Xiaotao Shen, Ph.D.

Postdoctoral Research Fellow, Prof. Michael Snyder's Lab, Department of Genetics, Stanford University 3165 Porter Drive, Palo Alto, CA 94304, USA.

✓ shenxt@stanford.edu fashenxt.info 1+1 571-267-9283 3Xiaotao Shen is jaspershen Xiaotao Shen is 0000-0002-9608-9964

Research Interests

- > Mass Spectrometry Data Processing Algorithms and Software Development
- Multi-omics Data Integration Methods Development >
- Precision Exposome and Multi-omics Integration for Healthcare
- > Multi-omics Profiling for Human Pregnancy-Related Disease Diagnosis and Mechanism Research
- > Aging and Neurodegenerative Diseases
- Wearable Data and Precision Medicine

Education & Research Experiences

Postdoctoral Research Fellow

2019/4–present, Stanford University

(Advisor: Prof. Michael Snyder)

Ph.D. in Bioinformatics and Metabolomics 2013/9-2018/12, Chinese Academy of Sciences

(Advisor: Prof. Zheng-Jiang Zhu)

B.S. in Biotechnology

2009/9-2013/6, Inner Mongolia University

Honors & Awards

1. SPORR 2023 Rigor and Reproducibility Awards

Stanford Program on Research Rigor and Reproducibility (2023)

2. Winner Selected by the Event Committee

3. Student Travel Award for Oral Presentation

4. International Conference Travel Award

5. China National Scholarship

6. Award for Outstanding Youth Report

7. Merit Student

8. Award for Outstanding Youth Report

9. Inner Mongolia Outstanding Graduate

10. 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 3rd 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+, R. Kellogg+, D. Panyard+, N. Bararpour+, 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*, Multi-omic Microsampling Captures Health Perturbations in A Lifestyle Context. Nature Biomedical Engineering, 2023, 10.1038/s41551-022-00999-8. (Citation: 4, IF: 29.2)

- 2. X. Shen+*, C. Wang+, M.P. Snyder*, massDatabase: Utilities for the Operation of the Public Compound and Pathway Database, *Bioinformatics*, 2022, btac546. (Citation: 1, IF: 6.9)
- 3. 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. (Citation: 1, IF: 14.0)
- 4. 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. (Citation: 11, IF: 17.7)
- 5. 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. ② (Citation: 15, IF: 9.4)
- 6. 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. (Citation: 18, IF: 6.9)
- 7. 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. *(Citation: 200, IF: 17.7)*
- 8. X. Shen and Z.-J. Zhu*, MetFlow: An Interactive and Integrated Workflow For Metabolomics Data Cleaning and Differential Metabolite Discovery, *Bioinformatics*, 2019, 35, 16. (Citation: 27, IF: 6.9)
- 9. 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. (Citation: 38, IF: 6.9)
- 10. 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. *②* (Citation: 109, IF: 4.7)
- 11. 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. (Citation: 144, IF: 4.7)

Collaborative Publications

- 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.
- 2. 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.
- 3. 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.
- 4. 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.

- 5. 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.
- 6. 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.
- 7. 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.
- 8. 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.
- 9. 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.
- 10. 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. *⊘*
- 11. 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 Publications

- +Co-first Author. *: Co-Corresponding Author
- 1. X. Shen+, C. Wang+, X. Zhou, W. Zhou, D. Hornburg, S. Wu, and M.P. Snyder*, **Nonlinear Dynamic Changes During Human Aging Revealed in Multi-omics Profiles. Submitted**.
- 2. X. Shen+*, M.P. Snyder*, microbiomeDataset: A tidyverse-style framework for organizing and processing microbiome data. Under review in *Bioinformatics*.
- 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. Under review in *Cell*.
- 4. S. Chen+, X. Shen+, L. Liang+, M. P. Snyder*, Longitudinal Urine Metabolic Profiling and Gestational Age Prediction in Pregnancy. Submitted to *Science Translational Medicine*. *⊘*
- 5. 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, **Methods for Evaluating Gestational Progress and Applications Thereof**, *2021*, USA.
- 3. Z-J. Zhu, X. Shen, A Method for Metabolite Annotation and Dysregulated Pathway Analysis, 2019, China.

□ Oral Presentations

- 1. Multi-omics Microsampling for The Profiling of Lifestyle-Associate Changes in Health. The 71th American Society for Mass Spectrometry Conference, 2023/6, Houston, USA.
- 2. Remote and Flexible Microsampling Multi-omics for Precision Medicine. Invited presentation, 2023/4, iPOP summit, Stanford University, USA.
- 3. Bioinformatics Algorithm Development for Mass Spectrometry Data and its Application to Precision Medicine.

 Invited presentation, 2023/3, Altos Labs, Redwood City, 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.
- 5. Multi-omics Microsampling for The Profiling of Lifestyle-Associate Changes in Health. Stanford Postdoc Symposium, 2023/2, Stanford, USA.
- 6. Bioinformatics Method Development for Mass Spectrometry and its Application to Precision Medicine. Stanford CVI Early Career Research Roundtable, 2022/11, Stanford, USA.
- 7. Deep Learning-based Pseudo-Mass Spectrometry Imaging Analysis for Precision Medicine. CASMS Virtual Conference, 2022/10, Virtual meeting.
- 8. TidyMass: an Object-oriented Reproducible Analysis Framework for LC-MS Data. ACS Fall 2022, 2022/8, Virtual meeting.
- 9. metID: an R Package for Automatable Compound Annotation for LC-MS-based Data. The 69th American Society for Mass Spectrometry Conference, 2021/11, Philadelphia, USA.
- 10. Decoding Links Between the Exposome and Health Outcomes by Multi-omics Analysis. Exposome Data Challenge Event, 2021/4, Virtual meeting.
- 11. Metabolic Reaction Network-based Recursive Metabolite Identification for Untargeted Metabolomics. The 14th International Conference of the Metabolomics Society, 2018/6, Seattle, USA.
- 12. Assessment of the Response to Neoadjuvant Chemo-Radiation in Rectal Cancer Patients based on a Metabolomics Approach. The 3rd China Mass Spectrometry Analysis Conference, 2017/12, Xiamen, China.
- 13. Normalization and Integration of Large-Scale Mass Spectrometry-based Metabolomics Data Using Support Vector Regression. The 34th China Mass Spectrometry Society Conference, 2016/9, Xining, China.
- 14. 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.

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Poster Presentations

1. TidyMass An Object-oriented Reproducible Analysis Framework for LC-MS Data. Stanford Data Science Conference, 2023/5, Stanford University, USA.

- 2. Deep Learning-based Pseudo-Mass Spectrometry Imaging Analysis for Precision Medicine. Stanford Genetics Retreat 2022, 2022/9, Monterey, USA.
- 3. Deep Learning-based Pseudo-Mass Spectrometry Imaging Analysis for Precision Medicine. Bay Area Metabolism Meeting (BAMM) 2022, 2022/9, Palo Alto, USA.
- 4. TidyMass An Object-oriented Reproducible Analysis Framework for LC-MS Data. The 70th American Society for Mass Spectrometry Conference, 2022/6, Minneapolis, USA.
- 5. Longitudinal Interactions Between Levels of Serum Cytokine and the Microbiome from Four Body Sites. IMMUNOLOGY2022, 2022/5, Portland, USA.
- 6. TidyMass An Object-oriented Reproducible Analysis Framework for LC-MS Data. Stanford Genetics Retreat 2021, 2021/9, Palo Alto, USA.
- 7. Longitudinal Urine Metabolic Profiling and Gestational Age Prediction in Pregnancy. The 17th International Conference of the Metabolomics Society, 2020/6, Virtual meeting.
- 8. Metabolic Reaction Network based Metabolite Annotation in Untargeted Metabolomics. The 13th International Conference of the Metabolomics Society, 2017/6, Brisbane, Austria.

Teaching Experience

> LC-MS Data Processing and Analysis Using R language

2022/9, Biotree Company

Responsibilities: Lecture

> R Language for Reproducible Data Analysis

Responsibilities: Lecture

2020/4, SCPA

> Stanford School of Medicine Intern

2019/8-Present, Stanford University

Responsibilities: Mentor

> Mass Spectrometry Analysis

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

Responsibilities: Guest lecturer

Volunteering

> 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

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

2013/9–2014/7, Student Association of IRCBC, Chinese Academy of Sciences

Journal Referee

Member

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- > Nature Biotechnology
- > Nature Communications
- > Briefing in Bioinformatics

- > Bioinformatics
- > GigaScience
- > PLOS one
- > Phytochemistry
- > Genomics, Proteomics&Bioinformatics
- > Communications Chemistry
- > Communications Biology
- > Frontiers Molecular Biosciences
- > iMeta
- > Proteomics

Technical Strength

- Languages: Mandarin (Very fluent), English (Fluent).
- ✓ Programming Languages: R[®], Python[®], HTML, Bash.
- **Bioinformatic Tools**: RNA-seq, Proteomics.
- Other Skills: Markdown, Photoshop, Illustrator, Linux, GitHub 🔾, Shiny 🥜

Referrers

> Professor Michael Snyder

Postdoctoral Advisor

Chair, Department of Genetics, Stanford University

Phone number: +1 (650) 723-4668

Email: mpsnyder@stanford.edu

> Professor Zheng-Jiang Zhu

Ph.D. Advisor

Director of Metabolomics Research Center, The Interdisciplinary Research Center on Biology and Chemistry, Chinese

Academy of Sciences

Phone number: +86 21-68582296

Email: jiangzhu@sioc.ac.cn

> Professor Caroline Johnson

Collaborator

Yale School of Public Health

Phone number: +1 (203) 785-2882 Email: caroline.johnson@yale.edu