CSE@UCR *colloquium*

Monday, February 28 | 11:00 – 11:50 AM | WCH 205

Computational Approaches for Biomedical Molecule Discovery

High-throughput mass spectrometry has enabled unprecedented depth and versatility to observe the molecules in the world around us. Traditionally, a handful of molecules were detected in a typical measurement. Today, this has grown to thousands of molecules in a few minutes. The growth in data presents new opportunities for discovery but also challenges in data analysis. The development of new computational approaches for mass spectrometry data has already accelerated drug discovery, revealed the chemical dialog of the microbiome, and characterized the molecular dynamics of our oceans due human activity.

I will describe the computational approaches, tools, and infrastructure that I have developed to transform mass spectrometry data analysis from a solitary activity to a community wide collaborative effort – crowd-sourcing mass spectrometry knowledge, reusing knowledge in an error-controlled fashion, and computationally amplifying knowledge to make new discoveries. I will discuss how these tools have transformed the community and how future computational work can further elucidate the mass spectrometry dark matter.

Dr. Mingxun Wang

UCSD

Dr. Wang received his BS summa cum laude in computer engineering at the University of Illinois Urbana Champaign. He earned his PhD with Prof. Nuno Bandeira in Computer Science at the University of California San Diego. Dr. Wang then turned to chemistry and pharmaceutical sciences in his postdoctoral studies with Prof. Pieter Dorrestein in the Skaggs School of Pharmacy and Pharmaceutical Sciences at the University of California San Diego. During his postdoctoral studies, Dr. Wang led the development of computational tools and infrastructure that resulted in the GNPS ecosystem – a web analysis and knowledge curation infrastructure that became the de facto standard tool for the natural products, metabolomics, and chemical ecology research communities. His computational tools are used by over 5,000 chemists and biologists from around the world each month. Dr. Wang co-founded Ometa Labs in 2017 that commercialized the computational tools he developed during his PhD and postdoctoral studies. Dr. Wang's research interests lie in bioinformatics, computational mass spectrometry, and analytical chemistry.