ODYSSEAS VAVOURAKIS

DPhil (PhD) Student, University of Oxford — Generative Antibody Design

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in 🗘 ovavourakis

EDUCATION

DPhil (PhD) - Department of Statistics University of Oxford (Balliol College), UK

- 🚞 Sep 2023 present
- focus on *De Novo* Antibody Design
- student in SABS: \mathbb{R}^3 CDT programme
- completed coursework in software engineering, mathematical modelling, structural drug discovery, data science, and scientific computing

M.Sc. Computational Biology & Bioinformatics **ETH Zürich, Switzerland**

- 🚞 Sep 2020 Aug 2023
- graduated with distinction; ranked 1st in my course
- top grade for thesis project (see right-hand column)
- **GPA: 5.9** / **6.0** (= μ + 1.75 σ); UK 1st class equivalent
- totalled $151\ /\ 120\ ECTS$ credits; extra coursework in RL & probabilistic ML, NLP, computational quantum chemistry and physics, game theory
- jointly awarded with Universities of Zurich and Basel

B.Sc. Biochemistry

Heidelberg University, Germany

🚞 Sep 2015 – Aug 2018

- **GPA 1.5** (best possible: 1.0)
- extra coursework on computational methods

PUBLICATIONS

Challenges and compromises: Predicting unbound antibody structures with deep learning

A. Greenshields-Watson, O. Vavourakis,

F.C. Spoendlin, M. Cagiada, C. M. Deane

- 2025
- \blacklozenge Curr. Opin. Struct. Biol.
- reviews the state of antibody structure prediction; highlights the need to model the unbound state, outlining current challenges; and points to generative models as promising solutions

Exact tunneling splittings from symmetrized path integrals

G. Trenins, L. Meuser, H. Bertschi, O. Vavourakis, R. Flütsch, and J. O. Richardson

- **i** 2023
- Journal of Chemical Physics
- a new path-integral molecular dynamics simulation technique to calculate exact ground-state tunnelling splitting patterns in small molecules without wavefunctions

RESEARCH EXPERIENCE

DPhil (PhD) Project

Mar 2024-present

De Novo Generative Antibody Design

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- OPIG, University of Oxford
- *in silico* sequence-structure co-design of antibody variable domains with a generative flow-matching model
- advised by Prof C. Deane, M. Raybould (University of Oxford); Dr R. Croasdale-Wood (AstraZeneca)

Master's Thesis Project

Boost-SE: Wide-Spectrum Enzyme-Substrate Interactions from Multi-Task Recommendations using Protein Language Models

i 7 months (2023)

- ♥ ETH AI Center, ETH Zürich
- recommendation system to propose likely-interacting enzyme-substrate pairs given a set of MACCS fingerprints + enzyme sequences
- enables inductive enzyme and compound discovery
- trained on binary, positive/unlabelled metabolic pathway data + auxiliary targets
- uses fine-tuned pLM sequence embeddings
- advised by Prof A. Krause, J. Rothfuss, M. Mutný

Master's Rotation Project

Calculating Tunnelling Splittings with Path-Integral Molecular Dynamics

- **i** 3.5 months (2022)
- D-CHAB, ETH Zurich
- built path-integral molecular dynamics simulation package from scratch
- co-developed, implemented and validated the mathematical method, sampling scheme and estimator
- see publication on left
- advised by Prof J. Richardson; Dr G. Trenins

Bachelor's Thesis Project

Spectrin-Repeat Mechanical Unfolding with Atomistic Force-Probe MD

a 3.5 months (2018)

- ♥ HITS, Heidelberg
- studied sequence determinants of unfolding behaviour and rupture force of spectrin repeat domains under mechanical tension with steered molecular dynamics
- advised by Prof F. Gräter; Dr C. Daday

INTERESTS & EXPERTISE

Computational Protein Design Generative Modelling Geometric Deep Learning Biomolecular ML Computational Biophysics Physical Chemistry

DISTINCTIONS



Oxford University Clarendon Scholar Oxford University Scatcherd European Scholar Balliol College John Henry Jones Scholar

2023-2028

Willi Studer Prize, as top graduate

of the year in my degree course at ETH Zürich. **■** 2024

 Scholar at Studienstiftung des deutschen Volkes (German Academic Scholarship Foundation)
 2015-2018 and 2020-2023 (B.Sc. and M.Sc.)

LAB EXPERIENCE

Sergeant (NATO OR-5; Military Service) Hellenic Air Force

i Nov 2018 - Nov 2019

- ov 2019 Athens, Greece
- Clinical Biochem General Air Force Hospital
 photometric/spectroscopic sample analysis, clinical assessment and reporting; responsible for ER samples; technical maintenance
- Fuel Chemist Eleusis Air Base
 - scanning electron microscopy of engine micro-debris for predictive maintenance
 - aircraft fuel and engine lubricant quality control and contamination assessment (i.a. optical emission spectroscopy)

Degree-Associated Practicals Heidelberg University

2015 - 2017

Heidelberg, Germany

- Biochemistry: experience in lipidomics; lipid click chemistry; FACS; CRISPR knockouts; immunoprecipitation (ChIP/qPCR); HPTLC; fluorescence microscopy; retroviral transduction; cloning; protein interaction & kinetic assays; protein purification; primer design
- (In)Organic Chemistry: AAS, IR, Raman, EI MS, 1D & 2D NMR; small molecule crystallography & theory; multi-stage organic and inorganic synthesis; classical quantitative analysis (potentiometry, conductometry, electrogravimetry etc.); non-spectroscopic inorganic analysis

- LEISURE
- online lectures/courses
- public lectures on international affairs and politics
- seminar talks, podcasts, non-fiction reading
- language learning, linguistics

ACADEMIC ROLES

Database Maintainer

Oxford Protein Informatics Group

- 2025-present
- upkeep and weekly updates to <u>SAbDab</u>, the largest annotated database of antibody structures in the world

Course Demonstrator (Teaching Assistant) Department of Statistics, University of Oxford

2024-present

- A12: Simulation and Statistical Programming
 led exercise groups & answered student questions
 - created learning material (e.g. jupyter notebooks)

SKILLS

Python & PyTorch R C++ Other Git, Shell & UNIX, Docker, IAT_EX

LANGUAGES

CO-CURRICULARS

Cooperativeness in Graph-Based Systems

Summer Game Theory Course Project

- studied collective phase changes in cooperative behaviour in agents facing iterated prisoner's dilemma interactions while interconnected in a dynamic random graph structure
- three-person group project; won best presentation

Information Theory & Evolution Summer School/Academic Retreat

Summer 2016

- ♥ Ftan, Switzerland
- two-week workshop on information-theoretic approaches to the evolution of intelligence
- gave introductory presentation on information theory
- co-wrote agent-based simulation framework to model emergence of intelligence (three-person group project)