Yuhui Hong

Website: josiehong.github.io
Email: yuhhong@iu.edu
GitHub: github.com/JosieHong
Google Scholar: Yuhui Hong
0000-0002-5647-9714

Education

Indiana University Bloomington — Bloomington, IN, US
Ph.D. Candidate in Computer Science — Sep. 2020 –Jun. 2025 (expect)

- My research delves into the intersection of **deep learning**, bioinformatics, and cheminformatics, with a concentrated emphasis on advancing the **identification of small molecules**. By leveraging cutting-edge deep learning techniques, I have pursued two synergistic approaches to molecular identification. The first involves predicting tandem mass spectra and other molecular properties from 3D conformational data, addressing the gaps—often referred to as the 'dark matter'—in existing spectral reference libraries. The second approach moves beyond traditional reliance on database-driven methods by predicting chemical formulas directly from tandem mass spectra. This enables a more accurate, de novo identification of molecules, offering a transformative alternative to conventional workflows.
  It is my honor to be guided by **Prof. Haixu Tang** during my research journey.

Xidian University — Xi'an, Shaanxi, China
B.E. in Computer Science and Technology — Sep. 2015–Jul. 2019

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

Research Experience

Indiana University Bloomington — Bloomington, IN, US
Research Assistant — 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 — Nanchang, Jiangxi, China
Research Intern — May 2021 –Jul. 2021

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

Xi'an Jiaotong University — Xi'an, Shaanxi, China
Research Assistant — Sep. 2019 –Jul. 2020

- Object tracking and segmentation in traffic images and videos.

Publications

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. [link] [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] [codes]
3. Zhang, Y., Hu, Z., Wang, X., **Hong, Y.**, Nan, Y., Wang, X., Cheng, J. and Xing, L., 2024, August. Navigating the Privacy Compliance Maze: Understanding Risks with Privacy-Configurable Mobile SDKs. In 33rd USENIX Security Symposium (USENIX Security 24). USENIX Association. [link]
4. 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]
5. 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] [codes]

6. 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] [codes]

Conference Presentations

1. 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]

2. 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]

3. Poster in 70th Conference on Mass Spectrometry and Allied Topics
   "Prediction of Molecular Tandem Mass Spectra Using 3-Dimensional Conformers" [poster]

Teaching

- **Co-author** of ACS in Focus Primer — Nov. 2024
  Neural Networks for Chemists, DOI forthcoming
- **Instructor** at Indiana University Bloomington — Fall 2024
  Machine Learning Bioinformatics (INFO-I529)
- **Assistant Instructor** at Indiana University Bloomington — Fall 2024
  Big Data Analytics (CSCI-D351)

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. Haixu 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
- **Second-class Scholarship of Xidian University** — 2018
  (Top 10% in the students)
  Academic Administration of Xidian University
- **Meritorious Winner of MCM (Mathematical Contest In Modeling)** — 2018
  (Top 10% in the 8085 teams)
  COMAP(the Consortium for Mathematics and Its Application)
- **Third-class Scholarship of Xidian University** — 2017
  (Top 15% in the students)
  Academic Administration of Xidian University