

# Yuhui Hong

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## EDUCATION

**Indiana University Bloomington**  
Ph.D. in Computer Science

Bloomington, IN, US  
Sep. 2020 –Jul. 2025 (expect)

**Xidian University**  
B.S. in Computer Science and Technology

Xi'an, Shaanxi, China  
Sep. 2015–Jul. 2019

## RESEARCH EXPERIENCE

**Indiana University Bloomington**  
Research Assistant

Bloomington, IN, US  
Sep. 2020 –Present

Advisor: Prof. Haixu Tang  
Area: Computational biology, Deep Learning, Small molecular mass spectrometry

**The First Affiliated Hospital of Nanchang University**  
Research Intern

Nanchang, Jiangxi, China  
May 2021 –Jul. 2021

Advisor: Prof. Sujun Li  
Area: MHC (Major Histocompatibility Complex) binding prediction

**Xi'an Jiaotong University**  
Research Assistant

Xi'an, Shaanxi, China  
Sep. 2019 –Jul. 2020

Advisor: Prof. Yaochen Li  
Area: Object tracking and segmentation in traffic scene

## TEACHING EXPERIENCE

**Instructor**  
DSCI-D590, Topics in Data Science

Indiana University Bloomington  
Spring 2025

**Instructor**  
INFO-I529, Machine Learning Bioinformatics

Indiana University Bloomington  
Fall 2024

**Assistant Instructor**  
DSCI-D351, Big Data Analytics  
Instructor: Prof. Haixu Tang

Indiana University Bloomington  
Aug.-Sep. 2024

## PUBLICATIONS

The deep learning models, 3DMolMS for retention time and collision-cross section [7] and 3DMolCSP for enantioselectivity [4], have been evaluated on internal data and positively considered for application by biotech, pharmaceutical and agricultural leaders, including **Amgen**, **Merck**, **AbbVie** and **Corteva**.

## BOOKS & PATENTS

- 1 Qingyang Xiao, Kaiyuan Liu, **Yuhui Hong** & Haixu Tang (2024). "Neural Networks for Chemists." *American Chemical Society*, DOI:10.1021/acsinfocus.7e8012. [Primer]
- 2 Haixu Tang, **Yuhui Hong**, & Sujun Li. "Method of predicting ms/ms spectra and properties of chemical compounds." US Patent No. WO2023239720A1, June 6, 2023.

## PEER-REVIEWED ARTICLES

- 3 **Yuhui Hong**, Yuzhen Ye & Haixu Tang (2025). "Machine Learning in Small-Molecule Mass Spectrometry." (Accepted by *Annual Review of Analytical Chemistry*, to be published on May 2025)
- 4 **Yuhui Hong**, Christopher J Welch, Patrick Piras, & Haixu Tang (2024). "Enhanced Structure-Based Prediction of Chiral Stationary Phases for Chromatographic Enantioseparation from 3D Molecular Conformations." *Analytical Chemistry*, 96(6), 2351-2359. [Paper] [Code]
- 5 Mahsa Monshizadeh\*, **Yuhui Hong**\*, & Yuzhen Ye (2024). "Multitask Knowledge-primed Neural Network for Predicting Missing Metadata and Host Phenotype based on Human Microbiome." *Bioinformatics Advances*, vbae203. [Paper] [Code]
- 6 Yifan Zhang, Zhaojie Hu, Xueqiang Wang, **Yuhui Hong**, Yuhong Nan, XiaoFeng Wang, Jiatao Cheng & Luyi Xing (2024). "Navigating the Privacy Compliance Maze: Understanding Risks with Privacy-Configurable Mobile SDKs." In *33rd USENIX Security Symposium*, pp. 6543-6560. [Paper]
- 7 **Yuhui Hong**, Sujun Li, Christopher J Welch, Shane Tichy, Yuzhen Ye, & Haixu Tang (2023). "3DMolMS: Prediction of Tandem Mass Spectra from Three Dimensional Molecular Conformations." *Bioinformatics*, btad354. [Paper] [Code] [PyPI package] [Service on GNPS] [Service on Konia]
- 8 Yaochen Li, **Yuhui Hong**, Yonghong Song, Chao Zhu, Ying Zhang, & Ruihao Wang (2022). "SiamPolar: Semi-supervised Realtime Video Object Segmentation with Polar Representation." *Neurocomputing*, 467, 491-503. [Paper] [Code]
- 9 Yaochen Li, Chao Zhu, Yuehu Liu, **Yuhui Hong**, & Jianji Wang (2021). "Geometric and Semantic Analysis of Road Image Sequences for Traffic Scene Construction." *Neurocomputing*, 465, 336-349. [Paper] [Code]

## ONGOING ARTICLES

- 10 **Yuhui Hong**, Sujun Li, Yuzhen Ye, & Haixu Tang (2024). "FIDDLE: a deep learning method for chemical formulas prediction from tandem mass spectra." *bioRxiv*, 2024-11. (Under review). [Preprint] [Code]
- 11 Ludwig Lautenbacher, Kevin L. Yang, Tobias Kockmann, Christian Panse, Wassim Gabriel, Dulguun Bold, Elias Kahl, Matthew Chambers, Brendan X. MacLean, Kai Li, Fengchao Yu, Brian C. Searle, Wilburn, Damien, Mohammad Reza Zare Shahneh, **Yuhui Hong**, Haixu Tang, Mingxun Wang, Ralf Gabriels, Robbin Bouwmeester, Robbe Devreese, Tobias K. Schmidt, Alexey I. Nesvizhskii, & Mathias Wilhelm (2024). "Koina: Democratizing machine learning for proteomics research." (Under review). [Website] [Code]
- 12 **Yuhui Hong**, & Haixu Tang (2025). "A Task-Specific Transfer Learning Approach to Enhancing Small Molecule Retention Time Prediction with Limited Data." (Under review). [Code]
- 13 Mahsa Monshizadeh, **Yuhui Hong**, & Yuzhen Ye (2025). "Confounder Free Predictive Models for Microbiome-based Host Phenotype Prediction." (Under review). [Code]

\*equal contribution as co-first authors

## CONFERENCE PRESENTATIONS

- 1 **Poster presentation**. "Predicting Compositional Fragments of Compounds from Their Tandem Mass Spectra Using Deep Neural Networks" [Poster]  
*72nd Conference on Mass Spectrometry and Allied Topics*. Jun. 2 - 6, 2024. Anaheim, CA.
- 2 **Poster presentation**. "3DMolMS: Prediction of Tandem Mass Spectra from 3D Molecular Conformations"  
*Turkey Run Analytical Chemistry Conference 2023*. Sep. 29 - 30, 2023. Marshall, IN.
- 3 **Oral Presentation** "A Machine Learning Model for Chemical Formula Prediction Using Tandem Mass Spectra of Compounds" [Slides]  
*71st Conference on Mass Spectrometry and Allied Topics*. Jun. 4 - 8, 2023. Houston, TX.
- 4 **Poster Presentation** "Prediction of Molecular Tandem Mass Spectra Using 3-Dimensional Conformers" [Poster]  
*70th Conference on Mass Spectrometry and Allied Topics*. Jun. 5 - 9, 2022. Minneapolis, MN.

## PROFESSIONAL SERVICES

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- **Reviewer:** Journal of Chromatography A, BMC Genomics, BMC Bioinformatics, IEEE Transactions on Computational Biology and Bioinformatics, Pharmaceutical Research, Beilstein Journal of Organic Chemistry, Chemical Physics Letters
- **Sub-reviewer:** (conferences) RECOMB 2025, ACM BCB 2024, ISMB 2023, RECOMB 2023, RECOMB 2022; (journals) Analytical Chemistry, International Journal of Mass Spectrometry  
*assisted in reviewing papers under the guidance of Prof. Haixu Tang*

## PROFESSIONAL AFFILIATIONS

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- American Society for Mass Spectrometry (ASMS), Member. 2022 - Present
- NSF Center for Bioanalytic Metrology (CBM), Student. 2022 - Present

## 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
- **Second-tier 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)