

# Yuanyue Li, Ph.D.

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## PERSONAL STATEMENT

Metabolites are the foundation of life. With its excellent sensitivity and accuracy, mass spectrometry has become the best tool for systematically measuring metabolites. Currently, only about 10% of detected metabolites can be annotated, leaving the rest unidentified metabolites as the “dark matters” in the life science. My research focuses on developing computational methods to enhance metabolite identification using mass spectrometry. I am particularly interested in leveraging public metabolomics repositories and applying machine learning and big data strategies to improve annotation rates.

## EDUCATION EXPERIENCE

<b>Ph.D. in Biochemistry and Molecular Biology</b>	2008.9-2014.6
Xiamen University, Xiamen, China	
Thesis title: A novel analysis method for data-independent acquisition MS data	
<b>B.Sc. in Life Science</b>	2004.9-2008.7
Xiamen University, Xiamen, China	

## RESEARCH EXPERIENCE

<b>Zhejiang University</b>	Zhejiang, China
ZJU 100 Young Professor	2025.1-now
<b>University of California, Davis</b>	Davis, United States
Postdoctoral Fellow, advisor: Dr. Oliver Fiehn	2020.1-2022.8
Assistant Project Scientist	2022.9-2024.12
<b>European Molecular Biology Laboratory</b>	Heidelberg, Germany
Postdoctoral Fellow, advisor: Dr. Peer Bork	2015.12-2019.3
<b>Xiamen University</b>	Xiamen, China
Graduate Student, advisor: Dr. Jiahuai Han	2008.9-2015.6

## PUBLICATIONS

### Main author publications:

6. **Yuanyue Li** & Oliver Fiehn. Flash entropy search to query all mass spectral libraries in real time. *Nature Methods* 20, 1475–1478 (2023).

5. **Yuanyue Li**, Tobias Kind, Jacob Folz, Arpana Vaniya, Sajjan Singh Mehta & Oliver Fiehn. Spectral entropy outperforms MS/MS dot product similarity for small-molecule compound identification. *Nature Methods* 18, 1524–1531 (2021).
4. **Yuanyue Li**, Michael Kuhn, Joanna Zukowska-Kasprzyk, Marco L. Hennrich, Panagiotis L. Kastiris, Francis J. O'Reilly, Prasad Phapale, Martin Beck, Anne-Claude Gavin & Peer Bork. Coupling proteomics and metabolomics for the unsupervised identification of protein–metabolite interactions in *Chaetomium thermophilum*. *PLOS ONE* 16, e0254429 (2021).
3. **Yuanyue Li**, Michael Kuhn, Anne-Claude Gavin & Peer Bork. Identification of metabolites from tandem mass spectra with a machine learning approach utilizing structural features. *Bioinformatics* 36, 1213–1218 (2020).
2. **Yuanyue Li**, Chuan-Qi Zhong, Xiaozheng Xu, Shaowei Cai, Xiurong Wu, Yingying Zhang, Jinan Chen, Jianghong Shi, Shengcai Lin & Jiahuai Han. Group-DIA: analyzing multiple data-independent acquisition mass spectrometry data files. *Nature Methods* 12, 1105–1106 (2015).
1. Chuan-Qi Zhong\*, **Yuanyue Li**\*, Daowei Yang, Na Zhang, Xiaozheng Xu, Yaying Wu, Jinan Chen & Jiahuai Han. Quantitative phosphoproteomic analysis of RIP3-dependent protein phosphorylation in the course of TNF-induced necroptosis. *Proteomics* 14, 713–724 (2014). (\* equal contributions)

#### Contributing author publications:

8. Fanzhou Kong, Tong Shen, **Yuanyue Li**, Amer Bashar, Susan Bird & Oliver Fiehn. Denoising Search doubles the number of metabolite and exposome annotations in human plasma using an Orbitrap Astral mass spectrometer. *Nature Methods*.
7. Elys P. Rodríguez, **Yuanyue Li**, Arpana Vaniya, Patrick M. Shih & Oliver Fiehn. Alternative Identification of Glycosides Using MS/MS Matching with an In Silico-Modified Aglycone Mass Spectra Library. *Analytical Chemistry* (2023) doi:10.1021/acs.analchem.3c00957.
6. Panagiotis L. Kastiris, Francis J. O'Reilly, Thomas Bock, **Yuanyue Li**, Matt Z. Rogon, Katarzyna Buczak, Natalie Romanov, Matthew J. Betts, Khanh Huy Bui, Wim J. Hagen, Marco L. Hennrich, Marie-Therese Mackmull, Juri Rappsilber, Robert B. Russell, Peer Bork, Martin Beck & Anne-Claude Gavin. Capturing protein communities by structural proteomics in a thermophilic eukaryote. *Molecular Systems Biology* 13, 936 (2017).
5. Xiurong Wu, Wan-Ting He, Shuye Tian, Dan Meng, **Yuanyue Li**, Wanze Chen, Lisheng Li, Lili Tian, Chuan-Qi Zhong, Felicia Han, Jianming Chen & Jiahuai Han. *pelo* Is Required for High Efficiency Viral Replication. *PLOS Pathogens* 10, e1004034 (2014).
4. Ting Wu, **Yuanyue Li**, Deli Huang, Felicia Han, Ying-Ying Zhang, Duan-Wu Zhang & Jiahuai Han. Regulator of G-Protein Signaling 19 (RGS19) and Its Partner  $G\alpha$ -Inhibiting Activity Polypeptide 3 (GNAI3) Are Required for zVAD-Induced Autophagy and Cell Death in L929 Cells. *PLOS ONE* 9, e94634 (2014).
3. Xiurong Wu, Lili Tian, Jie Li, Yingying Zhang, Victor Han, **Yuanyue Li**, Xiaozheng Xu, Hanjie Li, Xi Chen, Jinan Chen, Wenhai Jin, Yongming Xie, Jiahuai Han & Chuan-Qi Zhong. Investigation

of receptor interacting protein (RIP3)-dependent protein phosphorylation by quantitative phosphoproteomics. *Molecular & cellular proteomics* 11, 1640–1651 (2012).

2. Hanjie Li, Congting Ye, Guoli Ji, Xiaohui Wu, Zhe Xiang, **Yuanyue Li**, Yonghao Cao, Xiaolong Liu, Daniel C. Douek, David A. Price & Jiahuai Han. Recombinatorial Biases and Convergent Recombination Determine Interindividual TCR $\beta$  Sharing in Murine Thymocytes. *The Journal of Immunology* 189, 2404–2413 (2012).

1. Duan-Wu Zhang, Min Zheng, Jing Zhao, **Yuan-Yue Li**, Zhe Huang, Zhu Li & Jiahuai Han. Multiple death pathways in TNF-treated fibroblasts: RIP3- and RIP1-dependent and independent routes. *Cell Research* 21, 368–371 (2011).

## SELECTED PRESENTATIONS

### **Oral talks:**

2023.10	Metabolomics Association of North America SODAMeets
2023.08	3rd Chinese American Society for Mass Spectrometry Conference
2023.02	University of Ottawa
2022.06	JRNLclub.org
2022.03	National Center of Protein Sciences, China
2022.02	Metabolomics Association of North America SODAMeets
2021.10	Metabolomics Association of North America Annual Conference
2020.09	NIH Common Fund Metabolomics Consortium Meeting

### **Poster:**

2024.06	American Society for Mass Spectrometry Annual Conference
2023.10	38th Asilomar Conference on Mass Spectrometry
2022.10	2nd Chinese American Society for Mass Spectrometry Conference
2022.06	American Society for Mass Spectrometry Annual Conference