Shunyang Wang, Ph.D.

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Scientist, Computational Metabolomics at Brightseed

EDUCATION

Ph.D. in Chemistry **2019 - 2022**

University of California, Davis
Advisors: Dr. Oliver Fiehn, Dr. Dean J Tantillo, Dr. Tobias Kind
Dissertation: *Quantum chemistry explorations on compound identification in metabolomics*

B.S. in Chemistry **2014 - 2018**

Shandong University, Weihai, China

RESEARCH & EXPERIENCE

Computational Metabolomics, Brightseed 02/2023 – Current

Bioactive Nature Product Discovery

- Developed a mass spectrometry-based algorithm for bioactive prediction.
- Validated the model through collaboration with experimental teams, doubling the success rate and reducing screening time from months to weeks.
- Contributed numerous leads to preclinical and clinical studies.

Metabolomics Spectral Database

- Developed a fully automated data processing pipeline, serving as the core of company products.
- Built and maintain a spectral database of over 10 million entries for plant profiling.
- Optimized database search time, reducing it from hours to microseconds.

Retention Time Prediction of Small Molecules

- Created a graph neural network model with attention mechanism, achieving a 100-fold increase in prediction speed.
- Achieved a reduction in mean absolute error to within 10 seconds for a 10-minute method.
- Deployed an API and Docker environment for daily use by experimental researchers.

Doctoral Research, UC Davis 12/2018 –12/2022

Quantum Chemistry simulation of electron ionization mass spectra

- Developed the world's first in-silico mass spectral database using molecular dynamics.
- Created a cutting-edge excited-state molecular dynamics algorithm.
- Enhanced mass spectral prediction accuracy, surpassing all machine learning methods.

High-resolution mass spectral library

- Built a commercialized mass spectral library for Agilent Technologies.
- Led an interdisciplinary team of postdocs, lab managers, and undergraduates.
- Developed an algorithm for metabolite identification using chemical ionization.

PUBLICATIONS

Automatic Assignment of Molecular Ion Species to Elemental Formulas in Gas Chromatography/Methane Chemical Ionization Accurate Mass Spectrometry. **2023**

Shunyang Wang, Luis Valdiviez, Honglian Ye, Oliver Fiehn.
Metabolites: 13(8):962. DOI: 10.3390/metabo13080962

Quantum Chemical Prediction of Electron Ionization Mass Spectra of Trimethylsilylated Metabolites. **2022**

Shunyang Wang, Tobias Kind, Parker Ladd Bremer, Dean J. Tantillo, Oliver Fiehn.
Analytical Chemistry: 94, 3, 1559–1566. DOI: 10.1021/acs.analchem.1c02838

Beyond the ground state: electron ionization mass spectra quantum chemistry prediction. **2022**

Shunyang Wang, Dean J. Tantillo, Oliver Fiehn.
Journal of Chemical Information and Modeling: 62, 18, 4403–4410. DOI: 10.1021/acs.jcim.2c00597

Quantum Chemistry Calculations for Metabolomics. **2021**

Ricardo M. Borges, Sean M. Colby, Susanta Das et al. & **Shunyang Wang**, Ryan S. Renslow.
*Chemical Reviews:*121 (10), 5633-5670. DOI: 10.1021/acs.chemrev.0c00901

Predicting in silico electron ionization mass spectra using quantum chemistry. **2020**

Shunyang Wang, Tobias Kind, Dean J. Tantillo, Oliver Fiehn.
Journal of Cheminformatics: 12. DOI: 10.1186/s13321-020-00470-3

PRESENTATIONS

Predicting collision induced mass spectra using topological analysis **2022**
Poster presentation in *Houk research conference, Los Angeles, CA*

Beyond the ground state: electron ionization mass spectra quantum chemistry prediction **2021 & 2022**

Poster presentation in *69th ASMS Conference on Mass Spectrometry and Allied Topics*
Oral presentation in *NIH Common Fund Metabolomics Consortium Annual Meeting*

Quantum chemical prediction of electron ionization mass spectra of trimethylsilylated metabolites **2020**

Poster presentation in *Metabolomics Association of North America annual conference*
& in *NIH Common Fund Metabolomics Consortium Annual Meeting*
Oral presentation in *Quantum Mechanical Computing Working Group*

Predicting in silico electron ionization mass spectra using quantum chemistry **2019**
Poster presentation *in Metabolomics Association of North America annual conference, Atlanta*

OUTREACH AND VOLUNTEERING

Metabolomics Association of North America Early Career Members Council **2024**

Organizer in the following events:

- Early Career Researchers Networking Event: Navigating International Collaboration and International Mobility
- Meet with Recruiter Round Table: Diversity, Equity, and Inclusion
- Transition into Industry: How to Utilize Transferable Skills Gained from Ph.D. to Navigate the Future Careers

TEACHING AND MENTORING

TEACHING ASSISTANT

CHE 2B General Chemistry II	2019 Winter Quarter
CHE 107 Physical Chemistry for the Life Sciences	2018 Fall Quarter
CHE 8A Organic Chemistry: Brief Course	2018 Fall Quarter

MENTORING

Natural product team summer intern mentor (Ph.D. student)	2023 Summer Session
Computational metabolomics summer intern mentor (Master student)	2022 Summer Session

PROFESSIONAL AFFILIATIONS

ECM At-Large Council Members	2024 – Current
Chinese American Society for Mass Spectrometry (CASMS)	2022 - Current
American Society for Mass Spectrometry (ASMS)	2021 - Current
American Chemical Society (ACS)	2021 - Current

SKILLS

Computation Skills

- **Programming & Scripting**: Python, Fortran
- **Machine Learning & Cheminformatics**: PyTorch, RDKit, Chemaxon
- **High-Performance Computing**: AWS, Docker, Slurm
- **Computational Chemistry**: Gaussian, ORCA, Molecular Docking, OpenMM

Laboratory Skills

Gas chromatography-mass spectrometry, Liquid chromatography-mass spectrometry, Metabolomics Sample Preparation

HONORS

Edmund and Wilma Fink Memorial Award	2022
American Society for Mass Spectrometry Graduate Student Travel Award	2022
Metabolomics Service Cores Best Presentation Award, MANA	2021
China National Scholarship (Top 0.2%)	2015 & 2017

GRANTS

2024	Almond Board of California: Deep Metabolomic Profiling of Almonds	$250,000
2023	Brightseed products: Plant profiling for bioactivity	$300,000