CAMILLA CAPRAI

MSc in Quantitative Biology

RESEARCH INTERESTS

I am a Master's graduate in Quantitative Biology with a Bachelor's degree in Biological Sciences and a strong passion for computational biology. Over the past year, I have focused on high-performance computing (HPC) and large-scale molecular dynamics (LSMD). During this time, I also had the opportunity to work with advanced computational techniques such as Self-Organizing Maps (SOMs) and Markov State Models (MSMs) in the context of protein binding modes analysis. Having recently graduated, I am eager to pursue a PhD in Southern Europe, where I can further develop my expertise and contribute to innovative research. My primary interests lie in protein function analysis and design, with a particular emphasis on leveraging computational methods to understand and engineer biological molecules, especially for tailored drug design.

EDUCATION

Master's Degree in Quantitative Biology

Università degli Studi di Milano
(Average exam grade: 29.14/30 — Final grade: 110/110 cum laude)

Thesis title: Large Scale Molecular Dynamics Approaches to Data-Driven Binding Mode Identification and Classification.
This thesis presents the use of unbiased all-atom molecular dynamics simulations combined with advanced computational methods to study allosteric networks, ligand-receptor binding pathways, and binding pocket detection in proteins. The AlloViz tool was created to analyze allosteric networks, revealing key insights into protein dynamics. A new approach using self-organizing maps with Markov state models was applied to map ligand-receptor binding pathways. Additionally, a large-scale workflow was established for simulating protein databases, focusing on kinases. Lastly, an algorithm combining MDpocket with HDBSCAN clustering was developed to identify and analyze binding sites.
Thesis co-supervisors: Prof. Carlo Camilloni and Dott. Toni Giorgino

October 2022 — October 2024 Milan, Italy

- October 2023 — October 2024 Thesis Internship at Istituto di Biofisica CNR (IBF-CNR).
  Topic: Development and application of computational methods for classifying binding modes in biological molecules via large-scale molecular dynamics simulations. During this time, two projects I contributed to were published.
  Supervisor: Dott. Toni Giorgino
- September 2023 Short Internship at Istituto Nazionale Genetica Molecolare (INGM), Genome Biology Lab.
  Topic: I followed researchers in their daily routines, joining lab meetings, gaining insights into experiment design and time management. I dedicated substantial time to colony PCR and worked in the imaging facility, acquiring ISH (In Situ Hybridization) images and quantifying the associated signals.
  Supervisor: Prof. Beatrice Bodega

Bachelor's Degree in Biological Sciences

Università di Pisa
(Average exam grade: 27.93/30 — Final grade: 110/110)

Thesis title: Il Glutatione: Metabolismo ed Azione Antiossidante
Thesis supervisor: Prof. Roberta Moschini

September 2019 — July 2022 Pisa, Italy

- November 2021 Short Internship at the Biochemistry Department, Università di Pisa.
  Topic: Investigating the cellular response of tumor cell culture A549 to Daunorubicin and Doxorubicin treatment through viability assays (MTT, Crystal Violet).
  Supervisor: Prof. Roberta Moschini
- May 2021 — July 2021 Internship at the Biochemistry Department, Università di Pisa.
  Topic: Investigating the suitability of stable transfected Human Lens Epithelial Cells (HLEC) for studying NF-κB activation upon cellular stimulation.
  Supervisor: Prof. Roberta Moschini

LANGUAGES

Italian

English

COMPUTER SKILLS

Python
Data analysis and visualization, Molecular Dynamics, Biostatistics

Snakemake

HPC
Slurm

LaTeX

R
Data analysis and visualization, Bioinformatics

OTHER EDUCATION AND CERTIFICATIONS

Fundamentals of Accelerated Computing with CUDA Python
NVIDIA Deep Learning Institute
November 2024

One-day workshop offering theoretical and practical insights into GPU-accelerated Python with CUDA and Numba.

THE HORIZONS OF INTELLIGENCE. Knowledge and the Human-Technology Frontier
13th Edition of Trieste Next – Festival of Scientific Research
Trieste, Italy
27 – 29 September 2024

I participated in this festival as a selected student, awarded the *Trieste Next Academy* fellowship.

To publish or patent: when is the right time?
Fondazione Human Technopole
April 2024

Workshop on coordinating patents with publishing discoveries, focusing on balancing career goals and protecting intellectual property.

The drug discovery process: from lead optimization to the clinical candidate
Università degli Studi di Milano
Milan, Italy
February 2024

Seminar day for PhD students in Pharmaceutical Sciences, focused on drug discovery and hosted by professors and industry professionals.

Training School on Computational Tools to Study Non-Globular Proteins
ML4NGP - REFRACT
Carmona, Spain
13 – 16 February 2024

I was one of 25 selected participants in this training school and received a fellowship covering my expenses.

Fundamentals of Deep Learning
NVIDIA Deep Learning Institute
January 2024

One-day workshop to gain and refine insights into deep learning frameworks.

IELTS Academic - Band 8

British Council, IDP Education, Cambridge Assessment English

January 2024

IELTS Academic certification achieved with an overall band score of 8/9 (CEFR Level: C1, Proficient User).

QMB1: Quantitative Methods for Biology

Prof. Michael Springer, HarvardX

October 2021

Introductory course on MATLAB and its applications in the biological field that I took at the beginning of my final year of undergraduate studies to gain familiarity with the computational world.

INDUSTRIAL COLLABORATIONS

Part of my Master's thesis project (HPC automation, Snakemake workflow implementation, pockets characterization) has been developed in collaboration with Dompé Farmaceutici S.p.A.

MEETINGS

NEXT – Nurture EXscalate Technology meeting

Dompé Farmaceutici S.p.A.

Milan, Italy

11 – 12 November 2024

Internal meeting of Dompé and academic collaborators.

PUBLICATIONS

2. Callea L, **Caprai C**, Bonati L, Giorgino T, Motta S. Self-Organizing Maps of Unbiased Ligand-Target Binding Pathways and Kinetics. Journal of Chemical Physics. 2024 Oct.
1. Nerín-Fonz F, **Caprai C**, Morales-Pastor A, Lopez-Balastegui M, Aranda-García D, Giorgino T, Selent J. AlloViz: A Tool for the Calculation and Visualisation of Protein Allosteric Communication Networks. Computational and Structural Biotechnology Journal. 2024 Dec, 23:1938–1944.