

FEI WANG

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EDUCATION

University of Alberta

2020 - Present

Doctor of Philosophy in Computing Science

Supervised by Dr. Russell Greiner and Dr. David S. Wishart

University of Alberta

2016 - 2019

Master of Science in Computing Science

Supervised by Dr. Russell Greiner and Dr. David S. Wishart

Thesis: Learning Metabolite Mass Tandem Spectra Predictors From Molecular Graph Structure

University of Lethbridge

2013

Bachelor of Science, Computer Science with Co-op

Publications

- [1] Qiang, Hantao*, **Fei Wang***, Wenyun Lu, Xi Xing, Hahn Kim, Sandrine A. M. Mérette, Lucas B. Ayres, Eponine Oler, Jenna E. AbuSalim, Asael Roichman, Michael Neinast, Ricardo A. Cordova, Won Dong Lee, Ehud Herbst, Vishu Gupta, Samuel L. Neff, Mickel Hiebert-Giesbrecht, Adamo Young, Vasuk Gautam, Siyang Tian, Bo Wang, Hannes Röst, Jatinder Baidwan, Russell Greiner, Li Chen, Chad W. Johnston, Leonard J. Foster, Aaron M. Shapiro, David S. Wishart, Joshua D. Rabinowitz, and Michael A. Skinnider. “Language Model-Guided Anticipation and Discovery of Mammalian Metabolites”. In: *Nature* 651.8104 (2026).
- [2] Adamo Young*, **Fei Wang***, David Wishart, Bo Wang, Russell Greiner, and Hannes Rost. “FraGN-Net: a deep probabilistic model for tandem mass spectrum prediction”. en. In: *Transactions on Machine Learning Research* (2025).
- [3] Lingkai Cai, Rongjie Bai, Qiang Cao, Weijie Sun, **Fei Wang**, Xiaotong Liu, Bo Liang, Meihua Jiang, Gongcheng Wang, Qiang Shao, et al. “A non-invasive MRI-based multimodal fusion deep learning model (MF-DLM) for predicting overall survival in bladder cancer: a multicentre retrospective study”. In: *Eclinicalmedicine* 90 (2025).
- [4] Ray Kruger, Eponine Oler, Sukanta Saha, Jenna Poelzer, Scott Han, Mark Peter Punsalan, Brittany Green, Fahrin Bushra, Megane Kyes, Fehintola Disu, Julia Wakoli, Robyn Woudstra, Elykah Tejol, Omolola Fakutan, **Fei Wang**, Brian L Lee, Tanvir Sajed, Siyang Tian, Claudia Torres-Calzada, Mark Berjanskii, Scott MacKay, Naama Karu, Rima Kadurrah-Daouk, and David S Wishart. “MiMeDB 2.0: the human microbial metabolome database for 2026”. en. In: *Nucleic Acids Research* (2025).
- [5] Roman Bushuiev, Anton Bushuiev, Niek F de Jonge, Adamo Young, Fleming Kretschmer, Raman Samusevich, Janne Heirman, **Fei Wang**, Luke Zhang, Kai Dührkop, Marcus Ludwig, Nils A Haupt, Apurva Kalia, Corinna Brungs, Robin Schmid, Russell Greiner, Bo Wang, David S Wishart, Li-Ping Liu, Juho Rousu, Wout Bittremieux, Hannes Rost, Tytus D Mak, Soha Hassoun, Florian Huber, Sebastian Böcker, Josef Sivic, and Tomáš Pluskal. “MassSpecGym: A Benchmark for the Discovery and Identification of Molecules”. In: *Conference on Neural Information Processing Systems*. 2024.
- [6] Craig Knox, Mike Wilson, Christen M Klinger, Mark Franklin, Eponine Oler, Alex Wilson, Allison Pon, Jordan Cox, Na Eun (Lucy) Chin, Seth A Strawbridge, Marysol Garcia-Patino, Ray Kruger, Aadhavya Sivakumaran, Selena Sanford, Rahil Doshi, Nitya Khetarpal, Omolola Fatokun, Daphnee Doucet, Ashley Zubkowski, Dorsa Yahya Rayat, Hayley Jackson, Karxena Harford, Afia Anjum, Mahi Zakir, **Fei Wang**, Siyang Tian, Brian Lee, Jaanus Liigand, Harrison Peters, Ruo Qi (Rachel) Wang, Tue Nguyen, Denise So, Matthew Sharp, Rodolfo da Silva, Cyrella Gabriel, Joshua Scantlebury,

- Marissa Jasinski, David Ackerman, Timothy Jewison, Tanvir Sajed, Vasuk Gautam, and David S Wishart. "DrugBank 6.0: The DrugBank Knowledgebase for 2024". In: *Nucleic Acids Research* 52.D1 (2024).
- [7] Thomas O. Metz, Christine H. Chang, Vasuk Gautam, Afia Anjum, Siyang Tian, **Fei Wang**, Sean M. Colby, Jamie R. Nunez, Madison R. Blumer, Arthur S. Edison, Oliver Fiehn, Dean P. Jones, Shuzhao Li, Edward T. Morgan, Gary J. Patti, Dylan H. Ross, Madelyn R. Shapiro, Antony J. Williams, and David S. Wishart. *Introducing 'Identification Probability' for Automated and Transferable Assessment of Metabolite Identification Confidence in Metabolomics and Related Studies*. 2024.
- [8] Tanvir Sajed, Zinat Sayeeda, Brian L. Lee, Mark Berjanskii, **Fei Wang**, Vasuk Gautam, and David S. Wishart. "Accurate Prediction of ¹H NMR Chemical Shifts of Small Molecules Using Machine Learning". In: *Metabolites* 14.5 (2024).
- [9] Julia Wakoli, Afia Anjum, Tanvir Sajed, Eponine Oler, **Fei Wang**, Vasuk Gautam, Marcia LeVatte, and David S Wishart. "GCMS-ID: A Webserver for Identifying Compounds from Gas Chromatography Mass Spectrometry Experiments". In: *Nucleic Acids Research* 52.W1 (2024).
- [10] David S. Wishart, Mickel Hiebert-Giesbrecht, Gozal Incheborouni, Xuan Cao, An Chi Guo, Marcia A. LeVatte, Claudia Torres-Calzada, Vasuk Gautam, Mathew Johnson, Jaanus Liigand, **Fei Wang**, Shirin Zahraei, Sudarshana Bhumireddy, Yilin Wang, Jiamin Zheng, Rupasri Mandal, and Jason R. B. Dyck. "Chemical Composition of Commercial Cannabis". In: *Journal of Agricultural and Food Chemistry* 72.25 (2024).
- [11] Zehra Shah, Shi-Ang Qi, **Fei Wang**, Mahtab Farrokh, Mashrura Tasnim, Eleni Stroulia, Russell Greiner, Manos Plitsis, and Athanasios Katsamanis. "Exploring Language-Agnostic Speech Representations Using Domain Knowledge for Detecting Alzheimer's Dementia". In: *ICASSP 2023 - 2023 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*. Rhodes Island, Greece: IEEE, 2023. ISBN: 978-1-72816-327-7.
- [12] **Fei Wang**, Daniel Pasin, Michael A. Skinnider, Jaanus Liigand, Jan-Niklas Kleis, David Brown, Eponine Oler, Tanvir Sajed, Vasuk Gautam, Stephen Harrison, Russell Greiner, Leonard J. Foster, Petur Weihe Dalsgaard, and David S. Wishart. "Deep Learning-Enabled MS/MS Spectrum Prediction Facilitates Automated Identification Of Novel Psychoactive Substances". In: *Analytical Chemistry* 95.50 (2023).
- [13] **Fei Wang**, Dana Allen, Siyang Tian, Eponine Oler, Vasuk Gautam, Russell Greiner, Thomas O Metz, and David S Wishart. "CFM-ID 4.0 – a Web Server for Accurate MS-based Metabolite Identification". In: *Nucleic Acids Research* 50.W1 (2022).
- [14] David S Wishart, AnChi Guo, Eponine Oler, **Fei Wang**, Afia Anjum, Harrison Peters, Raynard Dizon, Zinat Sayeeda, Siyang Tian, Brian L Lee, Mark Berjanskii, Robert Mah, Mai Yamamoto, Juan Jovel, Claudia Torres-Calzada, Mickel Hiebert-Giesbrecht, Vicki W Lui, Dorna Varshavi, Dorsa Varshavi, Dana Allen, David Arndt, Nitya Khetarpal, Aadhavya Sivakumaran, Karxena Harford, Selena Sanford, Kristen Yee, Xuan Cao, Zachary Budinski, Jaanus Liigand, Lun Zhang, Jiamin Zheng, Rupasri Mandal, Naama Karu, Maija Dambrova, Helgi B Schiöth, Russell Greiner, and Vasuk Gautam. "HMDB 5.0: The Human Metabolome Database for 2022". In: *Nucleic Acids Research* 50.D1 (2022).
- [15] Ammar Hassanzadeh Keshteli, Dana Allen, Afia Anjum, Yashvi Patel, Aadhavya Sivakumaran, Siyang Tian, **Fei Wang**, Hao Wang, Mark A. Lewis, Russell Greiner, and David S. Wishart. "A Longitudinal Dataset of Incidence and Intervention Policy Impacts Regarding the COVID-19 Pandemic in Canadian Provinces". In: *Data in Brief* 38 (2021).
- [16] Michael A. Skinnider, **Fei Wang**, Daniel Pasin, Russell Greiner, Leonard J. Foster, Petur W. Dalsgaard, and David S. Wishart. "A Deep Generative Model Enables Automated Structure Elucidation of Novel Psychoactive Substances". In: *Nature Machine Intelligence* 3.11 (2021).
- [17] **Fei Wang**, Jaanus Liigand, Siyang Tian, David Arndt, Russell Greiner, and David S. Wishart. "CFM-ID 4.0: More Accurate ESI-MS/MS Spectral Prediction and Compound Identification". In: *Analytical Chemistry* 93.34 (2021).

Asterisks(*) indicates equal contribution.

Under Review

- [1] Vishu Gupta, Chencheng Xu, Ehud Herbst, **Fei Wang**, David S. Wishart, and Michael A. Skinnider. *Confronting Spurious Evaluations of Computational Methods in Small Molecule Mass Spectrometry*. 2026.

Asterisks(*) indicates equal contribution.

CONFERENCE PRESENTATIONS

- FraGNNNet: A Deep Probabilistic Model for Mass Spectrum Prediction, International Conference on Intelligent Systems for Molecular Biology Conference (2024)
- CFM-ID 4 Plus: An Improved MS/MS Prediction Tool, Metaboloimcs Conference (2023)
- Build Domain Specific ESI-MS/MS Prediction model from Pre-trained CFM-ID 4.0", 4th Annual MANA Annual Conference (2022)
- Accurate MSMS Spectral Prediction with CFM-ID 4.0, Metaboloimcs Conference (2020)
- Optical Character Recognition of Printed Mathematical Symbols using A Hierarchical Classifier, International Conference on Image Processing, Computer Vision, and Pattern Recognition (2012)

WORK EXPERIENCE

Software Engineer, Bioware ULC

2013 - 2015

- Implemented multiple ETL processes by using .Net, AngularJS, Elasticsearch
- Prototyped web service in microservice architecture by using Docker containers, Nginx, Mono, MVC framework and Consul.
- Contributed to Dragon Age Keep, web application as the franchise ecosystem to support Dragon Age, one of the most wanted franchise of the company with millions of users.
- Participated in developing Dragon Age Inquisition HQ, a web application to provide the companion experience for Dragon Age Inquisition
- Designed and implemented restful backend services and RESTful APIs by using PHP and Symfony 2 MVC framework.
- Successfully achieved automatic data transferring from complicated game data to web service via Python.

Associate Software Engineer, Electronic Arts

2013

- Frontend developer for the FIFA online team.
- Contributed in FIFA 14 for Xbox One and PlayStation 4 version, the first release of the biggest game franchise on the new generation of console platforms
- Successfully implemented game frontend for online game mode by using C++ and Actionscript.

Research Assistant, University of Lethbridge

2011-2013

- Acquired and leveraged comprehensive knowledge of OCR engine design and necessary knowledge of machine learning mechanism, such as K-means and SVM to build an OCR prototype for mathematical expression.
- Upgraded and modified a 3D graph drawing package named GLuskap with latest algorithm.
- Prototyped hand gesture input solution which leveraging the Microsoft Kinect, OpenCV library, and OpenNI library to recognize hand gestures as an input device for GLuskap.

TEACHING EXPERIENCE

Teaching Assistant, University of Alberta

2016 - Present

- CMPUT 174 - Introduction to the Foundations of Computation I
- CMPUT 175 - Introduction to the Foundations of Computation II
- CMPUT 201 - Practical Programming Methodology
- CMPUT 301 - Introduction to Software Engineering

SKILLS

Programming Languages

Python, C++

Libraries

PyTorch, NumPy, Pandas, rdkit, MPI

Software Development

Programming Paradigms, Git, Agile Methodology

Experienced With

Scientific Computing, Slurm, High Performance Computing, CUDA