

ODYSSEAS VAVOURAKIS

DPhil (PhD) Student, University of Oxford — Antibody Structure Modelling

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EDUCATION

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

-  Sep 2023 – present
- focus on *De Novo* Antibody Design
 - student in SABS:R³ 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** ($= \mu + 1.75\sigma$); 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. Spöndlin, M. Cagiada, C. M. Deane

-  2025  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

-  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
De Novo Generative Antibody Design

-  Mar 2024-present  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

-  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

-  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

-  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.)

CONFERENCE TALKS

In silico and ML Tools for Antibody Design and
Developability Prediction (Short Course)

PEGS Europe 2025

- course instructor; outlined array of SOTA tools and gave hands-on demonstrations

LAB EXPERIENCE

Sergeant (NATO OR-5; Military Service)

Hellenic Air Force

📅 Nov 2018 - Nov 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

ACADEMIC ROLES

Database Maintainer (SAbDab)

Oxford Protein Informatics Group

📅 2025-present

- upkeep and weekly updates to SAbDab, the largest annotated database of antibody structures in the world

Course Demonstrator (Teaching Assistant)

Department of Statistics, University of Oxford

📅 2025,2026

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

SKILLS

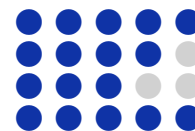
Python & PyTorch

R

C++

Other

Git, Shell & UNIX, Docker, L^AT_EX



LANGUAGES

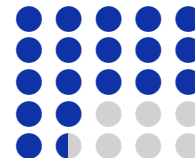
English

German

Modern Greek

Spanish

Latin



CO-CURRICULARS

Cooperativeness in Graph-Based Systems

Summer Game Theory Course Project

📅 Summer 2021 📍 ETH Zurich

- 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)