

Yuhui Hong

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EDUCATION

Indiana University Bloomington

Ph.D. Candidate in Computer Science

Bloomington, IN, US

Sep. 2020 –Jun. 2025 (expect)

- My research explores the intersection of **deep learning**, bioinformatics, and cheminformatics, with a focus on advancing the **identification of small molecules** in two key scenarios. The first involves predicting tandem mass spectra and other molecular properties from 3D structures, addressing gaps—often referred to as the “dark matter”—in existing spectral reference libraries. The second approach moves beyond the traditional reliance on database-driven methods by predicting chemical formulas directly from tandem mass spectra. Additionally, I am passionate about developing **reliable and interpretable** neural networks for real-world applications. It is my honor to be guided by **Prof. Haixu Tang** during my research journey.

Xidian University

B.E. in Computer Science and Technology

Xi'an, Shaanxi, China

Sep. 2015–Jul. 2019

- Thesis: “Point Detection of Traffic Objects in Road Scene Based on Convolutional Neural Network”

RESEARCH EXPERIENCE

Indiana University Bloomington

Research Assistant

Bloomington, IN, US

Sep. 2020 –Now

- Reliable prediction of tandem mass spectra from 3D molecular conformations.
- Prediction of chiral stationary phases for chromatographic enantioseparation from 3D molecular conformations.
- Chemical formula identification from molecular tandem mass spectra through deep learning methods.

The First Affiliated Hospital of Nanchang University

Research Intern

Nanchang, Jiangxi, China

May 2021 –Jul. 2021

- Major Histocompatibility Complex (MHC) binding prediction based on deep learning methods.

Xi'an Jiaotong University

Research Assistant

Xi'an, Shaanxi, China

Sep. 2019 –Jul. 2020

- Object tracking and segmentation in traffic images and videos.

PUBLICATIONS

BOOKS

1. Xiao Q., Liu K., **Hong, Y.** & Tang H. (2024). Neural Networks for Chemists. *American Chemical Society*. (In press, to be published November 2024)

PEER-REVIEWED ARTICLES

1. **Hong, Y.**, Welch, C. J., Piras, P., & Tang, H. (2024). “Enhanced Structure-Based Prediction of Chiral Stationary Phases for Chromatographic Enantioseparation from 3D Molecular Conformations.” *Analytical Chemistry*, 96(6), 2351-2359.
[link] [source codes]
2. **Hong, Y.**, Li, S., Welch, C. J., Tichy, S., Ye, Y., & Tang, H. (2023). “3DMolMS: Prediction of Tandem Mass Spectra from Three Dimensional Molecular Conformations.” *Bioinformatics*, btad354.
[link] [source codes] [PyPI package] [online service]

- Li, Y., **Hong, Y.**, Song, Y., Zhu, C., Zhang, Y., & Wang, R. (2022). "SiamPolar: Semi-supervised realtime video object segmentation with polar representation." *Neurocomputing*, 467, 491-503.
[link] [source codes]
- Li, Y., Zhu, C., Liu, Y., **Hong, Y.**, & Wang, J. (2021). "Geometric and semantic analysis of road image sequences for traffic scene construction." *Neurocomputing*, 465, 336-349.
[link] [source codes]

ARTICLES UNDER REVIEW

- Monshizadeh, M.*, **Hong, Y.***, & Ye, Y. (2024). "Multitask Knowledge-primed Neural Network for Predicting Missing Metadata and Host Phenotype based on Human Microbiome." *bioRxiv*, 2024-02. (* Equal contribution as co-first authors)
[link] [source codes]

CONFERENCE PRESENTATIONS

- Poster in 72nd Conference on Mass Spectrometry and Allied Topics
"Predicting compositional fragments of compounds from their tandem mass spectra using deep neural networks" [poster]
- Talk in 71st Conference on Mass Spectrometry and Allied Topics
"A Machine Learning Model for Chemical Formula Prediction Using Tandem Mass Spectra of Compounds" [slides]
- Poster in 70th Conference on Mass Spectrometry and Allied Topics
"Prediction of Molecular Tandem Mass Spectra Using 3-Dimensional Conformers" [poster]

TEACHING EXPERIENCE

- Instructor** of Machine Learning Bioinformatics (INFO-I529) Fall 2024, Indiana University Bloomington
Conducted an online course on machine learning techniques for bioinformatics, focusing on dimensionality reduction, clustering methods, Bayesian approaches, random forests, SVMs, and neural networks.
- Assistant Instructor** of Big Data Analytics (CSCI-D351) Fall 2024, Indiana University Bloomington
Assisted in teaching big data analytics, covering data processing, storage, and visualization techniques. Delivered an introductory lecture on Spark and provided one-on-one coding support to students during office hours.

PROFESSIONAL SERVICES

- Reviewer: IEEE/ACM Transactions on Computational Biology and Bioinformatics, BMC Genomics, BMC Bioinformatics, Pharmaceutical Research, Beilstein Journal of Organic Chemistry, Chemical Physics Letters
- Co-reviewer: Analytical Chemistry, International Journal of Mass Spectrometry
assisted in reviewing papers under the guidance of Prof. Hairu Tang
- Sub-reviewer: ISMB 2023, RECOMB 2023, RECOMB 2022

SKILLS

- Programming:** Python, R, C/C++, Java, Racket
- Deep Learning:** PyTorch, TensorFlow, Keras
- Tools/Techs:** LaTeX, Git, SQL

LANGUAGES

- English:** Proficient
- Chinese:** Mother tongue, native speaker

SCHOLARSHIPS AND AWARDS

- Special Academic Scholarship of Xi'an Jiao Tong University** 2019
(Top 20% in the students)
Academic Administration of Xi'an Jiao Tong University
- First-class Scholarship for New Students of Xi'an Jiao Tong University** 2019
(Top 40% in the recommended for exam-free graduate students)
Academic Administration of Xi'an Jiao Tong University
- Meritorious Winner of MCM (Mathematical Contest In Modeling)** 2018
(Top 10% in the 8085 teams)
COMAP(the Consortium for Mathematics and Its Application)