# 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 Consultant, WWomics LLC, San Diego

## Areas of specialization

Computer Engineering - Computer Science - Bioinformatics - Computational Mass Spectrometry

#### Education

PH.D. in Computer Science, UC San Diego
C PHIL. in Computer Science, UC San Diego
MS in Computer Science, UC San Diego
BS in Computer Engineering summa cum laude, University of Illinois

### Publications & Talks

JOURNAL ARTICLES

2019

2019

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** 

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** 

Melissa M Galey, Alexandria N Young, Valentina Z Petukhova, **Mingxun Wang**, Jian Wang, Amrita Salvi, Angela Russo, Joanna E Burdette, Laura M Sanchez. "Detection of Ovarian Cancer Using

Samples Sourced from the Vaginal Microenvironment" Journal of proteome research

2019

2019

2019

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2019

Alexey V Melnik, Yoshiki Vázquez-Baeza, Alexander A Aksenov, Embriette Hyde, Andrew C McAvoy, Mingxun Wang, Ricardo R da Silva, Ivan Protsyuk, Jason V Wu, Amina Bouslimani, Yan Wei Lim, Tal Luzzatto-Knaan, William Comstock, Robert A Quinn, Richard Wong, Greg Humphrey, Gail Ackermann, Timothy Spivey, Sharon S Brouha, Nuno Bandeira, Grace Y Lin, Forest Rohwer, Douglas J Conrad, Theodore Alexandrov, Rob Knight, Pieter C Dorrestein, Neha Garg. "Molecular and Microbial Microenvironments in Chronically Diseased Lungs Associated with Cystic Fibrosis" MSystems

Daniel Petras, Jeremiah J Minich, Emily Kunselman, **Mingxun Wang**, Margot E White, Eric E Allen, Lihini I Aluwihare, Pieter C Dorrestein. "Non-Targeted Metabolomics Enables the Prioritization and Tracking of Anthropogenic Pollutants in Coastal Seawater" *Preprint in ChemRxiv* 

Allegra T Aron, Emily Gentry, Kerry L McPhail, Louis Felix Nothias, Mélissa Nothias-Esposito, Amina Bouslimani, Daniel Petras, Julia M Gauglitz, Nicole Sikora, Fernando Vargas, J van der Hooft, Madeleine Ernst, Kyo Bin Kang, Christine M Aceves, Andrés Mauricio Caraballo-Rodríguez, Irina Koester, Kelly C Weldon, Samuel Bertrand, Catherine Roullier, Kunyang Sun, Richard M Tehan, Cristopher A Boya, H Christian Martin, Marcelino Gutiérrez, Aldo Moreno Ulloa, Javier Andres Tejeda Mora, Randy Mojica-Flores, Johant Lakey-Beitia, Victor Vásquez-Chaves, Angela I Calderón, Nicole Tayler, A Robert, Fidele Tugizimana Keyzers, Nombuso Ndlovu, Alexander A Aksenov, Alan K Jarmusch, Robin Schmid, Andrew W Truman, Nuno Bandeira, **Mingxun Wang**, Pieter Dorrestein. "Reproducible Molecular Networking Of Untargeted Mass Spectrometry Data Using GNPS" *Preprint in ChemRxiv* 

Evan Bolyen, Jai Ram Rideout, Matthew R Dillon, Nicholas A Bokulich, Christian C Abnet, Gabriel A Al-Ghalith, Harriet Alexander, Eric J Alm, Manimozhiyan Arumugam, Francesco Asnicar, Yang Bai, Jordan E Bisanz, Kyle Bittinger, Asker Brejnrod, Colin J Brislawn, C Titus Brown, Benjamin J Callahan, Andrés Mauricio Caraballo-Rodríguez, John Chase, Emily K Cope, Ricardo Da Silva, Christian Diener, Pieter C Dorrestein, Gavin M Douglas, Daniel M Durall, Claire Duvallet, Christian F Edwardson, Madeleine Ernst, Mehrbod Estaki, Jennifer Fouquier, Julia M Gauglitz, Sean M Gibbons, Deanna L Gibson, Antonio Gonzalez, Kestrel Gorlick, Jiarong Guo, Benjamin Hillmann, Susan Holmes, Hannes Holste, Curtis Huttenhower, Gavin A Huttley, Stefan Janssen, Alan K Jarmusch, Lingjing Jiang, Benjamin D Kaehler, Kyo Bin Kang, Christopher R Keefe, Paul Keim, Scott T Kelley, Dan Knights, Irina Koester, Tomasz Kosciolek, Jorden Kreps, Morgan GI Langille, Joslynn Lee, Ruth Ley, Yong-Xin Liu, Erikka Loftfield, Catherine Lozupone, Massoud Maher, Clarisse Marotz, Bryan D Martin, Daniel McDonald, Lauren J McIver, Alexey V Melnik, Jessica L Metcalf, Sydney C Morgan, Jamie T Morton, Ahmad Turan Naimey, Jose A Navas-Molina, Louis Felix Nothias, Stephanie B Orchanian, Talima Pearson, Samuel L Peoples, Daniel Petras, Mary Lai Preuss, Elmar Pruesse, Lasse Buur Rasmussen, Adam Rivers, Michael S Robeson, Patrick Rosenthal, Nicola Segata, Michael Shaffer, Arron Shiffer, Rashmi Sinha, Se Jin Song, John R Spear, Austin D Swafford, Luke R Thompson, Pedro J Torres, Pauline Trinh, Anupriya Tripathi, Peter J Turnbaugh, Sabah Ul-Hasan, Justin JJ van der Hooft, Fernando Vargas, Yoshiki Vázquez-Baeza, Emily Vogtmann, Max von Hippel, William Walters, Yunhu Wan, Mingxun Wang, Jonathan Warren, Kyle C Weber, Charles HD Williamson, Amy D Willis, Zhenjiang Zech Xu, Jesse R Zaneveld, Yilong Zhang, Qiyun Zhu, Rob Knight, J Gregory Caporaso. "Reproducible, interactive, scalable and extensible microbiome data science using QIIME 2" Nature Methods

Madeleine Ernst, Kyo Bin Kang, Andrés Mauricio Caraballo-Rodríguez, Louis-Felix Nothias, Joe Wandy, Christopher Chen, **Mingxun Wang**, Simon Rogers, Marnix H Medema, Pieter C Dorrestein, Justin JJ van der Hooft. "Molnetenhancer: enhanced molecular networks by integrating

metabolome mining and annotation tools" Metabolites

2019

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Alan K Jarmusch, Emmanuel O Elijah, Fernando Vargas, Amina Bouslimani, Ricardo R da Silva, Madeleine Ernst, **Mingxun Wang**, Krizia K del Rosario, Pieter C Dorrestein, Shirley M Tsunoda. "Initial Development Towards Non-Invasive Drug Monitoring via Untargeted Mass Spectrometric Analysis of Human Skin" *Analytical chemistry* 

Valentina Z Petukhova, Alexandria N Young, Jian Wang, **Mingxun Wang**, Andras Ladanyi, Rajul Kothari, Joanna E Burdette, Laura M Sanchez. "Whole Cell MALDI Fingerprinting Is a Robust Tool for Differential Profiling of Two-Component Mammalian Cell Mixtures" **Journal of The American Society for Mass Spectrometry** 

Andrea G Albarracín Orio, Daniel Petras, Romina A Tobares, Alexander Aksenov, **Mingxun Wang**, Florencia Juncosa, Pamela Sayago, Alejandro Moyano, Pieter C Dorrestein, Andrea M Smania, Daniel A Ducasse. "Fungal-bacterial interaction selects for quorum sensing mutants and a metabolic shift towards the production of natural antifungal compounds" *Preprint in Biorxiv* 

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 Neuweger, 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* 

Fernando Vargas, Kelly C Weldon, Nicole Sikora, **Mingxun Wang**, Zheng Zhang, Emily C Gentry, Morgan W Panitchpakdi, Mauricio Caraballo, Pieter C Dorrestein, Alan K Jarmusch. "Protocol for Community-created Public MS/MS Reference Library Within the GNPS Infrastructure." *Preprint in Biorxiv* 

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** 

Neha Garg, Alexey V Melnik, Yoshiki Vasquez-Baeza, Alexander Aksenov, Embriette R Hyde, Andrew C McAvoy, **Mingxun Wang**, Ricardo da Silva, Ivan Protsyuk, Jason V Wu, Amina Bouslimani, Yan Wei Lim, Tal Luzzatto-Knaan, William Comstock, Robert Andrew Quinn, Richard Wong, Greg Humphrey, Gail Ackermann, Timothy Spivey, Sharon S Brouha, Nuno Bandeira, Grace Y

Lin, Forest Rohwer, Douglas Conrad, Theodore Alexandrov, Pieter C Dorrestein, Rob Knight. "The Molecular and Microbial Microenvironments in Chronically Diseased Lungs." *Preprint in Biorxiv* 

- 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." *Preprint in Biorxiv*
- Mingxun Wang, Alan K. Jarmusch, Fernando Vargas, Alexander A. Aksenov, Julia Gauglitz, Kelly Weldon, Daniel Petras et al. "MASST: A Web-based Basic Mass Spectrometry Search Tool for Molecules to Search Public Data." Preprint in Biorxiv
- Valentina Z. Petukhova, Alexandria N. Young, Jian Wang, **Mingxun Wang**, Andras Ladanyi, Rajul Kothari, Joanna E. Burdette, and Laura M. Sanchez. "Whole Cell MALDI Fingerprinting Is a Robust Tool for Differential Profiling of Two-Component Mammalian Cell Mixtures.", **Journal of The American Society for Mass Spectrometry**
- Antonio Gonzalez, Jose A. Navas-Molina, Tomasz Kosciolek, 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**
- Ricardo R. da Silva, **Mingxun Wang**, Louis-Félix Nothias, Justin JJ van der Hooft, Andrés Mauricio Caraballo-Rodríguez, Evan Fox, Marcy J. Balunas, Jonathan L. Klassen, Norberto Peporine Lopes, and Pieter C. Dorrestein. "Propagating annotations of molecular networks using in silico fragmentation" **PLoS Computational Biology**
- 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**
- Mingxun Wang, Jian Wang, Jeremy Carver, Benjamin Pullman, Seong Cha, Nuno Bandeira, "Assembling the Community-Scale Discoverable Human Proteome", *Cell Systems*
- 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**
- Neha Garg, **Mingxun Wang**, Embriette Hyde, Ricardo R. da Silva, Alexey V. Melnik, Ivan Protsyuk, 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, Forest 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*

Tal Luzzatto Knaan, Neha Garg, **Mingxun Wang**, Evgenia Glukhov, Yao Peng, Gail Ackermann, Amnon Amir, Brendan M Duggan, Sergey Ryazanov, Lena Gerwick, Rob Knight, Theodore Alexandrov, Nuno Bandeira, William H Gerwick, Pieter C Dorrestein, "Digitizing mass spectrometry data to explore the chemical diversity and distribution of marine cyanobacteria and algae", *eLife* 

Yasset Perez-Riverol, Mingze Bai, Felipe da Veiga Leprevost, Silvano Squizzato, Young Mi Park, Kenneth Haug, Adam J Carroll, Dylan Spalding, Justin Paschall, **Mingxun Wang**, Noemi del-Toro, Tobias Ternent, Peng Zhang, Nicola Buso, Nuno Bandeira, Eric W Deutsch, David S Campbell, Ronald C Beavis, Reza M Salek, Ugis Sarkans, Robert Petryszak, Maria Keays, Ariana Barbera, Rafael C Jiménez, Alexey I Nesvizhskii, Susanna-Assunta Sansone, Christoph Steinbeck, Rodrigo Lopez, Juan Antonio Vizcaíno, Peipei Ping, Henning Hermjakob, "Omics Discovery Index – Discovering and Linking Public 'Omics' Datasets", **Nature Biotechnology** 

2016

2016

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2016

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 Sciences* 

Gert Wohlgemuth, Sajjan S Mehta, Ramon F Mejia, Steffen Neumann, Diego Pedrosa, Tomáš Pluskal, Emma L Schymanski, Egon L Willighagen, Michael Wilson, David S Wishart, Masanori Arita, Pieter C. Dorrestein, Nuno Bandeira, **Mingxun Wang**, Tobias Schulze, Reza M Salek, Christoph Steinbeck, Venkata Chandrasekhar Nainala, Robert Mistrik, Takaaki Nishioka, Oliver Fiehn, "SPLASH, A hashed identifier for mass spectra", *Nature Biotechnology* 

Eric W Deutsch, Attila Csordas, Zhi Sun, Andrew Jarnuczak, Yasset Perez-Riverol, Tobias Ternent, David S Campbell, Manuel Bernal-Llinares, Shujiro Okuda, Shin Kawano, Robert L Moritz, Jeremy J Carver, **Mingxun Wang**, Yasushi Ishihama, Nuno Bandeira, Henning Hermjakob, Juan Antonio Vizcaíno, "The ProteomeXchange consortium in 2017: supporting the cultural change in proteomics public data deposition", **Nucleic Acids Research** 

Mingxun Wang, Jeremy J Carver, Vanessa V Phelan, Laura M Sanchez, Neha Garg, Yao Peng, Don Duy Nguyen, Jeramie Watrous, Clifford A Kapono, Tal Luzzatto-Knaan, Carla Porto, Amina Bouslimani, Alexey V Melnik, Michael J Meehan, Wei-Ting Liu, Max Crüsemann, 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 Kleigrewe, 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 Mohimani, 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, Stefan Jenkins, Venkat Macherla, Thomas Hoffman, Vinayak Agarwal, Philip G Williams, Jingqui Dai, Ram Neupane, Joshua Gurr, Andrés MC Rodríguez, Anne Lamsa, Chen Zhang, Kathleen Dorrestein, Brendan M Duggan, Jehad Almaliti, Pierre-Marie Allard, Prasad Phapale, Louis-Felix Nothias, Theodore Alexandrov, Marc Litaudon, Jean-Luc Wolfender, Jennifer E Kyle, Thomas O Metz, Tyler Peryea, Dac-Trung Nguyen, Danielle VanLeer, Paul Shinn, Ajit Jadhay, Rolf Müller, Katrina M Waters, Wenyuan Shi, Xueting Liu, Lixin Zhang, Rob Knight, Paul R Jensen, Bernhard Ø Palsson, Kit Pogliano, Roger G Linington, 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 Biotechnology

- Waqas Nasir, Alejandro Gomez Toledo, Fredrik Noborn, Jonas Nilsson, Mingxun Wang, Nuno Bandeira, Goran Larson, "SweetNET: A bioinformatics workflow for glycopeptide MS/MS spectral analysis" Journal of Proteome Research
- Amina Bouslimani, Carla Porto, Christopher M Rath, Mingxun Wang, Yurong Guo, Antonio 2015 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
- Katherine R Duncan, Max Crüsemann, Anna Lechner, Anindita Sarkar, Jie Li, Nadine Ziemert, 2015 Mingxun Wang, Nuno Bandeira, Bradley S Moore, Pieter C Dorrestein, Paul R Jensen, "Molecular networking and pattern-based genome mining improves discovery of biosynthetic gene clusters and their products from Salinispora species", Chemistry Biology
- Hosein Mohimani, Roland D Kersten, Wei-Ting Liu, Mingxun Wang, Samuel O Purvine, Si Wu, 2014 Heather M Brewer, Ljiljana Pasa-Tolic, Nuno Bandeira, Bradley S Moore, Pavel A Pevzner, Pieter C Dorrestein, "Automated genome mining of ribosomal peptide natural products", ACS Chemical Biology
- Mingxun Wang, Nuno Bandeira, "Spectral library generating function for assessing spectrum-2013 spectrum match significance", Journal of Proteome Research

#### Conference Talks

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

#### POSTER PRESENTATIONS

2017

2016

2017 2016 2015	ASP - GNPS: High Throughput Mass Spectrometry Dereplication and Discovery with Molecular Networking and Crowd Sourced Annotation ASMS - Assembling the community-scale discoverable human proteome Gordon Research Seminar/Conference Chemistry Biology of Peptides - Exploring the Highly Post Translationally Modified Peptide Space with Molecular Networks ASMS - GNPS: Charting Molecular Families and Structure of Tens of Thousands of Mass Spectrometry Runs ASMS - GNPS: Global Natural Product Molecular Social Networking – Enabling High Throughput
2013 2012	Compound Discovery ASMS - Beyond Exact Match Spectral Library Search: Mutation Tolerant Search ASMS - Spectral Library Generating Function: Assessing the Signicance of Spectral Similarity
	Service
2017 2016 2016 2014/2015 2012 2012-2017	Session Moderator - US Human Proteome Organization (HUPO) - Metaproteomics Session Moderator - Summer Research Conference at UC San Diego Session Moderator - Gordon Research Seminar/Conference Chemistry Biology of Peptides Committee Member - Proteomics Standards Initiative - defined standard representation and file formats for bioinformatics tools in proteomics and metabolomics Organizing Committee - RECOMB Satellite Conference on Computational Proteomics 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
2015 - 2016 2015 - 2016 2015 - 2016 2014 - 2016 2013 - 2016 2010 - 2012	Bandeira Lab - Computer Science and Engineering - UC San Diego  Visualized microbe/molecular distribution of the lung in Cystic Fibrosis  Mapped microbe/molecular distribution in the gut microbiome  Developed algorithms to build peptide reference spectral libraries  Designed and developed mass spectrometry living data repository for Proteomics (MassIVE)  Designed and developed crowd sourced analysis platform for natural products research (GNPS)  Developed methods for assessing spectral matching significance in peptide library searches
2009 - 2010	<b>ZHONG LAB</b> - BIOENGINEERING - UNIVERSITY OF ILLINOIS  Developed software to map bisulfite reads to reference genomes to detect methylation patterns

# Teaching

UC SAN DIEGO

2015

structors: Nuno Bandeira and Debashis Sahoo **Instructor** - Extension Academic Connections - Introduction to Bioinformatics 2014/2015 Guest Lecturer - School of Pharmacy and Pharmaceutical Sciences 205 - Pharmacy Informatics 2014-2016 Guest Lecturer - Biology 4 - Introductory Biology Lab 2013-2016 University of Illinois Lab Tutor - ECE 391 - Computer Systems Engineering, Instructor: Nikita Borisov 2009 - Spring Lab Tutor - ECE 391 - Computer Systems Engineering, Instructor: Steve Lumetta 2009 - Fall Work Experience **Software Engineer** - Nuvixa Inc. (now Personify Inc.) 2010 **Software Engineer Intern** - Qualcomm Inc. Software Development Engineering Intern - Amazon.com 2008/2009 Extracurriculars UC SAN DIEGO CHAMBER SINGERS Ensemble Member 2013-2018 UC SAN DIEGO A CAPPELLA - ACAMAZING Founding Member 2010-2011 President and Musical Director 2011-2012 Leadership Mentor 2012-2013 Web Video Platform - Potato Surfer Project Leader - Designed and developed website, Android App, and Chromecast app. 2014 Folk Music Duo - Marlena and the Wang Arranged, rehearsed, performed, and recorded folk music as a folk music duo with Marlena Fecho. 2011/2012 ALAN ALDA CENTER FOR COMMUNICATING SCIENCE - STONY BROOK UNIVERSITY Trained to improve science communication skills using improvisation exercises 2015 REUBEN H. FLEET SCIENCE CENTER

Teaching Assistant - Computer Science and Engineering 100 - Advanced Data Structures, In-

Community Science Outreach - Two Scientists Walk into a Bar

2014-2016

## Honors and Awards

<sup>2014</sup> CSE 25th Anniversary - Excellent Presentation Award

San Diego Fellowship

UC San Diego CSE Department Fellowship E. C. Jordan Award

Brian Sophie Leung Scholarship
 Henry O. Koehler Merit Scholarship
 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