# ODYSSEAS VAVOURAKIS

**DPhil (PhD) Student, University of Oxford — ML for Biomolecular Structure**

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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$^3$ CDT programme
- completed coursework in software engineering, mathematical modelling, structural drug discovery, data science, and scientific computing

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### 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

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### 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

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### 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)

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### 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

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### 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

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### 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

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**Willi Studer Prize**, as top graduate
of the year in my degree course at ETH Zürich.

📅 2024

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Scholar at **Studienstiftung des deutschen Volkes**
(German Academic Scholarship Foundation)

📅 2015-2018 and 2020-2023 (B.Sc. and M.Sc.)

# WORK 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)

# 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

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## 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)
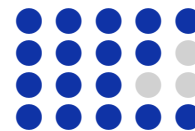
# SKILLS

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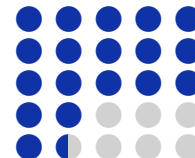**C++**
**Other**
Git, Shell & UNIX, Docker, LaTeX

# LANGUAGES

**English**
**German**
**Modern Greek**
**Spanish**
**Latin**

# LABORATORY EXPERIENCE

## 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