

Daniella Pretorius

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Education

Massachusetts Institute of Technology

Visiting PhD student in Professor Sergey Ovchinnikov group

- Research collaboration visit

Boston, U.S.A

Mar 2024 - May 2024

Imperial College London

PhD candidate in Dr. James W. Murray group

- EPSRC funded CDT programme in BioDesign Engineering

London, U.K

Oct 2021 - present

MRes in Systems and Synthetic Biology - Distinction

Oct 2020 - Aug 2021

- Top scholar of the year

BSc Biochemistry - First Class

Oct 2017 - Jun 2020

- Speciality in protein biochemistry, structural biology and biophysics

Research Experience

Imperial College London

PhD Researcher, Dr. James W. Murray group

London, U.K

Oct 2021 - present

Novel Solenoid Protein Generation via *in silico* Evolution

- Developed an *in-silico* protein evolution platform guided by a discrimination network to generate novel protein designs and implemented a selection pipeline to screen for quality, diversity, and novelty
- Comparative bioinformatic analysis on large-scale protein datasets for structure and sequence (AF-DB, PDB, UniProt) using techniques such as Multidimensional Scaling (MDS) and structural clustering
- Established an inexpensive moderate-throughput screening platform for synthetic gene libraries; linear gene fragments to purified protein in 5 days in batches of 96
- Experimentally validated novel solenoid designs; 6 with expected size exclusion chromatography and circular dichroism traces; 1 structure solved by X-ray crystallography to 3 Å with 0.9 Å RMSD to design

Functionalisable β -Solenoid Homo-Oligomer Toolkit

- Developed a pipeline to design a toolkit of oligomeric interfaces (C2-C5 symmetry) for a synthetic β -solenoid (PDB:4YC5), as well as *ad hoc* interface designs
- Experimentally validated 2 novel β -solenoid trimer designs with negative-stain electron microscopy to obtain 2D class averages and 3D *ab initio* reconstructed electron density maps that match the designs
- Characterised trimer designs incorporating N-terminal and internal SpyTag-SpyCatcher systems to form functionalisable assemblies and hydrogels

Masters Project, Dr. James W. Murray group

Oct 2020 - Sep 2021

Repeat Protein Parameterisation and Design

- Wrote Python programs to parametrise repeat proteins and design them from parameters
- Produced a repeat protein parameter dataset from the RepeatsDB database
- Analysed natural protein parameters by pairwise distributions and dimensionality reduction (PCA) to guide future repeat protein design

Collaborations

Massachusetts Institute of Technology

Visiting PhD student, Professor Sergey Ovchinnikov group

Boston, U.S.A

Aug 2023 - present

AlphaFold2 Diffusion Model

- Adapted AlphaFold2 into an open-source diffusion model for generative protein design by leveraging AlphaFold2's understanding of co-evolutionary information and protein structure
- Initiated and led collaborative efforts, resulting in a fully-funded, two-month research visit to MIT

Eden Bio

Research collaborator

London, U.K

July 2023 - Dec 2023

Innovate UK Grant: New Proteins for New Threads

- Contributed to successful Innovate UK grant application with Eden Bio for novel, industrially translatable protein-based fibre materials on the basis on my previous work
- Successfully produced novel protein fibre threads via wet-spinning method
- Delivered on all milestones in the work package timeline, ensuring project continuity and success

Work Experience

OpenCell

Head of Robotics and Automation

London, U.K / Jersey

Jul 2020 - Oct 2020

Set up automated COVID-19 diagnostic station for airport testing in Jersey.

- Involved in initial laboratory accreditation and acted as site project manager
- Composed official government documentation and SOPs for BSL2+ laboratory operation
- Wrote protocols and maintained liquid-handling robotics platforms (Opentrons, feliX)

Publications

1. **Daniella, Pretorius**, James W, Murray. *Novel Solenoid Protein Generation via in silico Evolution Platform* - Manuscript in preparation
2. **Daniella, Pretorius**, James W, Murray. *Functionalisable β -Solenoid Homo-Oligomer Toolkit* - Manuscript in preparation
3. **Daniella, Pretorius**, Fiazall, Tufail, James W, Murray. *Cheap, Robot-Free Moderate Throughput Protocol for Screening Protein Expression and Purification from Small Libraries of Synthetic Genes in Escherichia coli* - Manuscript in preparation for journal Bioprotocol.

Skills

Dry-lab

- **Platforms and Environments:** Linux, High-Performance Computing, Google Colaboratory
- **Scripting Languages:** Python (Pytorch, Pandas, NumPy), Bash
- **Protein Modelling and Design:** Structure prediction (Alphafold, Colabfold, ESMfold, Openfold), protein design software (RFdiffusion, ProteinGenerator, ProteinMPNN, Rosetta), molecular visualisation (PyMOL, ChimeraX)

Wet-lab

- **Micro and molecular biology:** Bacterial culture, restriction digest, primer design, transformation, Golden Gate cloning
- **Protein and DNA skills:** large- and small-scale protein production with *E. coli* (expression, purification and optimisation), Affinity chromatography, size exclusion chromatography, AKTA system, EMSAs
- **Analytical skills:** PCR, SDS-PAGE, Native-PAGE
- **Structural biology:** Crystallography (initial screening, crystal optimisation, data collection and processing), Negative Stain Electron Microscopy (grid preparation, Tecnai T12 operation)

Leadership experience

Imperial Graduate Biotechnology Society

Starting team member

London, U.K

Oct 2022 - present

- Interviewed high-profile speakers in fireside chats about the biotech industry
- Successfully organised and managed multiple events, achieving attendances of over 70 participants

Graduate teaching

- Supervised and mentored 2 Master's and 3 Undergraduate students in lab and computational research; all students achieved Distinction/First Class marks ;1 achieved top project of their cohort
- Acted as a Graduate Teaching Assistant for 5 university modules (62 hours)

Achievements and Honours

- Winter RosettaCon invited speaker (2024)
- Delivered SynBioUK workshop on protein design and engineering (2023)
- Invitation to deliver protein design lecture to Systems and Synthetic Biology MRes cohort (2023)
- Imperial Blyth Art scholarship award (2023)
- Awarded Innovate UK 6 month grant for novel protein-based fibre materials (2023)
- Best poster prize, Imperial Life Science Symposium (2023)
- Centenary Prize for MRes Systems and Synthetic Biology (2021)
- Imperial WOMEN SET Hackathon winner - best ARM related hack (2021)
- BBSRC Undergraduate Research Opportunities Programme (UROP) funding recipient (2019)