

## Yuanyue Li, Ph.D.

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### PERSONAL STATEMENT

Metabolites are fundamental components in biological processes, yet their large-scale detection remains a big challenge, limiting our understanding of metabolomics. My research aims to bridge this gap by integrating mass spectrometry with computational strategies to enhance metabolite identification techniques. I am interested in the development of innovative computational tools and the integration of machine learning strategies for large-scale metabolite structure identification. In tandem with this, I am interested in integrating metabolomics with other ‘omics’ like proteomics and genomics to better understand the function of metabolomics, thereby enhancing our knowledge of life science and human health.

### EDUCATION EXPERIENCE

**Ph.D. in Biochemistry and Molecular Biology** 2008.9-2014.6  
Xiamen University, Xiamen, China  
Thesis title: A novel analysis method for data-independent acquisition MS data

**B.Sc. in Life Science** 2004.9-2008.7  
Xiamen University, Xiamen, China

### RESEARCH EXPERIENCE

**University of California, Davis** Davis, United States  
Postdoctoral Fellow / Assistant Project Scientist, advisor: Dr. Oliver Fiehn 2020.1-now  
*Focus: Mass Spectrometry-based Metabolomics*

- Designed and implemented Flash entropy search algorithm, magnifying the speed of library searching by five orders of magnitude.
- Introduced the concept of spectral entropy and entropy similarity to the mass spectrometry field, reducing the false positive rate in metabolite identification by up to 40%.

**European Molecular Biology Laboratory** Heidelberg, Germany  
Postdoctoral Fellow, advisor: Dr. Peer Bork 2015.12-2019.3  
*Focus: Proteomics and Metabolomics*

- Invented SF-Matching, a machine learning-driven approach to improve metabolite identification.
- Established a strategy coupling proteomics and metabolomics techniques to unsupervised identify protein-metabolite interactions.

**Xiamen University**

Graduate Student, advisor: Dr. Jiahuai Han

Xiamen, China

2008.9-2015.6

*Focus: Mass Spectrometry-based Proteomics*

- Developed Group-DIA, an approach that enhances protein identification notably by grouping multiple mass spectrometry datasets.

## **PUBLICATIONS AND AWARDS**

### **Main author publications:**

6. **Yuanyue Li** & Oliver Fiehn. Flash entropy search to query all mass spectral libraries in real time. *Accepted by Nature Methods* (2023) doi:10.21203/rs.3.rs-2693233/v1.
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:**

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 Gα-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 TCRβ 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).

## PRESENTATIONS

### **Invited oral talk:**

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|---------|--|
| 2023.08 | (Upcoming) 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                  |

### **Oral talk:**

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| 2022.10 | Chinese American Society for Mass Spectrometry Conference   |
| 2021.10 | Metabolomics Association of North America Annual Conference |
| 2020.09 | NIH Common Fund Metabolomics Consortium Meeting             |

### **Poster:**

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| 2022.06 | American Society for Mass Spectrometry Annual Conference    |
| 2021.09 | NIH Common Fund Metabolomics Consortium Meeting             |
| 2020.09 | Metabolomics Association of North America Annual Conference |
| 2020.05 | American Society for Mass Spectrometry Annual Conference    |