Matt Ball

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Skills

Programming Languages: Python, SQL, Rust, Java
Libraries: PyTorch, Scikit-Learn, Polars (Pandas), NumPy, SciPy

Education

AstraZeneca / University of Strasbourg, PhD: Cheminformatics Sep 2024 - Present

- Thesis title: 'Prediction of optimal reaction conditions using artificial intelligence tools'.

University of Cambridge, M.Sci: Chemistry June 2024

- *Awards:* Ranked 2/72 across university cohort; received departmental prize in Physical Chemistry and college prizes for exceptional exam performance; re-elected to college scholarship.
- *Relevant Courses:* Specialised in Computational, Organic and Physical Chemistry.

University of Cambridge, B.A: Natural Sciences June 2023

- *Awards:* Ranked 5/111 across university cohort; received college prizes for exceptional exam performance and elected to college scholarship every year across 3 years.
- *Relevant Courses:* Computational, Organic and Physical Chemistry. Multivariate and Vector Calculus, Linear Algebra, Group Theory, Probability Theory and Statistics.

Experience

Academic Researcher, AstraZeneca – Gothenburg, SE Sep 2024 – Present

- PhD Student in MolecularAI Group at AstraZeneca.
- Planned projects combining expert quantum chemistry features with custom deep-learning architectures for improved predictions of reaction outcomes.
- Worked in a dynamic, cross-functional environment with chemists, process engineers and ML engineers.

Student Researcher, Sormanni Lab – Cambridge, UK Sep 2023 – June 2024

- Developed a computational pipeline to determine possible binding geometries of small, rigid affinity proteins, implemented using Rust.
- Created data analysis and visualisation pipelines to streamline analysis of results.

Full-Stack Software Developer Intern, TPP – Leeds, UK July 2023 – Sep 2023

- Contributed to all parts of the software development life cycle, including the ideation, design, development and testing of multiple features.
- Handled electronic patient records and enabling national level analytics with clinical reporting tools for over 53 million patient records.
- Developed backend code for one of the top 5 largest SQL databases in the world.
- Improved technologies that bolstered public health initiatives and streamline clinical trial processes globally, using Agile methodologies

Publications

- Ball, M. et al. Predicting reaction conditions: a data-driven perspective. *Chem. Sci.* 16, 17523-17541 DOI: 10.1039.D5SC03045E (2025).