

Xiaotao Shen, Ph.D.

Incoming Nanyang Assistant Professor, Lee Kong Chian School of Medicine, Nanyang Technological University, Singapore

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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
- Maternal and Child Health
- Wearable Data and Precision Medicine
- Environmental Health

Education & Research Experiences

- **Nanyang Assistant Professor** 2024/5–present, **Nanyang Technological University, Singapore**
- **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

- Young Investigator Award **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 **Exposome Data Challenge Event** (2021)
- Student Travel Award for Oral Presentation **The International Metabolomics Society** (2018)
- International Conference Travel Award **The Metabolites Journal** (2018)
- China National Scholarship **Ministry of Education of the People’s Republic of China** (2017)
- Award for Outstanding Youth Report **The 3<sup>rd</sup> China MS Analysis Conference** (2017)
- Merit Student **University of Chinese Academy of Sciences** (2016)
- Award for Outstanding Youth Report **The 34<sup>th</sup> China MS Society Conference** (2016)
- Inner Mongolia Outstanding Graduate **Inner Mongolia Autonomous Region** (2013)
- National Encouragement Scholarship **Inner Mongolia University** (2011)

First/Co-first Author Publications

+: Co-first Author. \*: Co-Corresponding Author

1. X. Zhou<sup>+</sup>, X. Shen<sup>+</sup>, 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.** Accepted *Cell Host&Microbe*.
2. X. Shen<sup>+</sup>, R. Kellogg<sup>+</sup>, D. Panyard<sup>+</sup>, N. Bararpour<sup>+</sup>, K. Castillo, B. Lee-McMullen, A. Delfarah, J. Ubellesker, 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. [↗](#)
3. X. Shen<sup>+</sup>, C. Wang<sup>+</sup>, M.P. Snyder\*, **massDatabase: Utilities for the Operation of the Public Compound and Pathway Database,** *Bioinformatics*, 2022, btac546. [↗](#)
4. X. Shen<sup>+</sup>, W. Shao<sup>+</sup>, C. Wang<sup>+</sup>, 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. [↗](#)
5. X. Shen<sup>+</sup>, H. Yan<sup>+</sup>, C. Wang<sup>+</sup>, P. Gao, C.H. Johnson\*, M.P. Snyder\*, **TidyMass an Object-oriented Reproducible Analysis Framework for LC-MS Data,** *Nature Communications*, 2022, 4365. [↗](#)
6. P. Gao<sup>+</sup>, X. Shen<sup>+</sup>, X. Zhang, C. Jiang, M. P. Snyder\*, **Precision Environmental Health Monitoring by Longitudinal Exposome and Multi-omics Profiling,** *Genome Research*, 2022, 32, 1199-1214. [↗](#)
7. X. Shen<sup>+</sup>, S. Wu<sup>+</sup>, 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. [↗](#)
8. 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. [↗](#)
9. X. Shen and Z.-J. Zhu\*, **MetFlow: An Interactive and Integrated Workflow For Metabolomics Data Cleaning and Differential Metabolite Discovery,** *Bioinformatics*, 2019, 35, 16. [↗](#)
10. H. Jia<sup>+</sup>, X. Shen<sup>+</sup>, 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. [↗](#)
11. J. Wang<sup>+</sup>, T. Zhang<sup>+</sup>, X. Shen<sup>+</sup>, 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. [↗](#)
12. 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. C. Peng, Q. Chen, S. Tan, X. Shen, C. Jiang. **Generalized Reporter Score-based Enrichment Analysis for Omics Data,** *BioRxiv*, 2023. [↗](#) Accepted *Briefing in Bioinformatics*
2. D. Ding, X. Shen, M.P. Snyder, R. Tibshirani, **Semi-supervised Cooperative Learning for Multiomics Data Fusion,** *arXiv*, 2023. [↗](#)
3. 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. [↗](#)
4. 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. [↗](#)
5. 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. [↗](#)
6. 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. [↗](#)
7. 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. [↗](#)
8. 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. [↗](#)
9. 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. [↗](#)
10. 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. [↗](#)
11. 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. [↗](#)
12. 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. [↗](#)
13. 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. [↗](#)
14. 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

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+Co-first Author. \*: Co-Corresponding Author

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>, C. Wang<sup>+</sup>, X. Zhou, W. Zhou, D. Hornburg, S. Wu, and M.P. Snyder<sup>\*</sup>, **Nonlinear Dynamic Changes During Human Aging Revealed in Multi-omics Profiles**. Submitted.
3. X. Shen<sup>+</sup>, M.P. Snyder<sup>\*</sup>, **microbiomeDataset: A Tidyverse-style Framework for Organizing and Processing Microbiome Data**. Submitted.
4. S. Chen<sup>+</sup>, X. Shen<sup>+</sup>, L. Liang<sup>+</sup>, M. P. Snyder<sup>\*</sup>, **Longitudinal Urine Metabolic Profiling and Gestational Age Prediction in Pregnancy**. Submitted to *Briefing in Bioinformatics*. [↗](#)
5. S. Chen<sup>+</sup>, G. Wang<sup>+</sup>, X. Shen<sup>+</sup>, D. Hornburg, S. Rego, R. Hoffman, S. Nevins, X. Cheng, M.P. Snyder<sup>\*</sup>, **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

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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

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1. **Nonlinear Dynamic Changes During Human Aging Revealed in Multi-omics Profiles**. Bay Area Metabolism Meeting (BAMM) 2023, 2022/9, 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. **Remote and Flexible Microsampling Multi-omics for Precision Medicine**. Invited presentation, 2023/4, iPOP summit, Stanford University, USA.
5. **Bioinformatics Algorithm Development for Mass Spectrometry Data and its Application to Precision Medicine**. Invited presentation, 2023/3, Altos Labs, Redwood City, USA.
6. **Multi-omics Microsampling for The Profiling of Lifestyle-Associate Changes in Health**. Invited presentation, 2023/2, Huazhong University of Science and Technology, China.
7. **Multi-omics Microsampling for The Profiling of Lifestyle-Associate Changes in Health**. Stanford Postdoc Symposium, 2023/2, Stanford, USA.
8. **Bioinformatics Method Development for Mass Spectrometry and its Application to Precision Medicine**. Stanford CVI Early Career Research Roundtable, 2022/11, Stanford, USA.
9. **Deep Learning-based Pseudo-Mass Spectrometry Imaging Analysis for Precision Medicine**. CASMS Virtual Conference, 2022/10, Virtual meeting.
10. **TidyMass: An Object-oriented Reproducible Analysis Framework for LC-MS Data**. ACS Fall 2022, 2022/8, Virtual meeting.

11. **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.
12. **Decoding Links Between the Exposome and Health Outcomes by Multi-omics Analysis.** Exposome Data Challenge Event, 2021/4, Virtual meeting.
13. **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.
14. **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.
15. **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.
16. **Normalization and Integration of Large-Scale MS-based Metabolomics Data Using Support Vector Regression.** The 64<sup>th</sup> American Society for Mass Spectrometry Conference, 2016/6, San Antonio, USA.

## Poster Presentations

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1. **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.
2. **TidyMass An Object-oriented Reproducible Analysis Framework for LC-MS Data.** Stanford Data Science Conference, 2023/5, Stanford University, USA.
3. **Deep Learning-based Pseudo-Mass Spectrometry Imaging Analysis for Precision Medicine.** Stanford Genetics Retreat 2022, 2022/9, Monterey, USA.
4. **Deep Learning-based Pseudo-Mass Spectrometry Imaging Analysis for Precision Medicine.** Bay Area Metabolism Meeting (BAMM) 2022, 2022/9, Palo Alto, USA.
5. **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.
6. **Longitudinal Interactions Between Levels of Serum Cytokine and the Microbiome from Four Body Sites.** IMMUNOLOGY2022, 2022/5, Portland, USA.
7. **TidyMass An Object-oriented Reproducible Analysis Framework for LC-MS Data.** Stanford Genetics Retreat 2021, 2021/9, Palo Alto, USA.
8. **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.
9. **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 Experience

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- **LC-MS Data Processing and Analysis Using R language** 2022/9, Biotree Company  
Responsibilities: Lecture
- **R Language for Reproducible Data Analysis** 2020/4, SCPA  
Responsibilities: Lecture
- **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

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- **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](#)
- **Member** 2019/7–2021/7, [Stanford Chinese Postdoctoral Association](#)
- **Member** 2013/9–2014/7, **Student Association of IRCBC, Chinese Academy of Sciences**





## Journal Referee

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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

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- **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

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- [\*\*Professor Michael Snyder\*\*](#)  
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