

Yuhui Hong

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EDUCATION

Indiana University Bloomington
Ph.D. in Computer Science

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

Xidian University
B.E. in Computer Science and Technology

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

RESEARCH EXPERIENCE

Indiana University Bloomington
Research Assistant
Advisor: Prof. Haixu Tang

Bloomington, IN, US
Sep. 2020 – Present

- Designed deep learning models (1) leveraging 3D molecular conformations to predict tandem mass spectra and chromatographic enantioseparation, and (2) identifying chemical formulas, advancing small compound identification and analysis.

The First Affiliated Hospital of Nanchang University
Research Intern
Mentor: Dr. Sujun Li

Nanchang, Jiangxi, China
May 2021 – Jul. 2021

- Implemented a machine learning model for Major Histocompatibility Complex (MHC) binding prediction based on Bidirectional Encoder Representations from Transformers (BERT).

Xi'an Jiaotong University
Research Assistant
Advisor: Prof. Yaochen Li

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

- Designed a point-based representation method and benchmarked state-of-the-art deep learning models for object tracking and segmentation in traffic images and videos.

PUBLICATIONS

BOOKS

1. Qingyang Xiao, Kaiyuan Liu, **Yuhui Hong** & Haixu Tang (2024). “Neural Networks for Chemists.” *American Chemical Society*. (In press, to be published on November 2024) DOI: 10.1021/acsinfocus.7e8012

PEER-REVIEWED ARTICLES

1. **Yuhui Hong**, Yuzhen Ye & Haixu Tang (2024). “Machine Learning in Small-Molecule Mass Spectrometry.” *Annual Review of Analytical Chemistry*. (In press, to be published on May 2025)
2. **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.
[link] [source codes]
3. **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.
[link] [source codes] [PyPI package] [online service]

4. 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 (USENIX Security 24)* (pp. 6543-6560).
[link]
5. 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.
[link] [source codes]
6. 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.
[link] [source codes]

ARTICLES UNDER REVIEW

1. Mahsa Monshizadeh*, **Yuhui Hong***, & Yuzhen Ye (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 REPRESENTATIONS

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.

TEACHING EXPERIENCE

Instructor INFO-I529, Machine Learning Bioinformatics	Indiana University Bloomington Fall 2024
Assistant Instructor CSCI-D351, Big Data Analytics Instructor: Prof. Haixu Tang	Indiana University Bloomington Fall 2024

PROFESSIONAL SERVICES

- **Reviewer:** BMC Genomics, BMC Bioinformatics, Pharmaceutical Research, Beilstein Journal of Organic Chemistry, Chemical Physics Letters
- **Sub-reviewer:** (conferences) 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

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

PROFESSIONAL AFFILIATIONS

American Society for Mass Spectrometry (ASMS), Member. 2022 - Present

LANGUAGE COMPETENCY

English: Proficient; **Chinese:** Native.