Shunyang Wang, Ph.D.

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Scientist, Computational Metabolomics at Brightseed

EDUCATION

Ph.D. in Chemistry, University of California, Davis   12/2022

Advisor: Dr. Oliver Fiehn, Dr. Dean J Tantillo, Dr. Tobias Kind

Dissertation: Quantum chemistry explorations on compound identification in metabolomics

B.S., Chemistry, Shandong University, Weihai, China   06/2018

RESEARCH& EXPERIENCE

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

Quantum chemistry prediction of electron ionization mass spectra

Deploy the calculation on high performance computering clusters; analyze and optimize the program; develop an excited-state molecular dynamics algorithm.

Build of high-resolution mass spectral library with Electron and Chemical Ionization source

Lead team collaboration with Agilent Technologies; run the instrument and process data; develop a method to analyze metabolomics data with both EI and CI spectra.

PUBLICATIONS

Wang, S., Kind, T., Tantillo, D.J. et al. Predicting in silico electron ionization mass spectra using quantum chemistry. J Cheminform 12, 63 2020.

Borges, R. M.; Colby, S. M.; Das, S.; Edison, A. S.; Fiehn, O.; Kind, T.; Lee, J.; Merrill, A. T.; Merz, K. M.; Metz, T. O.; Nunez, J. R.; Tantillo, D. J.; Wang, L.-P.; **Wang, S.**; Renslow, R. S., Quantum Chemistry Calculations for Metabolomics. Chemical Reviews 2021, 121 (10), 5633-5670.

Wang, S.; Kind, T.; Bremer, P. L.; Tantillo, D. J.; Fiehn, O., Quantum Chemical Prediction of Electron Ionization Mass Spectra of Trimethylsilylated Metabolites. Analytical Chemistry 2022.

Bremer PL, Vaniya A, Kind T, **Wang S**, Fiehn O. How Well Can We Predict Mass Spectra from Structures? Benchmarking Competitive Fragmentation Modeling for Metabolite Identification on Untrained Tandem Mass Spectra. J Chem Inf Model. 2022, 62, 17, 4049–4056

Wang, S.; Kind, T.; Tantillo, D. J.; Fiehn, O., Beyond the ground state: electron ionization mass spectra quantum chemistry prediction. J. Chem. Inf. Model. 2022, 62, 18, 4403–4410

PROFESSIONAL AFFILIATIONS

American Society for Mass Spectrometry (ASMS, since 2021)

American Chemical Society (ACS, since 2021)

PRESENTATIONS

Predicting in silico electron ionization mass spectra using quantum chemistry

- Metabolomics Association of North America annual conference 2019, Atlanta, poster
- Metabolomics Association of North America Summer Symposium 2019, poster

Quantum chemical prediction of electron ionization mass spectra of trimethylsilylated metabolites

- Metabolomics Association of North America annual conference 2020, Virtual, poster
- Quantum Mechanical Computing Working Group 2020, Virtual, oral presentation
- NIH Common Fund Metabolomics Consortium Annual Meeting 2020, poster

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

- Metabolomics Association of North America annual conference 2021, Virtual, poster
- 69th ASMS Conference on Mass Spectrometry and Allied Topics 2021, Philadelphia, poster
- NIH Common Fund Metabolomics Consortium Annual Meeting 2022, oral presentation

Predicting collision induced mass spectra using topological analysis

- Houk research conference 2022, Los Angeles, poster

SKILLS

Computation: Python, Fortran, High performance computing, Machine Learning, Gaussian, ORCA, Cloud Computing, Docker

Lab: Gas chromatography-mass spectrometry, Metabolomics Sample Preparation

HONORS

2015&2017 | China National Scholarship (Top 0.2%)

2021 | Metabolomics Service Cores Best Presentation Award, Metabolomics Association of North America annual conference

2022 | American Society for Mass Spectrometry Graduate Student Travel Award

2022 | Edmund and Wilma Fink Memorial Award

TEACHING AND MENTORING

2018 Fall | 25% Teaching assistant (UC Davis). CHE107 Physical Chemistry for the Life Sciences

2018 Fall | 25% Teaching assistant (UC Davis). CHE8A Organic Chemistry: Brief Course

2019 Winter | 50% Teaching assistant (UC Davis). CHE2B General Chemistry II