Shipei Xing

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Research Interests

Mass spectrometry, Bioinformatics, Metabolomics, Molecule discovery

Employment

2023.8 – Present **Univeristy of California, San Diego** – La Jolla, US
Postdoctoral scholar
Supervisor: Pieter C. Dorrestein

Education

2019.1 – 2023.4 **University of British Columbia** – Vancouver, Canada
PhD in Chemistry
Supervisor: Tao Huan

2014.9 – 2018.6 **Zhejiang University** – Hangzhou, China
BSc in Chemistry (Chu Kochen Honors College)
Supervisor: Zhan Lu, Feihe Huang

2017.3 – 2017.9 **University of Utah** – Salt Lake City, US
Visiting scholar
Supervisor: Peter J. Stang

Featured Publications

See Google Scholar here.

2023 Shipei Xing, Sam Shen, Banghua Xu, Xiaoxiao Li, Tao Huan. BUDDY: molecular formula discovery via bottom-up MS/MS interrogation. ***Nature Methods***.

2026 Shipei Xing, Abubaker Patan, Julius Agongo, Harsha Gouda, Vincent Charron-Lamoureux, Yasin El Abiead, Zhewen Hu, Haoqi Nina Zhao, Ipsita Mohanty, Jasmine Zemlin, Wilhan Donizete Gonçalves Nunes, Lindsey A. Burnett, Mingxun Wang, Dionicio Siegel, Pieter C. Dorrestein. Navigating the conjugated metabolome. ***bioRxiv, manuscript in review at Nature***.

2025 Abubaker Patan†, Shipei Xing† (co-first), Vincent Charron-Lamoureux†, Zhewen Hu, Victoria Deleray, Julius Agongo, Yasin El Abiead, Helena Mannochio-Russo, Ipsita Mohanty, Harsha Gouda, Jasmine Zemlin, Prajit Rajkumar, Carlynda Lee, Daniel Leanos, Noah Weimann, Wataru Tsuda, Sadie Giddings, Tammy Bui, Kine Eide Kvitne, Haoqi Nina Zhao, Simone Zuffa, Vivian Nguyen, Aileen Andrade, Wilhan Donizete Gonçalves Nunes, Andrés M. Caraballo-Rodríguez, Lurian Caetano David, Jeremy Carver, Nuno Bandeira, Mingxun Wang, Lindsey Burnett, Dionicio Siegel, Pieter C. Dorrestein. Charting the undiscovered metabolome with synthetic multiplexing. ***bioRxiv***.

2024 Shipei Xing, Vincent Charron-Lamoureux, Måns Ekelöf, Yasin El Abiead, Huaxu Yu, Oliver Fiehn, Theodore Alexandrov, Pieter C. Dorrestein. Structural annotation of full-scan MS data: A unified solution for LC-MS and MS imaging analyses. ***Nature Communications, in revision***.

2025 Shipei Xing, Vincent Charron-Lamoureux, Haoqi Zhao, Yasin El Abiead, Mingxun Wang, Pieter C. Dorrestein. Reverse spectral search reimagined: a simple but overlooked solution for chimeric spectral annotation. ***Analytical Chemistry***.

2021 Shipei Xing, Yibo Jiao, Melody Salehzadeh, Kiran K Soma, Tao Huan. SteroidXtract: deep learning-based pattern recognition enables comprehensive and rapid extraction of steroid-like metabolic features for automated biology-driven metabolomics. ***Analytical Chemistry***.

2020 Shipei Xing, Yan Hu, Zixuan Yin, Min Liu, Xiaoyu Tang, Mingliang Fang, Tao Huan. Retrieving and utilizing hypothetical neutral losses from tandem mass spectra for spectral similarity analysis and unknown metabolite annotation. ***Analytical Chemistry***.

2022 Shipei Xing, Tao Huan. Radical fragment ions in collision-induced dissociation-based tandem mass spectrometry. ***Analytica Chimica Acta***.

2021 Shipei Xing, Huaxu Yu, Min Liu, Qingquan Jia, Zhi Sun, Mingliang Fang, Tao Huan. Recognizing contamination fragment ions in liquid chromatography–tandem mass spectrometry data. ***Journal of the American Society for Mass Spectrometry***. (JASMS 'Emerging Investigators' section)

Selected Co-authored Publications

2025 Haoqi Nina Zhao, Kine Eide Kvitne, Corinna Brungs, Siddharth Mohan, Vincent Charron-Lamoureux, Wout Bittremieux, Runbang Tang, Robin Schmid, Santosh Lamichhane, Shipei Xing, Yasin El Abiead, Mohammadsobhan S Andalibi, Helena Mannochio-Russo, Madison Ambre, Nicole E Avalon, MacKenzie Bryant, Lindsey A Burnett, Andrés Mauricio Caraballo-Rodríguez, Martin Casas Maya, Loryn Chin, Lluís Corominas, Ronald J Ellis, Donald Franklin, Sagan Girod, Paulo Wender P Gomes, Lauren Hansen, Robert K Heaton, Jennifer E Iudicello, Alan K Jarmusch, Lora Khatib, Scott Letendre, Sarolt Magyari, Daniel McDonald, Ipsita Mohanty, Andrés Cumsille, David J Moore, Prajit Rajkumar, Dylan H Ross, Harshada Sapre, Mohammad Reza Zare Shahneh, Ruben Gil-Solsona, Sydney P Thomas, Caitlin Tribelhorn, Helena M Tubb, Corinn Walker, Crystal X Wang, Jasmine Zemlin, Simone Zuffa, David S Wishart, Pablo Gago-Ferrero, Rima Kaddurah-Daouk, Mingxun Wang, Manuela Raffatellu, Karsten Zengler, Tomáš Pluskal, Libin Xu, Rob Knight, Shirley M Tsunoda, Pieter C Dorrestein. A resource to empirically establish drug exposure records directly from untargeted metabolomics data. ***Nature Communications***.

2025 Yasin El Abiead, Michael Strobel, Thomas Payne, Eoin Fahy, Claire O'Donovan, Shankar Subramamiam, Juan Antonio Vizcaíno, Ozgur Yurekten, Victoria Deleray, Simone Zuffa, Shipei Xing, Helena Mannochio-Russo, Ipsita Mohanty, Haoqi Nina Zhao, Andres M Caraballo-Rodriguez, Paulo Wender P. Gomes, Nicole E Avalon, Trent R Northen, Benjamin P Bowen, Katherine B Louie, Pieter C. Dorrestein, Mingxun Wang. Enabling pan-repository reanalysis for big data science of public metabolomics data. ***Nature Communications***.

2025 Vincent Charron-Lamoureux, Helena Mannochio-Russo, Santosh Lamichhane, Shipei Xing, Abubaker Patan, Paulo Wender Portal Gomes, Prajit Rajkumar, Victoria Deleray, Andrés Mauricio Caraballo-Rodríguez, Kee Voon Chua, Lye Siang Lee, Zhao Liu, Jianhong Ching, Mingxun Wang, Pieter C. Dorrestein. A guide to reverse metabolomics—a framework for big data discovery strategy. ***Nature Protocols***.

2025 Yasin El Abiead, Adriano Rutz, Simone Zuffa, Bashar Amer, Shipei Xing, Corinna Brungs, Robin Schmid, Mario SP Correia, Andres Mauricio Caraballo-Rodriguez, Amir Zarrinpar, Helena Mannochio-Russo, Michael Witting, Ipsita Mohanty, Tomáš Pluskal, Wout Bittremieux, Rob Knight, Andrew D Patterson, Justin JJ van der Hooft, Sebastian Böcker, Warwick B Dunn, Roger G Linington, David S Wishart, Jean-Luc Wolfender, Oliver Fiehn, Nicola Zamboni, Pieter C. Dorrestein. Discovery of metabolites prevails amid in-source fragmentation. ***Nature Metabolism***.

2024 Ipsita Mohanty, Helena Mannochio-Russo, Joshua V Schweer, Yasin El Abiead, Wout Bittremieux, Shipei Xing, Robin Schmid, Simone Zuffa, Felipe Vasquez, Valentina B Muti, Jasmine Zemlin, Omar E Tovar-Herrera, Sarah Moraïs, Dhimant Desai, Shantu Amin, Imhoi Koo, Christoph W Turck, Itzhak Mizrahi, Penny M Kris-Etherton, Kristina S Petersen, Jennifer A Fleming, Tao Huan, Andrew D Patterson, Dionicio Siegel, Lee R Hagey, Mingxun Wang, Allegra T Aron, Pieter C. Dorrestein. The underappreciated diversity of bile acid modifications. ***Cell***.

2023 Wout Bittremieux, Nicole E Avalon, Sydney P Thomas, Sarvar A Kakhkhorov, Alexander A Aksenov, Paulo Wender P Gomes, Christine M Aceves, Andrés Mauricio Caraballo-Rodríguez, Julia M Gauglitz, William H Gerwick, Tao Huan, Alan K Jarmusch, Rima F Kaddurah-Daouk, Kyo Bin Kang, Hyun Woo Kim, Todor Kondić, Helena Mannochio-Russo, Michael J Meehan, Alexey V Melnik, Louis-Felix Nothias, Claire O'Donovan, Morgan Panitchpakdi, Daniel Petras, Robin Schmid, Emma L Schymanski, Justin JJ van der Hooft, Kelly C Weldon, Heejung Yang, Shipei Xing, Jasmine Zemlin, Mingxun Wang, Pieter C Dorrestein. Open access repository-scale propagated nearest neighbor suspect spectral library for untargeted metabolomics. ***Nature Communications***.

2023 Fanrong Zhao, Li Li, Penghui Lin, Yue Chen, Shipei Xing, Huili Du, Zheng Wang, Junjie Yang, Tao Huan, Cheng Long, Limao Zhang, Bin Wang, Mingliang Fang. HExpPredict: in vivo exposure prediction of human blood exposome using a random forest model and its application in chemical risk prioritization. ***Environmental Health Perspectives***.

2022 Daniel GC Treen, Mingxun Wang, Shipei Xing, Katherine B Louie, Tao Huan, Pieter C Dorrestein, Trent R Northen, Benjamin P Bowen. SIMILE enables alignment of tandem mass spectra with statistical significance. ***Nature Communications***.

2021 Fanrong Zhao, Li Li, Yue Chen, Yichao Huang, Tharushi Prabha Keerthisinghe, Agnes Chow, Ting Dong, Shenglan Jia, Shipei Xing, Benedikt Warth, Tao Huan, Mingliang Fang. Risk-based chemical ranking and generating a prioritized human exposome database. ***Environmental Health Perspectives***.

Honors and Awards

2022 Canadian Society of Mass Spectrometry (CSMS) Lake Louise Travel Award (sponsored by Thermo).

2022 – 2023 Affiliated Fellowship, UBC.

2022 Pei-Huang Tung and Tan-Wen Tung Graduate Fellowship, UBC.

2022 Gladys Estella Laird Research Fellowship, UBC.

2022 C L Wang Memorial Scholarship, UBC.

2022 Dr. Arnold By Travel Fellowship, UBC Chemistry.

2022 Graduate Student Travel Award, UBC.

2021 Sandra Morris and Richard Tillyer Scholarship in Chemistry, UBC Chemistry.

2021 Best Poster Award. 1st Chinese American Society for Mass Spectrometry (CASMS) Virtual Conference.

2020 – 2022 President's Academic Excellence Initiative PhD Award, UBC.

2019 – 2022 Faculty of Science PhD Tuition Award, UBC.

2019 – 2022 International Tuition Award, UBC.

2018 Outstanding Thesis Award, ZJU.

Conference Presentations

2024 **Poster presentation**. Discovering and annotating new molecules in untargeted metabolomics through structural coupling.
72nd ASMS Conference on Mass Spectrometry and Allied Topics. Anaheim, US.

2022 **Oral presentation**. Molecular formula discovery via bottom-up MS/MS interrogation.
34th Lake Louise Tandem MS Workshop. Lake Louise, Canada.

2022 **Lightning talk & poster presentation**. BUDDY: Bottom-up MS/MS interrogation enables large-scale discovery of unreported molecular formulae with significance control.
2nd CASMS Virtual Conference.

2022 **Poster presentation**. Radical Fragment Ions in Collision-Induced Dissociation-based Tandem Mass Spectrometry.
70th ASMS Conference on Mass Spectrometry and Allied Topics. Minneapolis, US.

2021 **Lightning talk & poster presentation**. Radical Fragment Ions in Collision-Induced Dissociation Mass Spectrometry.
1st CASMS Virtual Conference.

Service

Reviewer

• Co-reviewer: *Nature*, *Cell*, and *Nature Microbiology*

• Independent reviewer: *Nature Communications*, *Analytical Chemistry*, *BMC Bioinformatics*, *Journal of Cheminformatics*, and others

Editorial Board Member

• *BMC Chemistry*

Teaching Experience

2022 Teaching assistant (lecture), CHEM 211: Analytical Chemistry.

2020 Teaching assistant (lab), CHEM 154: Chemistry for Engineering.

2019 & 2021 Teaching assistant (lab), CHEM 123: Thermodynamics, Kinetics and Organic Chemistry.

Professional Affiliations

2020 – Present American Society for Mass Spectrometry (ASMS), Member.

2021 – Present Chinese American Society for Mass Spectrometry (CASMS), Member.

2022 – Present Canadian Society for Mass Spectrometry (CSMS), Member.