Society Conference, 2016/9, Xining, China.
- 13. Normalization and Integration of Large-Scale MS-based Metabolomics Data Using Support Vector Regression.

  The 64th American Society for Mass Spectrometry Conference, 2016/6, San Antonio, USA.

#### **Poster Presentations**

- 1. Nonlinear Dynamic Changes During Human Aging Revealed in Multi-omics Profiles. The 72<sup>nd</sup> American Society for Mass Spectrometry Conference, 2024/6, Anaheim, California, USA.
- 2. Nonlinear Dynamic Changes During Human Aging Revealed in Multi-omics Profiles. Stanford Bio-X Interdisciplinary Initiatives Seed Grants Program Symposium 2023. 2023/9, Stanford, USA.
- 3. TidyMass An Object-oriented Reproducible Analysis Framework for LC-MS Data. Stanford Data Science Conference, 2023/5, Stanford University, USA.
- 4. Deep Learning-based Pseudo-Mass Spectrometry Imaging Analysis for Precision Medicine. Stanford Genetics Retreat 2022, 2022/9, Monterey, USA.
- 5. Deep Learning-based Pseudo-Mass Spectrometry Imaging Analysis for Precision Medicine. Bay Area Metabolism Meeting (BAMM) 2022, 2022/9, Palo Alto, USA.
- 6. TidyMass An Object-oriented Reproducible Analysis Framework for LC-MS Data. The 70<sup>th</sup> American Society for Mass Spectrometry Conference, 2022/6, Minneapolis, USA.
- 7. Longitudinal Interactions Between Levels of Serum Cytokine and the Microbiome from Four Body Sites. IMMUNOLOGY2022, 2022/5, Portland, USA.
- 8. TidyMass An Object-oriented Reproducible Analysis Framework for LC-MS Data. Stanford Genetics Retreat 2021, 2021/9, Palo Alto, USA.
- 9. Longitudinal Urine Metabolic Profiling and Gestational Age Prediction in Pregnancy. The 17<sup>th</sup> International Conference of the Metabolomics Society, 2020/6, Virtual meeting.
- 10. Metabolic Reaction Network based Metabolite Annotation in Untargeted Metabolomics. The 13<sup>th</sup> International Conference of the Metabolomics Society, 2017/6, Brisbane, Austria.

## **Teaching**

LC-MS Data Processing and Analysis Using R language

2022/9, **Biotree Company** 

Responsibilities: Lecture

R Language for Reproducible Data Analysis

**Stanford School of Medicine Intern** 

2020/4, **SCPA** 

2019/8-Present, Stanford University

Responsibilities: Mentor

Responsibilities: Lecture

Mass Spectrometry Analysis

2014/9-2014/12, Chinese Academy of Sciences

Responsibilities: Guest lecturer

## Volunteering

Member of Editorial Board

2023/8-present, npj Women's health

Member of Youth Editorial Board

2023/2-present, Phenomics

Member of Youth Editorial Board

2023/1-present, Brain-X

Member of Youth Editorial Board

2022/7-present, iMeta

Co-chair 2021/7–2022/8, Stanford Chinese Postdoctoral Association

• Organizer 2020/2–2021/12, Stanford Chinese Postdoctoral Oral Presentation Improvement

2019/7–2021/7, Stanford Chinese Postdoctoral Association

Member

## **Journal Referee**

 Nature Biotechnology, Nature Methods, Nature Genetics, Nature Communications, Briefing in Bioinformatics, Bioinformatics, GigaScience, PLOS one, Phytochemistry, Genomics, Proteomics& Bioinformatics, Communications Chemistry, Communications Biology, Frontiers Molecular Biosciences, iMeta, iMetaOmics, Proteomics, BMC Bioinformatics, Proteomics, Cell Systems, Journal of Integrative Plant Biology, Cell Reports Medicine, Cell Reports Methods, Advanced Science

#### Referrers

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