Audrius Kalpokas

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Computational chemist specializing in the intersection of biomolecular simulation and rigorous binding affinity prediction methods. Proven track record of developing robust, open-source software and scalable simulation protocols to accelerate the discovery of therapeutics.

Research Experience

PhD Researcher in Computational Chemistry — Edinburgh, UK
University of Edinburgh — *Sept 2022 – Present*

- Spearheaded the development of advanced biomolecular simulation methodologies (FEP/MD) for computational drug discovery.
- Established novel protocols for predicting drug resistance in highly flexible proteins and binding affinity for macrocyclic peptides, achieving state-of-the-art accuracy.
- Collaborated with industrial partners to integrate cutting-edge FEP methods into automated, proprietary drug discovery platforms.
- Contributed collaboratively via GitHub to major open-source scientific software packages, employing rigorous development practices including code reviews, unit testing, Docker, and CI/CD pipelines.
- Disseminated research findings through oral presentations and posters at major national and international conferences.

Computational Chemistry Intern — Cambridge, UK (Remote)
Cresset Biomolecular Discovery Ltd. — *Oct 2024 – Jan 2025*

- Designed and prototyped automated Python and Flare-based computational pipelines for predicting the 3D structures of PROTAC-induced ternary complexes.
- Contributed to protein-protein docking algorithms that were successfully integrated into the flagship product, Flare, directly enhancing predictive capabilities for customers.

Research Associate — Cardiff, UK
Cardiff University — *Jun 2021 – Sept 2022*

- Characterized the complex folding landscape of Ubiquitin using advanced enhanced-sampling molecular dynamics (Metadynamics/Umbrella Sampling), under the supervision of Dr. Stefano Leoni.
- Collaborated on the validation and conceptual development of a novel, Rust-based molecular dynamics engine.

Undergraduate Research Student — Maynooth, Ireland
Maynooth University — *Jun 2019 – Sept 2019*

- Investigated the catalytic mechanisms of transition metal organometallic compounds using Density Functional Theory (DFT), under the supervision of Dr. Tobias Krämer.
- Executed high-performance quantum chemical calculations using Gaussian 09 on the ICHEC Kay supercomputer to model complex reaction pathways.

Publications

Comparison of Scaffold Hopping Transformation Approaches for Relative Binding Free Energy Predictions — Expected Q3 2026

Modelling Macrocyclic Peptide PCSK9 Inhibitors with Alchemical Free Energy Calculations — Expected Q3 2026

Accurate Prediction of Drug Resistance for Intrinsically Disordered Protein Regions — 2025

- **A. Kalpokas**, M. Mackey, J. Michel; *J. Chem. Theory Comput.* 21 (24), 12497-12507

A shape changing tandem Rh (CNC) catalyst: preparation of bicyclo [4.2. 0] octa-1, 5, 7-trienes from terminal aryl alkynes — 2020

- C.M. Storey, **A. Kalpokas**, M.R. Gyton, T. Krämer, A.B. Chaplin; *Chemical Science* 11 (8), 2051-2057

Education

University of Edinburgh — Edinburgh, UK
Doctor of Philosophy in Computational Chemistry — *Sept 2022 – Expected Sept 2026*

Cardiff University — Cardiff, UK
MSc in Medicinal Chemistry — *Sept 2021 – Sept 2022*
Grade: Distinction

Maynooth University — Maynooth, Ireland
BSc (Hons) in Chemistry — *Sept 2016 – Sept 2020*

Leadership & Awards

Research Supervision: Mentored and supervised BSc, MSc, and PhD students, guiding them through computational workflows and project planning.

EPSRC iCASE Scholarship: Awarded competitive funding for PhD research on protein covalent modifications and machine learning.

Conference Awards:

- Best Poster Award at UK-QSAR 2026 Spring Meeting.
- Best Poster Runner-up (Physical Chemistry) at Joseph Black Conference 2025.
- Selected for Oral Presentation at YMF 2025.

Academic Service: Elected Class Representative during BSc and MSc studies, acting as the primary liaison between the student cohort and faculty.

Technical Skills

Languages: Python, C++, Bash, Cypher
Simulation & Modelling: OpenMM, GROMACS, BioSimSpace, Sire
Data Science & ML: Pandas, NumPy, Scikit-learn, Neo4j, Matplotlib
Cheminformatics: RDKit, PyMOL
Software Development & HPC: Git, Docker, CI/CD, Slurm, Linux

References

Prof. Julien Michel | Academic PhD Supervisor — University of Edinburgh
- Email: julien.michel@ed.ac.uk

Dr. Mark Mackey | Industrial PhD Supervisor — Cresset Biomolecular Discovery Ltd.
- Email: mark.mackey@cresset-group.com