

Pengfei Tian

EXPERIENCE

- **Principal Scientist**, Lila Sciences [🌐] 2022 - Now
Machine learning for protein and mRNA therapeutics design Boston, USA
- **Senior Data Scientist**, Novozymes A/S, Enzyme Research [🌐] 2019 - 2022
Generative model for enzyme engineering Copenhagen, Denmark
- **Postdoc**, National Institutes of Health (NIH) 2015 - 2018
Advisor: Robert Best [🌐] Bethesda, USA

EDUCATION

- **PhD in Physics**, Niels Bohr Institute, University of Copenhagen 2011 - 2014
Advisors: Kresten Lindorff-Larsen [🌐], Mogens Høgh Jensen [🌐] Copenhagen, Denmark
- **Exchange PhD**, Lund University Feb-May 2012
Advisor: Anders Irbäck Lund, Sweden
- **MSc in Mechatronics Engineering**, University of Southern Denmark 2008 - 2010
Profile: Mathematical Modeling Sønderborg, Denmark
- **BSc in Applied Mathematics**, Northwestern Polytechnical University 2004 - 2008
Profile: Information and Computing Science Xi'An City, China

PATENTS

- [1] Pengfei Tian, Thomas Lenhard, Anders Sandström, and Jonatan Fangel. “[Mannanase Variants and Polynucleotides Encoding Same](#)”. In: WIPO (PCT) Patent Application WO2023247348A1 (2023)
- [2] Jesper Frickmann, Esben Friis, Pengfei Tian, Trine Soerensen, Weijian Lai, Lars Anderson, Mateusz Dyla, and Stefanie Neun. “[Carbonic anhydrase variants and polynucleotides encoding same](#)”. In: WIPO (PCT) Patent Application WO2024118901A2 (2023)
- [3] Jesper Vind, Trine Soerensen, Lars Hylling Christensen, Pengfei Tian, Jan Vester, and Jesper Rung. “[DNase variants and compositions](#)”. In: WIPO (PCT) Patent Application WO2023165950A1 (2023)
- [4] Jesper Vind, Trine Soerensen, Pengfei Tian, Jesper Rung, and Annemarie Schoenfeld. “[Polypeptide variants](#)”. In: WIPO (PCT) Patent Application WO2022189521A1 (2022)
- [5] Vasudeva Rao, Geetha Mendez, Christian Joergensen, Akshatha Venugopalan, Naveen Raikar, Silja Poulose, Lars Olsen, Allan Svendsen, Jonatan Fangel, Subith Krishna, Pengfei Tian, and Rajendra Sainathan. “[Mannanase variants and polynucleotides Encoding Same](#)”. In: WIPO (PCT) Patent Application WO2021152123A1 (2021)
- [6] Sune Christensen, Vibeke Nielsen, Lone Baunsgaard, Jesper Vind, Lars Iversen, Matias Moses, Lene Cesar, and Pengfei Tian. “[Lipase variants and compositions comprising such lipase variants](#)”. In: WIPO (PCT) Patent Application WO2022090361A2 (2021)
- [7] Kenneth Jensen, Lars Anderson, Svend Kaasgaard, Jonatan Fangel, Frank Rasmussen, Pengfei Tian, and Christian Joergensen. “[Carbohydrate binding module variants](#)”. In: WIPO (PCT) Patent Application WO2021204838A1 (2020)

PUBLICATIONS

- [1] Richard Michael, Jacob Kæstel-Hansen, Peter Mørch Groth, Simon Bartels, Jesper Salomon, Pengfei Tian, Nikos S Hatzakis, and Wouter Boomsma. “[A systematic analysis of regression models for protein engineering](#)”. In: PLOS Computational Biology 20.5 (2024), e1012061
- [2] Peter Mørch Groth, Richard Michael, Jesper Salomon, Pengfei Tian, and Wouter Boomsma. “[Flop: Tasks for fitness landscapes of protein wildtypes](#)”. In: bioRxiv (2023), pp. 2023–06
- [3] Pengfei Tian, Adrien Lemaire, Fabien Sénéchal, Olivier Habrylo, Viviane Antonietti, Pascal Sonnet, Valérie Lefebvre, Frederikke Isa Marin, Robert B Best, Jérôme Pelloux, et al. “[Design of a Protein with Improved Thermal Stability by an Evolution-Based Generative Model](#)”. In: Angewandte Chemie 134.50 (2022), e202202711
- [4] Tomas Laursen, Hiu Yue Monatrice Lam, Kasper Kildegaard Sørensen, Pengfei Tian, Cecilie Cetti Hansen, Jay T Groves, Knud Jørgen Jensen, and Sune M Christensen. “[Membrane anchoring facilitates colocalization of enzymes in plant cytochrome P450 redox systems](#)”. In: Communications Biology 4.1 (2021), p. 1057

- [5] Florian Wruck, Pengfei Tian, Renuka Kudva, Robert B Best, Gunnar von Heijne, Sander J Tans, and Alexandros Katranidis. [“The ribosome modulates folding inside the ribosomal exit tunnel”](#). In: *Communications biology* 4.1 (2021), p. 523
- [6] Pengfei Tian and Robert B Best. [“Exploring the sequence fitness landscape of a bridge between protein folds”](#). In: *PLoS computational biology* 16.10 (2020), e1008285
- [7] Xiakun Chu, Yong Wang, Pengfei Tian, Wenfei Li, and Davide Mercadante. [“Advanced Sampling and Modeling in Molecular Simulations for Slow and Large-Scale Biomolecular Dynamics”](#). In: *Frontiers in Molecular Biosciences* 8 (2021), p. 795991
- [8] Grant Kemp, Ola B Nilsson, Pengfei Tian, Robert B Best, and Gunnar von Heijne. [“Cotranslational folding cooperativity of contiguous domains of \$\alpha\$ -spectrin”](#). In: *Proceedings of the National Academy of Sciences* 117.25 (2020), pp. 14119–14126
- [9] Aleix Lafita, Pengfei Tian, Robert B Best, and Alex Bateman. [“TADOSS: computational estimation of tandem domain swap stability”](#). In: *Bioinformatics* 35.14 (2019), pp. 2507–2508
- [10] Aleix Lafita, Pengfei Tian, Robert B Best, and Alex Bateman. [“Tandem domain swapping: determinants of multidomain protein misfolding”](#). In: *Current Opinion in Structural Biology* 58 (2019), pp. 97–104
- [11] Yong Wang, Pengfei Tian, Wouter Boomsma, and Kresten Lindorff-Larsen. [“Monte Carlo sampling of protein folding by combining an all-atom physics-based model with a native state bias”](#). In: *The Journal of Physical Chemistry B* 122.49 (2018), pp. 11174–11185
- [12] Pengfei Tian, Annette Steward, Renuka Kudva, Ting Su, Patrick J Shilling, Adrian A Nickson, Jeffrey J Hollins, Roland Beckmann, Gunnar Von Heijne, Jane Clarke, et al. [“Folding pathway of an Ig domain is conserved on and off the ribosome”](#). In: *Proceedings of the National Academy of Sciences* 115.48 (2018), E11284–E11293
- [13] Emily J Guinn, Pengfei Tian, Mia Shin, Robert B Best, and Susan Marqusee. [“A small single-domain protein folds through the same pathway on and off the ribosome”](#). In: *Proceedings of the National Academy of Sciences* 115.48 (2018), pp. 12206–12211
- [14] Renuka Kudva, Pengfei Tian, Fátima Pardo-Avila, Marta Carroni, Robert B Best, Harris D Bernstein, and Gunnar Von Heijne. [“The shape of the bacterial ribosome exit tunnel affects cotranslational protein folding”](#). In: *Elife* 7 (2018), e36326
- [15] Pengfei Tian, John M Louis, James L Baber, Annie Aniana, and Robert B Best. [“Co-evolutionary fitness landscapes for sequence design”](#). In: *Angewandte Chemie* 130.20 (2018), pp. 5776–5780
- [16] Pengfei Tian and Robert B Best. [“How many protein sequences fold to a given structure? A coevolutionary analysis”](#). In: *Biophysical journal* 113.8 (2017), pp. 1719–1730
- [17] Pengfei Tian, Richard W Jones, and Fei Yu. [“Elliptical modelling of hysteresis operating characteristics in a dielectric elastomer tubular actuator”](#). In: *Smart Materials and Structures* 25.7 (2016), p. 075038
- [18] Pengfei Tian and Robert B Best. [“Structural determinants of misfolding in multidomain proteins”](#). In: *PLOS Computational Biology* 12.5 (2016), e1004933
- [19] Pengfei Tian, Kresten Lindorff-Larsen, Wouter Boomsma, Mogens Høgh Jensen, and Daniel Erik Otzen. [“A Monte Carlo study of the early steps of functional amyloid formation”](#). In: *PloS one* 11.1 (2016), e0146096
- [20] Jesper Tranekjær Jørgensen, Kamilla Norregaard, Pengfei Tian, Poul Martin Bendix, Andreas Kjaer, and Lene B Oddershede. [“Single particle and PET-based platform for identifying optimal plasmonic nano-heaters for photothermal cancer therapy”](#). In: *Scientific Reports* 6.1 (2016), p. 30076
- [21] Pengfei Tian, Wouter Boomsma, Yong Wang, Daniel E Otzen, Mogens H Jensen, and Kresten Lindorff-Larsen. [“Structure of a functional amyloid protein subunit computed using sequence variation”](#). In: *Journal of the American Chemical Society* 137.1 (2015), pp. 22–25
- [22] Wouter Boomsma, Pengfei Tian, Jes Frellsen, Jesper Ferkinghoff-Borg, Thomas Hamelryck, Kresten Lindorff-Larsen, and Michele Vendruscolo. [“Equilibrium simulations of proteins using molecular fragment replacement and NMR chemical shifts”](#). In: *Proceedings of the National Academy of Sciences* 111.38 (2014), pp. 13852–13857
- [23] Pengfei Tian, Sigurður Jónsson, Jesper Ferkinghoff-Borg, Sergei Krivov, Kresten Lindorff-Larsen, and Wouter Boomsma. [“Robust estimation of diffusion-optimized ensembles for enhanced sampling”](#). In: *Biophysical Journal* 106.2 (2014), 640a
- [24] Jan B Valentin, Christian Andreetta, Wouter Boomsma, Sandro Bottaro, Jesper Ferkinghoff-Borg, Jes Frellsen, Kanti V Mardia, Pengfei Tian, and Thomas Hamelryck. [“Formulation of probabilistic models of protein structure in atomic detail using the reference ratio method”](#). In: *Proteins: Structure, Function, and Bioinformatics* 82.2 (2014), pp. 288–299
- [25] Haiyan Ma, Pengfei Tian, Josselin Pello, Poul Martin Bendix, and Lene B Oddershede. [“Heat generation by irradiated complex composite nanostructures”](#). In: *Nano letters* 14.2 (2014), pp. 612–619

- [26] Wouter Boomsma, Jes Frellsen, Tim Harder, Sandro Bottaro, Kristoffer E Johansson, Pengfei Tian, Kasper Stovgaard, Christian Andreetta, Simon Olsson, Jan B Valentin, et al. “[PHAISTOS: a framework for Markov chain Monte Carlo simulation and inference of protein structure](#)”. In: *Journal of computational chemistry* 34.19 (2013), pp. 1697–1705
- [27] Pengfei Tian, Gang Li, and Richard W Jones. “[Ellipse-based modelling of hysteresis in a smart actuator](#)”. In: *2010 IEEE/ASME International Conference on Advanced Intelligent Mechatronics*. IEEE. 2010, pp. 872–877

HONORS AND AWARDS

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|--|------|
| • Awarded a research grant as the Principal Investigator
<i>Innovation Fund Denmark, Denmark</i> | 2022 |
| • The Fellows Award for Research Excellence
<i>National Institutes of Health (NIH), USA</i> | 2017 |
| • The Fellows Award for Research Excellence
<i>National Institutes of Health (NIH), USA</i> | 2016 |

PRESENTATIONS

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|---|------|
| • 10th International Conference on Bioinformatics and Computational Biology, Virtual. | 2022 |
| • Structural Bioinformatics Course, University of Copenhagen, Denmark. | 2021 |
| • Sorbonne Université, France. | 2020 |
| • The 62nd Biophysical Society Annual Meeting, San Francisco, USA. | 2018 |
| • Gordon Research Conference, Galveston, USA. | 2018 |
| • The 61st Biophysical Society Annual Meeting, New Orleans, USA. | 2017 |
| • Gordon Research Conference, Galveston, USA. | 2016 |
| • The 251st American Chemical Society National Meeting; Exposition, San Diego, USA. | 2016 |
| • The 59th Biophysical Society Annual Meeting, Baltimore, USA. | 2015 |
| • Barcelona BioMed Conference: Frontiers in dynamics simulations of biological molecules, Barcelona, Spain. | 2013 |

OUTREACH

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|---|-----------|
| • Platform Co-chair , The 58th Biophysical Society Annual Meeting. San Francisco, USA. | 2014 |
| • Fellows Advisory Board , NIDDK, National Institute of Health(NIH). Bethesda, USA. | 2015-2017 |
| • Platform Moderator , The 12th Annual NIDDK Scientific Conference (NIH). Bethesda, USA. | 2017 |
| • Topic Editor , Journal Frontiers in Molecular Biosciences. | 2021 |
| • Mentor , Copenhagen Bioinformatics Hackathon, Denmark. | 2021 |
| • Career Mentor , Integrative Structural Biology Section, University of Copenhagen, Denmark. | 2021 |

MENTORING

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|--|---------------------|
| • PhD project Supervisor , Novozymes A/S, Denmark. | Apr 2022 - Oct 2022 |
| • Master Thesis Supervisor , Novozymes A/S, Denmark. | Feb 2020 - Aug 2021 |
| • Mentor , Community College Summer Enrichment Program, NIH, USA. | Summer 2018 |