Yuhui Hong

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Education

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

- My research focuses on applying **deep learning** to bioinformatics and cheminformatics, particularly in **identification of small molecules**.
  I developed models to predict **tandem mass spectra** and other properties from molecular 3D conformations, highlighting the 'dark matter' in reference libraries. To improve **reliability**, I worked on explaining deep neural networks to provide human-understandable annotations and confidence scores. Additionally, I combined deep learning with knowledge-based post-processing to predict **chemical formulas** from mass spectra.
  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