Mahdi Hijazi

Computational lead

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Profile

Computational scientist specializing in molecular simulations, mathematical modeling, and software development. Extensive experience in developing in-house software packages, optimizing high-performance computing environments, and generating molecular dynamics datasets, thus providing tailored solutions for project and team requirements. Certified communicator, excelling in bridging computational and experimental domains. Keen learner and enthusiastic teacher with substantial experience in mentoring and project management.

Work Experience

Jan–Sep 2024 **Computational lead - postdoctoral researcher at EPFL, Laboratory of Protein and Cell Engineering**, *Advisor: Prof. Patrick Barth*

- Advising on protein dynamics and G-protein-coupled receptor (GPCR)-specific mechanisms in collaborations inside and outside EPFL
- Building a database for molecular dynamics simulations in the lab that will streamline generation of new data and link it to the lab's electronic notebook (SLIMS) through an API
- Training group members in utilizing EPFL infrastructure, conducting molecular simulations, protein modeling, and designing GPCRs

Jan 2019–Dec 2023 **PhD at EPFL, Laboratory of Protein and Cell Engineering**, *Advisor: Prof. Patrick Barth*

Computational protein design

- Designed allosteric signaling in GPCRs *in silico* to make them selective to specific drugs using molecular dynamics simulations, Rosetta software suite, and graph theoretic metrics
- Modeled proteins in different states and bound to various binding partners, ranging from small molecule ligands to intracellular protein partners, using AI structural methods, homology modeling, and loop modeling
- Collaborated with wet lab scientists to validate designed proteins using cell-based assays

Method development

- Developed metrics from molecular simulations that correlate with experimental observables, including NMR chemical shifts, ligand potencies, and ligand efficacies in GPCRs.
- Created a comprehensive computational package to describe the elusive phenomenon of allostery in proteins and design allosteric mechanisms by considering both structural and dynamic perturbations

Molecular simulations and high performance computing

- Generated extensive molecular dynamics datasets for GPCRs to address diverse research questions such as receptor activation, drug-receptor interactions, ligand selectivity, allosteric modulation, and effector bias
- Utilized high-performance computing clusters (SLURM) and optimized simulation performance on GPU servers to enhance computational efficiency
- Established and managed a comprehensive simulation pipeline in the laboratory, encompassing software installation, script development, hardware optimization, the creation of analytical techniques, development of analysis software, and simulation design

March–August 2018 **Master thesis at IBM Research Zurich**, *Academic advisor: Prof. Nicola Marzari, IBM supervisor: Dr. Teodoro Laino*

- Simulated quantum biological systems using a sparse matrix-matrix multiplication algorithm with unprecedented massive scalability
- Re-parameterized the in-house developed semi-empirical molecular dynamics (SEMD) for biological applications

Education

2019–2023 **EPFL**, *PhD in Materials Science and Engineering*, Laboratory of Protein and Cell Engineering

2016–2018 **EPFL**, *MSc in Materials Science and Engineering*, Cumulative GPA of 5.42/6

2011–2015 **American University of Beirut (AUB)**, *BEn in Mechanical Engineering*, Cumulative GPA of 88.83/100, equivalent to 3.91/4.0

Other Experience

Teaching

Spring 2020 2021 — Taught synthetic biology to senior undergraduate students at EPFL, tasks included: lecturing, exam writing and marking, and project design

Autumn 2020 — Scientific literature analysis to masters students in computational biology at EPFL, tasks included: report grading, presentation evaluation, and mentoring on reading scientific literature

Supervision

Feb–July 2022 — Supervised Simon Lietar (Masters project at EPFL) with project titled: *Quantification of mutual information significance in allosteric pathway calculations in proteins*

Selected Publications

- **Mahdi Hijazi***, Daniel Keri*, Aurélien Oggier*, Melina Agosto, Theodore Wensel, and Patrick Barth, "Computational design of allosteric pathways reprograms ligand-selective GPCR signaling," under review in *Science*. *: co-first authorship
- Robert E Jefferson, Aurélien Oggier, Andreas Füglistaler, Nicolas Camviel, **Mahdi Hijazi**, Ana Rico Villarreal, Caroline Arber, and Patrick Barth, "Computational design of dynamic receptor—peptide signaling complexes applied to chemotaxis," *Nature Communications* **14**(1), 2875 (2023)
- Lucas SP Rudden, **Mahdi Hijazi**, and Patrick Barth, "Deep learning approaches for conformational flexibility and switching properties in protein design," *Frontiers in Molecular Biosciences* **840** (2022)
- Jie Yin, Kuang-Yui M Chen, Mary J Clark, **Mahdi Hijazi**, Punita Kumari, Xiao-chen Bai, Roger K Sunahara, Patrick Barth, and Daniel M Rosenbaum, "Structure of a D2 dopamine receptor-G-protein complex in a lipid membrane," *Nature* **584**(7819), 125-129 (2020)
- **Mahdi Hijazi**, David M. Wilkins, and Michele Ceriotti, "Fast-Forward Langevin Dynamics with Momentum Flips," *Journal of Chemical Physics* **148**(18), 184109 (2018). Awarded editor's pick

Awards

2024 — Nominated for the doctoral program EDMX Distinction 8% student prize at EPFL.

Sept 2022 — Best poster award at the "Understanding function of G-Protein Coupled Receptors by atomistic and multiscale simulations," CECAM worksop, Lugano, Switzerland.

2016–2018 — EPFL Excellence Fellowship for the academic years of 2016/2017 and 2017/2018.

June 2016 — Advanced Communicator Bronze award, *Toastmasters International*, with specializations in "professionally speaking" and "storytelling".

Nov 2015 — Advanced Leader Bronze award, *Toastmasters International*.

May 2015 — AUB High Distinction honor awarded on graduation. (GPA above 90/100 for the last two years of study)

Skills

Bash, Matlab, Python (inc. NumPy, Pandas, SciPy, and PyTorch), Molecular dynamics simulations (GROMACS, OpenMM, and NAMD), Enhanced sampling simulations (steered MD, metadynamics), Free energy perturbation (alchemical and geometric methods), Protein modeling and design (Rosetta software suit), protein structure prediction (Alphafold, RoseTTAFold), Molecular visualization (VMD and Pymol), High performance computing (Slurm and GPU servers), SLIMS, Git, C++, R, SQL

Extracurricular Activities

Feb 2024 — **My thesis in 180 seconds (EPFL):** participated in a competition to present my research, in simple language, to a non-specialist audience in three minutes.

Oct 2015–Feb 2016 — **Trainer and Advisor at Olayan School of Business (AUB):** Trained a group of five Masters of Finance students for the Chartered Financial Analyst (CFA) Institute Research Challenge in order to improve their professional business communication and presentation skills.

Languages

Arabic (Mother language), **English** (Bilingual Fluency), **French** (Level B2)