Zhidian Zhang

zhidianz@mit.edu
+41786764103

Academic

Massachusetts Institute of Technology (MIT), USA
- Postdoc, Biology and Artificial Intelligence May 2024 – Present

École Polytechnique Fédérale de Lausanne (EPFL), Switzerland
- Doctoral Assistant, Computational and Quantitative Biology Sep 2019 – Feb 2024

Harvard University, USA
- Visiting Scholar, Systems Biology. Feb 2023 – Aug 2023

McGill University, Canada
- Master of Science, Biochemistry Jan 2018 – May 2019
- Bachelor of Science, Major Biochemistry, Minor Mathematics Sep 2015 – Dec 2017

Honours and Awards

- MIT-Novo Nordisk Artificial Intelligence Postdoctoral Fellows (182k USD) Jun 2025
- Swiss National Science Foundation (SNSF) PostDocMobility Grant (136k CHF) Jun 2024
- Swiss National Science Foundation (SNSF) Mobility Grants in Projects (20k CHF) Jun 2022
- Student Research Achievement Award for Biophysical Society Annual Meeting 2022 Feb 2022
- Traveling Award for Biophysical Society Annual Meeting 2022 Dec 2021
- EPFL Ignition Grant (30k CHF), Enable Grant (30k CHF), Innosuisse (283k CHF), awarded to co-founded startup 2020-23
- Graduate Excellence Award (12k CAD) Jan 2018 – May 2019
- Faculty of Science Dean's Multidisciplinary Undergraduate Research List Jun 2018
- 2 * Tomlinson Engagement Award for Mentoring, Ordinary Differential Equations Course Sep 2016 – May 2017

Research Experiences

Postdoc Fellow in Biology and Artificial Intelligence
Sergey Ovchinnikov Lab, MIT, Boston, USA May 2024 – Present
Predicting physiological structures of biomolecular assemblies
- Developing methods to predict protein homo-oligomerisation and alternative conformations
- Modeling structural changes in response to post-translational modifications (PTMs) and environmental perturbations
- Predicting RNA structures using machine learning and high-throughput experimental data

SNSF Visiting Scholar in Systems Biology
Sergey Ovchinnikov Lab, FAS Center for Systems Biology, Harvard University, Boston, USA Feb 2023 – Aug 2023
Interpretability Study of Protein Language Models (pLMs)
- Led comprehensive interpretability studies on pLMs and identified limitations of current models
- Developed an unsupervised method for probing pLMs coevolutionary signals, now adopted widely for benchmarking and interpreting protein and genomic language models

PhD in Computational Biology
Laboratory for biomolecular modelling, Institute of Bioengineering, EPFL, Lausanne, Switzerland Sep 2019 – Feb 2024
Laboratory for neurobiology and neuroproteomic, Neuroscience – Brain Mind Institute, EPFL, Lausanne, Switzerland
The Intra-molecular and Inter-molecular Effects of PTM Cross-talks on Proteins Involved in Neurodegenerative Diseases
- Elucidated the molecular basis of PTMs' effects on the structure, aggregation, and membrane interactions of proteins by combining molecular simulations and biophysical experiments
- Identified 100k PTM sites at intermolecular interfaces with interface prediction machine learning methods

Master's in Biochemistry
Dr. Kalle Gehring Lab, Department of Biochemistry, McGill University, Montreal, QC, Canada Jan 2018 – May 2019
Mechanism of Inhibition of PRL Phosphatases by Thienopyridones and Its Derivatives
- Elucidated the mechanisms of potential therapeutic agents targeting the oncogenic PRL phosphatases
- Designed novel high-throughput screening methods for high-specificity drugs targeting PRL-CNNM interaction

Independent Research Student in Cancer Genetics
Dr. Patricia Tonin Lab, Research Institute of McGill University Health Centre, Montreal, QC, Canada Jan 2017 – May 2017
Bioinformatics Analyses for New Candidate Hereditary Ovarian Cancer Risk Genes
- Conducted data analysis for whole-exome sequencing data from French Canadian cohorts and from families with multi-case of hereditary ovarian cancer

Conference Talks

RosettaCON 2023: Interpretability study of protein language models
Biophysical Society Annual Meeting 2022: The role of PTM crosstalks in HTTex1 structure, aggregation, and membrane interaction

Intelligent Systems for Molecular Biology (ISMB) 2025, RosettaCON 2025
Probing Homo-Oligomeric Interaction Signals in Protein Language Models

Conference Organization

Winter RosettaCON 2025: Session Chair for 'Stability and conformational changes in proteins'
Summer RosettaCON 2025: Co-chair for 'Protein Language Models'
NeurIPS 2025 Co-localised Machine Learning in Structural Biology Workshop: Organizer

Teaching Assistant Experiences

Teaching: Artificial Intelligence for Protein Structure Prediction and Design **(University of Gothenburg)**, Science in the Age of AI **(Harvard)**
Course TA: Biomolecular Structure and Mechanics, New Tools & Research Strategies in Personalized Health, Biomaterials, Scientific Literature Analysis in Bioengineering (**EPFL)** Ordinary Differential Equations (**McGill)**
Supervised projects: Generative protein and genomic language models interpretability analysis (Xiaonan Liu, MIT Ph.D), Scaling down protein language modeling with MSA Pairformer (Yo Akiyama, MIT Ph.D), Adapting genomic language models for gene assembly (Anna Mikulevica, MIT B.Sc), Protein contact prediction (Samarth Jajoo, MIT B.Sc), Protein language model interpretability (Garyk Brixi, Harvard BSc), Phosphorylation site prediction (EPFL machine learning course project), Bioinformatics analysis on the roles of post-translation modification in phase separation (Laurent Pierre Brock, EPFL B.Sc).

Other Experiences

Co-founder

NanoDecoder, Lausanne, Switzerland Sep 2020 – Dec 2022

- Led team to utilize engineered bionanopores for polymer-based data storage and PTM biomarker detection
- Conducted molecular simulations and data analysis for the rational design of bionanopores
- Awarded EPFL Enable grant, EPFL Ignition grant, and Innosuisse

Head of Speaker Relations Team

TEDxEcublens, Lausanne, Switzerland Dec 2019 – Jul 2022

- Curated TEDx talks, and organized workshops or events for sponsors and students

Submitted

[1] Hit or Miss: Understanding Emergence and Absence of Homo-oligomeric Contacts in Protein Language Models. **Zhidian Zhang,** Yo Akiyama, Yehlin Cho, Samarth Jajoo, Sergey Ovchinnikov (bioRxiv 2025)

[2] Scaling Down Protein Language Modeling with MSA Pairformer. Yo Akiyama, **Zhidian Zhang**, Milot Mirdita, Martin Steinegger, Sergey Ovchinnikov (bioRxiv 2025)

[3] Boltzdesign1: Inverting All-Atom Structure Prediction Model for Generalized Biomolecular Binder Design. Yehlin Cho, Martin Pacesa, **Zhidian Zhang**, Bruno E. Correia, Sergey Ovchinnikov (bioRxiv 2025)

Publications

[1] Protein Language Models Learn Evolutionary Statistics of Interacting Sequence Motifs. **Zhidian Zhang**, Hannah K. Wayment-Steele, Garyk Brixi, Dorothee Kern, Sergey Ovchinnikov (PNAS 2024)

[2] AI Methods for Protein Folding and Design. **Zhidian Zhang**, Chenxi Ou, Yehlin Cho, Yo Akiyama, Sergey Ovchinnikov (Current Opinion in Structural Biology 2025)

[3] Differential Effects of Posttranslational Modifications on the Membrane Interaction of Huntingtin Protein. **Zhidian Zhang**, Charlotte Gehin, Luciano A Abriata, Matteo Dal Peraro, Hilal Lashuel (ACS Chemical Neuroscience 2024)

[4] Bicc1 ribonucleoprotein complexes specifying organ laterality are licensed by ANKS6-induced structural remodeling of associated ANKS3. Benjamin Rothé, Yayoi Ikawa, **Zhidian Zhang**, Takanobu A Katoh, Eriko Kajikawa, Katsura Minegishi, Sai Xiaorei, Simon Fortier, Matteo Dal Peraro, Hiroshi Hamada, Daniel B Constam (PLoS Biology, 2023)

[5] Crosstalk Among PTMs Provides Novel Insight Into the Structural Basis Underlying the Differential Effects of Nt17 PTMs on Mutant Httex1 Aggregation. Anass Chiki, **Zhidian Zhang (co-first),** Kolla Rajasekhar, Luciano A Abriata, Iman Rostami, Lucien F Krapp, Driss Boudeffa, Matteo Dal Peraro, Hilal A Lashuel (Front Mol Biosci, 2021)

[6] PRL oncogenicity is mediated through direct binding to CNNM Mg2+ transporter PRL3 pseudophosphatase activity is necessary and sufficient to promote metastatic growth. Guennadi Kozlov , Yosuke Funato , Yu Seby Chen , **Zhidian Zhang** , Katalin Illes , Hiroaki Miki, Kalle Gehring (JBC, 2020)

[7] Mechanism of thienopyridone and iminothienopyridinedione inhibition of protein phosphatases. **Zhidian Zhang**, Guennadi Kozlov, Kalle Gehring (MedChemComm, 2019)

[8] Conformational changes in the cytosolic domains of CNNM, a Mg^{2+} transporter, provide insight into Mg^{2+}-ATP sensing. Yu Seby Chen, Guennadi Kozlov, Rayan Fakih, Meng Yang, **Zhidian Zhang**, Evgenii L. Kovrigin, Kalle Gehring (Structure, 2019)