

# ODYSSEAS VAVOURAKIS

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

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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:R<sup>3</sup> 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. Spoendlin, 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

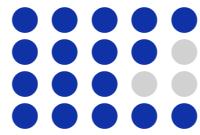
Python & PyTorch

R

C++

Other

Git, Shell & UNIX, Docker, L<sup>A</sup>T<sub>E</sub>X



# LANGUAGES

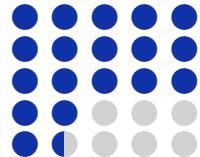
English

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)