

# Yuhui Hong

Website: [josiehong.github.io](https://josiehong.github.io)  
Email: [yuhhong@iu.edu](mailto:yuhhong@iu.edu)  
GitHub: [github.com/JosieHong](https://github.com/JosieHong)  
ORCID: 0000-0002-5647-9714



## EDUCATION

### Indiana University Bloomington

Ph.D. Candidate in Computer Science

Bloomington, IN, US

Sep. 2020 – Jun. 2025 (expect)

- My research interests focus on deep learning and its applications in cheminformatics and bioinformatics. I am passionate about molecular representation learning, structural bioinformatics, and tackling intricate tasks related to analytical chemistry. 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

- 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

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)
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

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1. Poster in ASMS 2024, "Predicting compositional fragments of compounds from their tandem mass spectra using deep neural networks" [\[poster\]](#)
2. Talk in ASMS 2023, "A Machine Learning Model for Chemical Formula Prediction Using Tandem Mass Spectra of Compounds" [\[slides\]](#)
3. Poster in ASMS 2022, "Prediction of Molecular Tandem Mass Spectra Using 3-Dimensional Conformers" [\[poster\]](#)

## TEACHING

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- **Instructor** at Indiana University Bloomington Fall 2024  
*Machine Learning Bioinformatics (INFO I529)*
- **Guest Lecture** at Indiana University Bloomington Fall 2024  
*Big Data Analytics (CSCI D351)*

## PROFESSIONAL SERVICES

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- Reviewer: IEEE/ACM Transactions on Computational Biology and Bioinformatics, BMC Genomics, BMC Bioinformatics, Pharmaceutical Research, Beilstein Journal of Organic Chemistry, Chemical Physics Letters
- Sub-reviewer: ISMB 2023, RECOMB 2023, RECOMB 2022

## SKILLS

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

## LANGUAGES

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

## SCHOLARSHIPS AND AWARDS

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- **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