Shipei Xing

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Research Interests

Mass spectrometry informatics, Metabolomics, Analytical chemistry

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
Research: *Towards accurate compound annotation in mass spectrometry-based global metabolomics*
Supervisor: Tao Huan

2014.9 – 2018.6 **Zhejiang University** – Hangzhou, China
BSc in Chemistry (Qiushi Honors Program, Chu Kochen Honors College)
Research: *Synthesis of Chiral Imidazoline Iminopyridine Ligands* (Outstanding thesis award)
Supervisor: Zhan Lu

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

Featured Publications

See Google Scholar here.

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. ***Manuscript submitted to Nature***.

2025 Shipei Xing, Abubaker Patan, Yasin El Abiead, Vincent Charron-Lamoureux, Julius Agongo, Zhewen Hu, Harsha Gouda, Haoqi Nina Zhao, Ipsita Mohanty, Pieter C. Dorrestein. Navigating the pan-repository conjugated metabolome. ***Manuscript in final preparation***.

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. ***bioRxiv (in revision at Nature Communications***).

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

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)

Co-authored Publications

2025 Harsha Gouda, Julius Agongo, Patricia Kelly, Marta Sala-Climent, Wilhan Gonçalves Nunes, Konstantinos Gkikas, Shipei Xing, Victoria Deleray, Crystal Wang, Vincent Charron-Lamoureux, Haoqi Nina Zhao, Ipsita Mohanty, Aubreyana McMaugh, Meera Sharma, An Nguyen, Jennifer Fleming, Mingxun Wang, Nicholas Rattray, Richard Russell, Konstantinos Gerasimidis, Monica Guma, Pieter C. Dorrestein. Learning molecular fingerprints of foods to decode dietary intake. ***Research Square***.

2025 Helena Mannochio-Russo, Wilhan D Gonçalves Nunes, Haoqi Nina Zhao, Kine Eide Kvitne, Shipei Xing, Harsha Gouda, Julius Agongo, Ipsita Mohanty, Vincent Charron-Lamoureux, Prajit Rajkumar, Abzer K Pakkir Shah, Axel Walter, Rithi Krishnaraj, Yasin El Abiead, Patrick C Ferreira, Simone Zuffa, Abubaker Patan, Andrés Mauricio Caraballo-Rodríguez, Wout Bittremieux, Daniel Petras, Mingxun Wang, Pieter C. Dorrestein. Bridging Complexity and Accessibility in Metabolomics with MetaboApps. ***chemRxiv***.

2025 Ipsita Mohanty, Shipei Xing, Vanessa Castillo, Julius Agongo, Abubaker Patan, Yasin El Abiead, Helena Mannochio-Russo, Simone Zuffa, Jasmine Zemlin, Alexandre Tronel, Audrey Le Gouellec, Thomas Soranzo, Crystal X Wang, Jennifer E Iudicello, Mohammadsobhan S Andalibi, Ronald J Ellis, David J Moore, Donald R Franklin Jr, Marta Sala-Climent, Monica Guma, Robin M Voigt, Rima Kaddaruh-Dauok, Dionicio Siegel, Mingxun Wang, Lee R Hagey, Pieter C. Dorrestein. MS/MS Mass Spectrometry Filtering Tree for Bile Acid Isomer Annotation. ***bioRxiv***.

2025 Julius Agongo, Harsha Gouda, Aubreyana E McMaugh, Celeste Allaband, Seyedeh Mehrnaz Aghili, Marta Sala-Climent, Shipei Xing, Jennifer Cao, Jasmine Zemlin, Mingxun Wang, Kathleen Dorrestein, Tiffany Holt, Rob Knight, Brigid S Boland, Monica Guma, Pieter C. Dorrestein. Quantitative Food Biomarkers Enable Dietary Ontology Referencing Across 500 Foods and Human Plasma. ***chemRxiv***.

2025 Yasin El Abiead, Ipsita Mohanty, Shipei Xing, Adriano Rutz, Vincent Charron-Lamoureux, Tito Damiani, Wenyun Lu, Gary J Patti, Nicola Zamboni, Oscar Yanes, Pieter C. Dorrestein. A Perspective on Unintentional Fragments and their Impact on the Dark Metabolome, Untargeted Profiling, Molecular Networking, Public Data, and Repository Scale Analysis. ***Journal of the American Chemical Society, just accepted***.

2025 Haoqi Nina Zhao, Kine Eide Kvitne, Corinna Brungs, Siddharth Mohan, Vincent Charron-Lamoureux, Wout Bittremieux, Runbang Tang, Robin Schmid, Santosh Lamichhane, Yasin El Abiead, Mohammadsobhan S Andalibi, Helena Mannochio-Russo, Madison Ambre, Nicole E Avalon, MacKenzie Bryant, Andrés Mauricio Caraballo-Rodríguez, Martin Casas Maya, Loryn Chin, Ronald J Ellis, Donald Franklin, Sagan Girod, Paulo Wender P Gomes, Lauren Hansen, Robert 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, Sydney P Thomas, Caitlin Tribelhorn, Helena M Tubb, Corinn Walker, Crystal X Wang, Shipei Xing, Jasmine Zemlin, Simone Zuffa, David S Wishart, Rima Kaddurah-Daouk, Mingxun Wang, Manuela Raffatellu, Karsten Zengler, Tomáš Pluskal, Libin Xu, Rob Knight, Shirley M Tsunoda, Pieter C. Dorrestein Empirically establishing drug exposure records directly from untargeted metabolomics data. ***Nature Communications, just accepted***.

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 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***.

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 Zixuan Zhang, Xin Xu, Shipei Xing, Changzhi Shi, Zecang You, Xiaojun Deng, Ling Tan, Zhe Mo, Mingliang Fang. PAH-Finder: A Pattern Recognition Workflow for Identification of PAHs and Their Derivatives. ***Analytical Chemistry***.

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***.

2024 Tingting Zhao, Nicholas JP Wawryk, Shipei Xing, Brian Low, Gigi Li, Huaxu Yu, Yukai Wang, Qiming Shen, Xing-Fang Li, Tao Huan. ChloroDBPFinder: Machine Learning-Guided Recognition of Chlorinated Disinfection Byproducts from Nontargeted LC-HRMS Analysis. ***Analytical Chemistry***.

2024 Paulo Wender P Gomes, Helena Mannochio-Russo, Robin Schmid, Simone Zuffa, Tito Damiani, Luis-Manuel Quiros-Guerrero, Andrés Mauricio Caraballo-Rodríguez, Haoqi Nina Zhao, Heejung Yang, Shipei Xing, Vincent Charron-Lamoureux, Desnor N Chigumba, Brian E Sedio, Jonathan A Myers, Pierre-Marie Allard, Thomas V Harwood, Giselle Tamayo-Castillo, Kyo Bin Kang, Emmanuel Defossez, Hector HF Koolen, Milton Nascimento da Silva, Consuelo Yumiko Yoshioka e Silva, Sergio Rasmann, Tom WN Walker, Gaëtan Glauser, José Miguel Chaves-Fallas, Bruno David, Hyunwoo Kim, Kyu Hyeong Lee, Myeong Ji Kim, Won Jun Choi, Young-Sam Keum, Emilly JSP de Lima, Lívia Soman de Medeiros, Giovana A Bataglion, Emmanoel V Costa, Felipe MA da Silva, Alice Rhelly V Carvalho, José Diogo E Reis, Sônia Pamplona, Eunah Jeong, Kyungha Lee, Geum Jin Kim, Yun-Seo Kil, Joo-Won Nam, Hyukjae Choi, Yoo Kyong Han, Si Young Park, Ki Yong Lee, Changling Hu, Yilun Dong, Shengmin Sang, Colin R Morrison, Ricardo Moreira Borges, Andrew Magno Teixeira, Seo Yoon Lee, Bum Soo Lee, Se Yun Jeong, Ki Hyun Kim, Adriano Rutz, Arnaud Gaudry, Edouard Bruelhart, Iris F Kappers, Rumyana Karlova, Mara Meisenburg, Roland Berdaguer, J Sebastián Tello, David Henderson, Leslie Cayola, S Joseph Wright, David N Allen, Kristina J Anderson-Teixeira, Jennifer L Baltzer, James A Lutz, Sean M McMahon, Geoffrey G Parker, John D Parker, Trent R Northen, Benjamin P Bowen, Tomáš Pluskal, Justin JJ van der Hooft, Jeremy J Carver, Nuno Bandeira, Benjamin S Pullman, Jean-Luc Wolfender, Roland D Kersten, Mingxun Wang, Pieter C Dorrestein. plantMASST-Community-driven chemotaxonomic digitization of plants. ***bioRxiv***.

2024 Abzer K Pakkir Shah, Axel Walter, Filip Ottosson, Francesco Russo, Marcelo Navarro-Diaz, Judith Boldt, Jarmo-Charles J Kalinski, Eftychia Eva Kontou, James Elofson, Alexandros Polyzois, Carolina González-Marín, Shane Farrell, Marie R Aggerbeck, Thapanee Pruksatrakul, Nathan Chan, Yunshu Wang, Magdalena Pöchhacker, Corinna Brungs, Beatriz Cámara, Andrés Mauricio Caraballo-Rodríguez, Andres Cumsille, Fernanda de Oliveira, Kai Dührkop, Yasin El Abiead, Christian Geibel, Lana G Graves, Martin Hansen, Steffen Heuckeroth, Simon Knoblauch, Anastasiia Kostenko, Mirte CM Kuijpers, Kevin Mildau, Stilianos Papadopoulos Lambidis, Paulo Wender Portal Gomes, Tilman Schramm, Karoline Steuer-Lodd, Paolo Stincone, Sibgha Tayyab, Giovanni Andrea Vitale, Berenike C Wagner, Shipei Xing, Marquis T Yazzie, Simone Zuffa, Martinus de Kruijff, Christine Beemelmanns, Hannes Link, Christoph Mayer, Justin JJ van der Hooft, Tito Damiani, Tomáš Pluskal, Pieter Dorrestein, Jan Stanstrup, Robin Schmid, Mingxun Wang, Allegra Aron, Madeleine Ernst, Daniel Petras. Statistical analysis of feature-based molecular networking results from non-targeted metabolomics data. ***Nature Protocols***.

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 Kirstin L Brown, Jessica MC Krekhno, Shipei Xing, Tao Huan, Lindsay D Eltis. Cholesterol-Mediated Coenzyme A Depletion in Catabolic Mutants of Mycobacteria Leads to Toxicity. ***ACS Infectious Diseases***.

2023 Tingting Zhao, Shipei Xing, Huaxu Yu, Tao Huan. De novo cleaning of chimeric MS/MS spectra for LC-MS/MS-based metabolomics. ***Analytical Chemistry***.

2023 Ting Fu, Tao Huan, Gibraan Rahman, Hui Zhi, Zhenjiang Xu, Tae Gyu Oh, Jian Guo, Sally Coulter, Anupriya Tripathi, Cameron Martino, Justin L McCarville, Qiyun Zhu, Fritz Cayabyab, Brian Low, Mingxiao He, Shipei Xing, Fernando Vargas, T Yu Ruth, Annette Atkins, Christopher Liddle, Janelle Ayres, Manuela Raffatellu, Pieter C Dorrestein, Michael Downes, Rob Knight, Ronald M Evans. Paired microbiome and metabolome analyses associate bile acid changes with colorectal cancer progression. ***Cell Reports***.

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***.

2023 Tingting Zhao, Kristin Carroll, Caley Craven, Nicholas JP Wawryk, Shipei Xing, Jian Guo, Xing-Fang Li, Tao Huan. HDPairFinder: A data processing platform for hydrogen/deuterium isotopic labeling-based nontargeted analysis of trace-level amino-containing chemicals in environmental water. ***Journal of Environmental Sciences***.

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***.

2022 Jian Guo, Huaxu Yu, Shipei Xing, Tao Huan. Addressing big data challenges in mass spectrometry-based metabolomics. ***Chemical Communications***.

2022 Jian Guo, Sam Shen, Min Liu, Chenjingyi Wang, Brian Low, Ying Chen, Yaxi Hu, Shipei Xing, Huaxu Yu, Yu Gao, Mingliang Fang, Tao Huan. JPA: joint metabolic feature extraction increases the depth of chemical coverage for LC-MS-Based metabolomics and exposomics. ***Metabolites***.

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***.

2021 Jian Guo, Sam Shen, Shipei Xing, Ying Chen, Frank Chen, Elizabeth M Porter, Huaxu Yu, Tao Huan. EVA: evaluation of metabolic feature fidelity using a deep learning model trained with over 25000 extracted ion chromatograms. ***Analytical Chemistry***.

2021 Jian Guo, Sam Shen, Shipei Xing, Huaxu Yu, Tao Huan. ISFrag: de novo recognition of in-source fragments for liquid chromatography–mass spectrometry data. ***Analytical Chemistry***.

2021 Ying Chen, Jian Guo, Shipei Xing, Huaxu Yu, Tao Huan. Global-scale metabolomic profiling of human hair for simultaneous monitoring of endogenous metabolome, short-and long-term exposome. ***Frontiers in Chemistry***.

2021 Jian Guo, Sam Shen, Shipei Xing, Tao Huan. DaDIA: hybridizing data-dependent and data-independent acquisition modes for generating high-quality metabolomic data. ***Analytical Chemistry***.

2021 Polina Beskrovnaya, Doaa Fakih, Isabelle Morneau, Ameena Hashimi, Dainelys Guadarrama Bello, Shipei Xing, Antonio Nanci, Tao Huan, Elitza I Tocheva. No Endospore Formation Confirmed in Members of the Phylum Proteobacteria. ***Applied and Environmental Microbiology***.

2020 Huaxu Yu, Shipei Xing, Lorenz Nierves, Philipp F Lange, Tao Huan. Fold-change compression: an unexplored but correctable quantitative bias caused by nonlinear electrospray ionization responses in untargeted metabolomics. ***Analytical Chemistry***.

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 for *Nature*, *Cell*, and *Nature Microbiology*

• Independent reviewer for *Nature Communications*, *BMC Bioinformatics*, *Journal of Cheminformatics*, and others

Editorial Board Member

• *BMC Chemistry*

Teaching Experience

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

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

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

Professional Affiliations

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

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

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