

Mingxun Wang

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Current position

Post Doctoral Scholar, Skaggs School of Pharmacy and Pharmaceutical Sciences, UC San Diego

Founder, Ometa Labs LLC, San Diego

Areas of specialization

Computer Engineering - Computer Science - Bioinformatics - Computational Mass Spectrometry

Education

- 2017 Ph.D. in Computer Science, UC San Diego
- 2014 C PHIL. in Computer Science, UC San Diego
- 2013 MS in Computer Science, UC San Diego
- 2009 BS in Computer Engineering summa cum laude, University of Illinois

Publications & Talks

Full publication list can be found [here](#).

SELECTED JOURNAL ARTICLES

- 2020 **Mingxun Wang**, Alan K. Jarmusch, Fernando Vargas, Alexander A. Aksenov, Julia Gauglitz, Kelly Weldon, Daniel Petras et al. "Mass spectrometry searches using MASST." *Nature Biotechnology*
- 2019 James T Morton, Alexander A Aksenov, Louis Felix Nothias, James R Foulds, Robert A Quinn, Michelle H Badri, Tami L Swenson, Marc W Van Goethem, Trent R Northen, Yoshiki Vazquez-Baeza, **Mingxun Wang**, Nicholas A Bokulich, Aaron Watters, Se Jin Song, Richard Bonneau, Pieter C Dorrestein, Rob Knight. "Learning representations of microbe-metabolite interactions" *Nature Methods*
- 2019 Jeffrey A van Santen, Grégoire Jacob, Amrit Leen Singh, Victor Aniebok, Marcy J Balunas, Derek Bunsko, Fausto Carnevale Neto, Laia Castaño-Espriu, Chen Chang, Trevor N Clark, Jessica L Cleary Little, David A Delgadillo, Pieter C Dorrestein, Katherine R Duncan, Joseph M Egan, Melissa M Galey, FP Jake Haeckl, Alex Hua, Alison H Hughes, Dasha Iskakova, Aswad Khadilkar, Jung-Ho Lee, Sanghoon Lee, Nicole LeGrow, Dennis Y Liu, Jocelyn M Macho, Catherine S McCaughey, Marnix H Medema, Ram P Neupane, Timothy J O'Donnell, Jasmine S Paula, Laura M Sanchez, Anam F Shaikh, Sylvia Soldatou, Barbara R Terlouw, Tuan Anh Tran, Mercia Valentine, Justin JJ van der Hooft, Duy A Vo, **Mingxun Wang**, Darryl Wilson, Katherine E Zink, Roger G Linington. "The

natural products atlas: an open access knowledge base for microbial natural products discovery”
ACS Central Science

- 2019 Louis Felix Nothias, Daniel Petras, Robin Schmid, Kai Dührkop, Johannes Rainer, Abinesh Sarvepalli, Ivan Protsyuk, Madeleine Ernst, Hiroshi Tsugawa, Markus Fleischauer, Fabian Aicheler, Alexander Aksenov, Oliver Alka, Pierre-Marie Allard, Aiko Barsch, Xavier Cachet, Mauricio Caraballo, Ricardo R Da Silva, Tam Dang, Neha Garg, Julia M Gauglitz, Alexey Gurevich, Giorgis Isaac, Alan K Jarmusch, Zdeněk Kameník, Kyo Bin Kang, Nikolas Kessler, Irina Koester, Ansgar Korf, Audrey Le Gouellec, Marcus Ludwig, Martin H Christian, Laura-Isobel McCall, Jonathan McSayles, Sven W Meyer, Hosein Mohimani, Mustafa Morsy, Oriane Moyne, Steffen Neumann, Heiko Neuweiger, Ngoc Hung Nguyen, Melissa Nothias-Esposito, Julien Paolini, Vanessa V Phelan, Tomáš Pluskal, Robert A Quinn, Simon Rogers, Bindesh Shrestha, Anupriya Tripathi, Justin JJ van der Hooft, Fernando Vargas, Kelly C Weldon, Michael Witting, Heejung Yang, Zheng Zhang, Florian Zubeil, Oliver Kohlbacher, Sebastian Böcker, Theodore Alexandrov, Nuno Bandeira, **Mingxun Wang**, Pieter C Dorrestein. "Feature-based Molecular Networking in the GNPS Analysis Environment" *Preprint in Biorxiv*
- 2019 Alan K Jarmusch, **Mingxun Wang**, Christine M Aceves, Rohit S Advani, Shaden Aguire, Alexander A Aksenov, Gajender Aleti, Allegra T Aron, Anelize Bauermeister, Sanjana Bolleddu, Amina Bouslimani, Andres Mauricio Caraballo-Rodriguez, Rama Chaar, Roxana Coras, Emmanuel O Elijah, Madeleine Ernst, Julia M Gauglitz, Emily C Gentry, Makhai Husband, Scott A Jarmusch, Kenneth L Jones, Zdenek Kamenik, Audrey Le Gouellec, Aileen Lu, Laura-Isobel McCall, Kerry L McPhail, Michael J Meehan, Alexey V Melnik, Riya C Menezes, Yessica Alejandra Montoya-Giraldo, Ngoc Hung Nguyen, Louis Felix Nothias, Melissa Nothias-Esposito, Morgan Panitchpakdi, Daniel Petras, Robert Quinn, Nicole Sikora, Justin JJ van der Hooft, Fernando Vargas, Alison Vrbanac, Kelly Weldon, Rob Knight, Nuno Bandeira, Pieter C Dorrestein. "Repository-scale Co-and Re-analysis of Tandem Mass Spectrometry Data" *Preprint in Biorxiv*
- 2019 Robert A. Quinn, Alison Vrbanac, Alexey V. Melnik, Kathryn A. Patras, Mitchell Christy, Andrew T. Nelson, Alexander Aksenov, Anupriya Tripathi, Greg Humphrey, Ricardo da Silva, Robert Bussell, Taren Thron, **Mingxun Wang**, Fernando Vargas, Julia M. Gauglitz, Michael J. Meehan, Orit Poulsen, Brigid S. Boland, John T. Chang, William J. Sandborn, Meerana Lim, Neha Garg, Julie Lumeng, Barbara I. Kazmierczak, Ruchi Jain, Marie Egan, Kyung E. Rhee, Gabriel G. Haddad, Dionicio Siegel, Sarkis Mazmanian, Victor Nizet, Rob Knight, Pieter C. Dorrestein. "Chemical Impacts of the Microbiome Across Scales Reveal Novel Conjugated Bile Acids." *Nature*
- 2018 Antonio Gonzalez, Jose A. Navas-Molina, Tomasz Kosciolk, Daniel McDonald, Yoshiki Vázquez-Baeza, Gail Ackermann, Jeff DeReus, Stefan Janssen, Austin D. Swafford, Stephanie B. Orchanian, Jon G. Sanders, Joshua Shorenstein, Hannes Holste, Semar Petrus, Adam Robbins-Pianka, Colin J. Brislawn, **Mingxun Wang**, Jai Ram Rideout, Evan Bolyen, Matthew Dillon, J. Gregory Caporaso, Pieter C. Dorrestein, and Rob Knight. "Qiita: rapid, web-enabled microbiome meta-analysis", *Nature Methods*
- 2018 Louis-Félix Nothias, Mélissa Nothias-Esposito, Ricardo da Silva, **Mingxun Wang**, Ivan Protsyuk, Zheng Zhang, Abi Sarvepalli et al. "Bioactivity-based molecular networking for the discovery of drug leads in natural product bioassay-guided fractionation." *Journal of natural products*
- 2018 **Mingxun Wang**, Jian Wang, Jeremy Carver, Benjamin Pullman, Seong Cha, Nuno Bandeira, "Assembling the Community-Scale Discoverable Human Proteome", *Cell Systems*
- 2017

- Kerstin Scheubert, Franziska Hufsky, Daniel Petras, **Mingxun Wang**, Louis-Felix Nothias, Kai Duehrkop, Nuno Bandeira, Pieter Dorrestein, Sebastian Boecker, "Significance estimation for large scale untargeted metabolomics annotations", *Nature Communications*
- 2017 Neha Garg, **Mingxun Wang**, Embriette Hyde, Ricardo R. da Silva, Alexey V. Melnik, Ivan Prot-syuk, Amina Bouslimani, Yan Wei Lim, William Comstock, Richard Wong, Greg Humphrey, James Gaffney, Gail Ackermann, Timothy Spivey, Sharon S. Brouha, Nuno Bandeira, Grace Y. Lin, For-est Rohwer, Douglas J. Conrad, Theodore Alexandrov, Rob Knight, Pieter C. Dorrestein, "Three dimensional volume cartography of microbiome and metabolome data onto radiological images of the human lung", *Cell Host Microbe*
- 2016 Amina Bouslimania, Alexey V Melnik, Zhenjiang Xu, Amnon Amir, Ricardo R da Silva, **Mingxun Wang**, Nuno Bandeira, Theodore Alexandrov, Rob Knight, and Pieter C. Dorrestein, "Lifestyle chemistries from phones for individual profiling", *Proceedings of the National Academy of Sci-ences*
- 2016 **Mingxun Wang**, Jeremy J Carver, Vanessa V Phelan, Laura M Sanchez, Neha Garg, Yao Peng, Don Duy Nguyen, Jeramie Watrous, Clifford A Kapon, Tal Luzzatto-Knaan, Carla Porto, Amina Bouslimani, Alexey V Melnik, Michael J Meehan, Wei-Ting Liu, Max Crusemann, Paul D Boudreau, Eduardo Esquenazi, Mario Sandoval-Calderón, Roland D Kersten, Laura A Pace, Robert A Quinn, Katherine R Duncan, Cheng-Chih Hsu, Dimitrios J Floros, Ronnie G Gavilan, Karin Kleigrew, Trent Northen, Rachel J Dutton, Delphine Parrot, Erin E Carlson, Bertrand Aigle, Charlotte F Michelsen, Lars Jelsbak, Christian Sohlenkamp, Pavel Pevzner, Anna Edlund, Jeffrey McLean, Jörn Piel, Brian T Murphy, Lena Gerwick, Chih-Chuang Liaw, Yu-Liang Yang, Hans-Ulrich Humpf, Maria Maansson, Robert A Keyzers, Amy C Sims, Andrew R Johnson, Ashley M Sidebottom, Brian E Sedio, Andreas Klitgaard, Charles B Larson, Daniel Torres-Mendoza, David J Gonzalez, Denise B Silva, Lucas M Marques, Daniel P Demarque, Egle Pociute, Ellis C O'Neill, Enora Briand, Eric JN Helfrich, Eve A Granatosky, Evgenia Glukhov, Florian Ryffel, Hailey Houson, Hosein Mohi-mani, Jenan J Kharbush, Yi Zeng, Julia A Vorholt, Kenji L Kurita, Pep Charusanti, Kerry L McPhail, Kristian Fog Nielsen, Lisa Vuong, Maryam Elfeki, Matthew F Traxler, Niclas Engene, Nobuhiro Koyama, Oliver B Vining, Ralph Baric, Ricardo R Silva, Samantha J Mascuch, Sophie Tomasi, Ste-fan Jenkins, Venkat Macherla, Thomas Hoffman, Vinayak Agarwal, Philip G Williams, Jingqui Dai, Ram Neupane, Joshua Gurr, Andrés MC Rodriguez, Anne Lamsa, Chen Zhang, Kathleen Dor-restein, Brendan M Duggan, Jehad Almaliti, Pierre-Marie Allard, Prasad Phapale, Louis-Felix Noth-ias, Theodore Alexandrov, Marc Litaudon, Jean-Luc Wolfender, Jennifer E Kyle, Thomas O Metz, Tyler Peryea, Dac-Trung Nguyen, Danielle VanLeer, Paul Shinn, Ajit Jadhav, Rolf Müller, Katrina M Waters, Wenyuan Shi, Xueting Liu, Lixin Zhang, Rob Knight, Paul R Jensen, Bernhard Ø Pals-son, Kit Pogliano, Roger G Lington, Marcelino Gutiérrez, Norberto P Lopes, William H Gerwick, Bradley S Moore, Pieter C Dorrestein, Nuno Bandeira, "Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking", *Nature Biotech-nology*
- 2015 Amina Bouslimani, Carla Porto, Christopher M Rath, **Mingxun Wang**, Yurong Guo, Antonio Gonzalez, Donna Berg-Lyon, Gail Ackermann, Gitte Julie Moeller Christensen, Teruaki Nakatsuji, Lingjuan Zhang, Andrew W Borkowski, Michael J Meehan, Kathleen Dorrestein, Richard L Gallo, Nuno Bandeira, Rob Knight, Theodore Alexandrov, Pieter C Dorrestein, "Molecular cartography of the human skin surface in 3D", *Proceedings of the National Academy of Sciences*
- 2013 **Mingxun Wang**, Nuno Bandeira, "Spectral library generating function for assessing spectrum-spectrum match significance", *Journal of Proteome Research*

CONFERENCE TALKS

- 2019 Skin Beauty Congress in San Francisco
- 2019 Microbiome Movement - Workshop in San Diego
- 2019 Skin Beauty Congress in San Francisco
- 2018 Skin Microbiome Congress in San Francisco
- 2018 ASP 2018 - Introduction to Global Natural Product Social (GNPS) Molecular Networking and 3D Visualization of Natural Product Data Workshop
- 2018 Metabolomics 2018 - Compound Identification Workshop
- 2018 ASM Oral Presentation - Sharing and Community Curation of Mass Spec Data with GNPS
- 2018 Skin Microbiome Congress in Boston
- 2017 ASMS Workshop - MassIVE Big Data Workshop
- 2017 ASM Workshop - Qiita and GNPS Analysis Workshop
- 2016 ASMS Oral - Collaborative Human Computing: The Next Generation Paradigm in Metabolomics
- 2016 ASMS Workshop - Big Data Workshop
- 2016 Sloan Microbiology of the Built Environment Data Analysis Workshop - Introduction to GNPS
- 2015 Plant Animal Genome Conference - GNPS - A Preview of the Future of Community Wide Collaboration and the Power of Social Networking in Mass Spectrometry
- 2013 RECOMB 2013 - Spectral Library Generating Function for Assessing Spectrum-Spectrum Match Significance

POSTER PRESENTATIONS

- 2017 ASP - GNPS: High Throughput Mass Spectrometry Dereplication and Discovery with Molecular Networking and Crowd Sourced Annotation
- 2017 ASMS - Assembling the community-scale discoverable human proteome
- 2016 Gordon Research Seminar/Conference Chemistry Biology of Peptides - Exploring the Highly Post Translationally Modified Peptide Space with Molecular Networks
- 2015 ASMS - GNPS: Charting Molecular Families and Structure of Tens of Thousands of Mass Spectrometry Runs
- 2014 ASMS - GNPS: Global Natural Product Molecular Social Networking – Enabling High Throughput Compound Discovery
- 2013 ASMS - Beyond Exact Match Spectral Library Search: Mutation Tolerant Search
- 2012 ASMS - Spectral Library Generating Function: Assessing the Significance of Spectral Similarity

SERVICE

- 2018 - Present **Organizer** - Online GNPS Office Hours
- 2020 **Organizer** - Online Spectral Library Upload GNPS Workshop/Hackathon
- 2019 **Organizer** - Metabolomics 2019 GNPS Workshop
- 2019 **Organizer** - Prague GNPS Workshop
- 2019 **Organizer** - ASP GNPS Workshop
- 2018 **Organizer** - ASP GNPS Workshop
- 2018 **Organizer** - CCMS Natural Products Workshop
- 2017 **Session Moderator** - US Human Proteome Organization (HUPO) - Metaproteomics
- 2016 **Session Moderator** - Summer Research Conference at UC San Diego
- 2016 **Session Moderator** - Gordon Research Seminar/Conference Chemistry Biology of Peptides
- 2014/2015 **Committee Member** - Proteomics Standards Initiative - defined standard representation and file formats for bioinformatics tools in proteomics and metabolomics
- 2012 **Organizing Committee** - RECOMB Satellite Conference on Computational Proteomics

2012-2017 **Reviewer** - RECOMB - Research in Computational Molecular Biology
Reviewer - Nature Methods
Reviewer - Molecular Cellular Proteomics
Reviewer - Journal of Proteome Research
Reviewer - Bioinformatics
Reviewer - Organic Geochemistry
2013-2016 **Community Science Outreach** - Fleet Science Center

Research Experience

DORRESTEIN LAB - SKAGGS SCHOOL OF PHARMACY AND PHARMACEUTICAL SCIENCES - UC SAN DIEGO

2017 - Present Building GNPS into a global data centric platform

BANDEIRA LAB - COMPUTER SCIENCE AND ENGINEERING - UC SAN DIEGO

2015 - 2016 Visualized microbe/molecular distribution of the lung in Cystic Fibrosis
2015 - 2016 Mapped microbe/molecular distribution in the gut microbiome
2015 - 2016 Developed algorithms to build peptide reference spectral libraries
2014 - 2016 Designed and developed mass spectrometry living data repository for Proteomics (MassIVE)
2013 - 2016 Designed and developed crowd sourced analysis platform for natural products research (GNPS)
2010 - 2012 Developed methods for assessing spectral matching significance in peptide library searches

ZHONG LAB - BIOENGINEERING - UNIVERSITY OF ILLINOIS

2009 - 2010 Developed software to map bisulfite reads to reference genomes to detect methylation patterns

Teaching

UC SAN DIEGO

2015 **Teaching Assistant** - Computer Science and Engineering 100 - Advanced Data Structures, Instructors: Nuno Bandeira and Debashis Sahoo
2014/2015 **Instructor** - Extension Academic Connections - Introduction to Bioinformatics
2014-2016 **Guest Lecturer** - School of Pharmacy and Pharmaceutical Sciences 205 - Pharmacy Informatics
2013-2016 **Guest Lecturer** - Biology 4 - Introductory Biology Lab

UNIVERSITY OF ILLINOIS

2009 - Spring **Lab Tutor** - ECE 391 - Computer Systems Engineering, Instructor: Nikita Borisov
2009 - Fall **Lab Tutor** - ECE 391 - Computer Systems Engineering, Instructor: Steve Lumetta

Work Experience

2010 **Software Engineer** - Nuvixa Inc. (now Personify Inc.)
2010 **Software Engineer Intern** - Qualcomm Inc.
2008/2009 **Software Development Engineering Intern** - Amazon.com

Extracurriculars

UC SAN DIEGO CHAMBER SINGERS

2013-2018 Ensemble Member

UC SAN DIEGO A CAPPELLA - ACAMAZING

2010-2011 Founding Member
2011-2012 President and Musical Director
2012-2013 Leadership Mentor

WEB VIDEO PLATFORM - POTATO SURFER

2014 Project Leader - Designed and developed website, Android App, and Chromecast app.

FOLK MUSIC DUO - MARLENA AND THE WANG

2011/2012 Arranged, rehearsed, performed, and recorded folk music as a folk music duo with Marlena Fecho.

ALAN ALDA CENTER FOR COMMUNICATING SCIENCE - STONY BROOK UNIVERSITY

2015 Trained to improve science communication skills using improvisation exercises

REUBEN H. FLEET SCIENCE CENTER

2014-2016 Community Science Outreach - Two Scientists Walk into a Bar

Honors and Awards

2019 Nvidia GPU Grant Recipient
2014 CSE 25th Anniversary - Excellent Presentation Award
2012 San Diego Fellowship
2010/2011 UC San Diego CSE Department Fellowship E. C. Jordan Award
2009 Brian Sophie Leung Scholarship
2008 Henry O. Koehler Merit Scholarship
2006 University Achievement Scholarship

Societies and Honoraries

Tau Beta Pi, Engineering Honor Society Historian

IEEE, Institute of Electrical and Electronics Engineers Publicity Chair

Eta Kappa Nu, Electrical Engineering Honor Society Member

Language Competency

English - Native

Mandarin - Conversational