Yang Zhang

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Education

- **03/2020 - Now: Ph.D. in Biomolecular Structure and Mechanism**, Joint program offered by University of Zurich and ETH Zurich, Zurich, Switzerland
  Research interests: *Computer-aided drug discovery; Molecular dynamics (MD) simulation; Geometric deep learning; Molecular interaction pattern recognition; High-performance computing;*
  Supervisor: Prof. Dr. Amedeo Caflisch; Co-supervisor: Dr. Andreas Vitalis
- **09/2018 - 11/2019: M.Phil. in Pharmacy and Pharmaceutical Sciences**, Division of Pharmacy and Optometry, University of Manchester, Manchester, UK
  Thesis title: *Simulation of protein dynamics for mechanistic insight and drug design.*
  Supervisor: Dr. Richard Bryce
- **09/2014 - 09/2018**: **B.Eng. in Pharmaceutical Engineering**, Joint program offered by Shandong Academy of Medical Sciences and University of Jinan, Jinan, China
  Thesis title: *Structural modification of Qumai diacid.* Supervisor: Dr. Jingyong Sun
  Ranked top 5% with average score

Professional and Research Experience

- **04/2020 – Now: Development of a browser-based drug discovery platform (ACGui)**, Ph.D. in Caflisch group, Department of Biochemistry, University of Zurich, Zurich, Switzerland
  - Automated batch MD system construction and developed a trajectory visualizer to dynamically request and render molecular models on the browser
  - Developed web utilities for trajectory analysis and interactive plotting that could control playback and highlight relevant component
  - Integrated the AutoDock Vina for docking and administered a PostgreSQL compound database
  - Collaborated and managed the project via git and employed feature branching
- **10/2021 - Now: Augmenting molecular recognition pattern with MD trajectories**, Same role in UZH
  - Developed a Python framework to extract dynamic/static features from the stream of trajectories
  - Implemented molecule block alignment using enhanced ICP algorithms
  - Optimized performance-critical C++ code using OpenMP and CUDA, exposed via Python bindings
- **10/2021 - Now: Small-molecule binder identification against multiple targets**, Same role in UZH
  - Conducted high-throughput virtual screening and MD simulations on HPC for targets including: *YTHDC1*, *YTHDF2*, *BCL2A1(BFL-1)*, and *METTL1*
  - Utilized Saturation transfer difference (STD) in NMR for ligand binding test
  - Developed tools to prepare combinatorial ligand library and commercial availability query
- **09/2018-10/2019: Small-molecule binder identification against R-spondin**, M.Phil. in Bryce group, Division of Pharmacy and Optometry, University of Manchester, Manchester, UK
  - Performed high-throughput virtual screening(1.3 billion compounds) against R-Spondin via molecular property/ADME filtration, molecular docking, MD simulation, and free energy computation
  - Specialized in HPC for task array optimization and large-scale file management
- **05/2019 - 10/2019: Exploration of pH sensing mechanism of calcium-sensing receptor (CaSR)**, Collaborated with Prof. Donald Ward and Dr. Patricia Centeno at the University of Manchester
  - Performed molecular dynamics simulations to study the allosteric behavior of multiple Calcium-sensing receptor (CaSR) mutants in the presence of different cofactors
- **03/2018 - 07/2018: Natural product purification and modification**, Intern, Institute of Materia Medica, Shandong Academy of Medical Sciences, Jinan, China
  - Isolated quillaic acid from *Gypsophila paniculata L.*, synthesized two new triterpenoid compounds, and characterized their structures using TLC, LCMS, and NMR techniques

Training and Conferences

- **10/2023: Advanced C++ on HPC**, Advanced Workshop, Swiss National Supercomputing Centre, Lugano, Switzerland
- **06/2023: High-Performance Computing with Python**, Advanced Workshop, Swiss National Supercomputing Centre, Lugano, Switzerland
- **09/2022: International Symposium on Medicinal Chemistry (EFMC-ISMC 2022)**, Poster: *A versatile browser-based platform for molecular dynamics simulation and visualization*, Nice, France
- **09/2021: Mathematics of life: Modelling molecular mechanisms**, Advanced Workshop, EMBL-EBI, UK
- **08/2019: International Congress of Radiation Research (ICRR 2019)**, Organizing Team, Manchester, UK
- **07/2019: International Conference on Medicinal Chemistry (RICT 2019)**, Poster: *In silico design of anti-cancer compounds targetting R-spondin using molecular dynamics*, Nantes, France
- **04/2019: Doctoral Academy Graduate Society Conference**, Poster: same as RICT 2019, Manchester, UK

Publications

- **Zhang Y**, Vitalis A, & Caflisch A. Closing the loop on MD: A graphical interface for setting up, running, storing, and analyzing molecular simulations. *in preparation*
- **Zhang Y**, Radler F, Langini C, Vitalis A, & Caflisch A. A visualization-driven approach to perform virtual screens and inspect their results. *in preparation*
- Vargas-Rosales, P.A., D'Addio, A., **Zhang Y** & Caflisch, A. (2023). Disrupting Dimeric β-Amyloid by Electric Fields. *ACS Physical Chemistry Au*.
- **Zhang Y.** (2020). Simulation of protein dynamics for mechanistic insight and drug design, *MPhil Thesis, The University of Manchester(United Kingdom)*.
- **Zhang Y.**, Zhang H., Hao B., & Sun J. (2019Kingdom). Advances in Pharmacological Activity and Action Mechanism of Myricetin. *Food and Drug*, 21(1), 75-80.

Teaching and Student Supervision

- **09/2022: Pablo Angelo Cristian Lugon**, MSc Biochemistry, Research Project, *High-throughput virtual screening of small-molecule ligands to human METTL1 with SEED and VINA*.
- **06/2022: Ruth Esser** and **Tim Schlatter**, BSc Biochemistry, Bachelor Thesis, *Structure-based virtual ligand screening of the human METTL1 protein*.
- **01/2022: Alessio D'Addio**, MSc Biochemistry, Advanced Protein Engineering, *High-throughput fragment docking on human YTHDC1 and analysis of interaction patterns with MD simulation*.
- **08/2021: Niklas Senning**, MSc Biochemistry, Research Project, *In silico high-throughput screening for METTL3 inhibitory fragments with SEED*.
- **2021, 2022: Biochemistry Experiment**, Teaching assistant, Department of Biochemistry, UZH.
- **10/2020: Siri Peter**, MSc Biochemistry, Research Project, *In-silico structure identification of human YTHDC1 inhibitors with SEED*.

Honors and Awards

- Annual Excellence Scholarship, University of Jinan (Top 15%) | 2015, 2016, 2017, 2018
- Outstanding Student Cadre, University of Jinan | 2015, 2018

Skills and Interests

- **Programming:** Python, C++/OpenMP/CUDA/pybind, Shell, JavaScript, HTML/CSS, SQL, LaTeX
- **Academic software:** GROMACS, AMBER, CAMPARI, CPPTRAJ, SEED, OpenBabel, AutoDock Vina, UCSF Chimera, MOE, OpenEye, AlphaFold
- **Academic packages:** RDKit, Pytraj, Open3D, OpenMM, Numpy, Matplotlib, Scikit-learn, Jax/Optax/Flax, PyTorch, 3DMol.js, Three.js, Plotly.js, MathJax
- **Languages:** Native speaker of Mandarin, proficient in English, and basic in German and French
- **Interests:** Photography, cooking, table tennis, trail running, rope skipping, kondi