Daniella Pretorius

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Education

Massachusetts Institute of Technology   **Boston, U.S.A**
Visiting PhD student   *Mar 2024 - May 2024*
- Research collaboration visit

Imperial College London   **London, U.K**
PhD candidate in computational protein design and structural biology   *Oct 2021 - present*
- BioDesign CDT programme - EPSRC scholarship

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   **London, U.K**
PhD Researcher, Dr. James W. Murray group   *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   **Boston, U.S.A**
Visiting PhD student, Professor Sergey Ovchinnikov group   *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   **London, U.K**
Research collaborator   *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   **London, U.K / Jersey**
Head of Robotics and Automation   *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 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   **London, U.K**
Starting team member   *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 4 Undergraduate students in lab and computational research
- 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 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)