

# ODYSSEAS VAVOURAKIS

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

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🌐 [ovavourakis.github.io](https://ovavourakis.github.io)

🐦 [@ovavourakis](https://twitter.com/ovavourakis)

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## EDUCATION

SABS R<sup>3</sup> EPSRC CDT - DPhil (PhD) Programme  
Balliol College, University of Oxford, UK

📅 Sep 2023 – present

- currently first-year, looking for rotation projects
- pursuing 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; GPA 5.9 / 6.0** ( $= \mu + 1.75\sigma$ ); UK 1st class equivalent
- passed **thesis project** (on right) **without corrections**
- total of **151 / 120 ECTS credits**; additional coursework on RL & probabilistic ML, NLP, computational quantum chemistry and physics, game theory
- degree jointly awarded with University of Zurich and University of Basel

B.Sc. Biochemistry

Heidelberg University, Germany

📅 Sep 2015 – Aug 2018

- **GPA 1.5** (UK 1st class equivalent; best possible: 1.0)
- additional coursework on programming foundations and computational methods

## PUBLICATIONS

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

- <https://doi.org/10.1063/5.0158879>
- a new path-integral molecular dynamics simulation technique to calculate exact ground-state tunnelling splitting patterns in small molecules without wavefunctions

## INTERESTS

Biomolecular ML

Comp. Protein Design

Bayesian ML

Evolutionary & Learning Dynamics

Generalisation in ML

Comp. Biophys.

Phys. Chem.

## RESEARCH EXPERIENCE

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

Lab Rotation Project

**Calculating Tunnelling Splittings with Path-Integral Molecular Dynamics**

📅 3.5 months (2022)

📍 D-CHAB, ETH Zurich

- helped develop the mathematical method, implemented and validated the sampling scheme and estimator
- built path-integral molecular dynamics simulation package from scratch
- 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 rupture force and sequence determinants of unfolding behaviour of spectrin repeat domains under mechanical tension with force-probe molecular dynamics (GROMACS)
- advised by Prof. F. Gräter; Dr. C. Daday

## DISTINCTIONS

Oxford University Clarendon Scholar



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

📅 2023-2028



Scholar at **Studienstiftung des deutschen Volkes**  
(Germany's single most prestigious scholarship)

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

## 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)

## WORK EXPERIENCE

### Staff 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)

## 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

## SKILLS

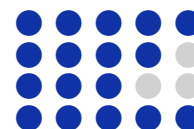
### Python & PyTorch

R

C++

Other

Git, Shell & UNIX, Docker,  $\LaTeX$



## LANGUAGES

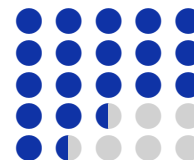
English

German

Modern Greek

Latin

Spanish



## LEISURE

- online lectures/courses
- seminar talks, podcasts, non-fiction books
- language learning
- swimming