

Audrius Kalpokas

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Computational chemist specializing in the intersection methodology development for rigorous binding affinity prediction methods and software engineering. 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

University of Edinburgh

Edinburgh, UK

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

Cresset Biomolecular Discovery Ltd.

Cambridge, UK (Remote)

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 University

Cardiff, UK

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 University

Maynooth, Ireland

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.

TECHNICAL SKILLS

Languages: Python, C++, Bash, Cypher

Simulation & Modelling: OpenMM, GROMACS, BioSimSpace, Sire

Data Science & ML: Pandas, NumPy, Scikit-learn, Neo4j, Matplotlib, LangGraph, MCP

Cheminformatics: RDKit, PyMOL

Software Development & HPC: Git, Docker, CI/CD, Slurm, Linux

PUBLICATIONS

The Logic of Alchemical Scaffold Hopping Transformations

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*Doctor of Philosophy in Computational Chemistry*

Edinburgh, UK

*Sept 2022 – Expected Sept 2026***Cardiff University***MSc in Medicinal Chemistry*

Grade: Distinction

Cardiff, UK

*Sept 2021 – Sept 2022***Maynooth University***BSc (Hons) in Chemistry*

Maynooth, Ireland

Sept 2016 – Sept 2020

LEADERSHIP & AWARDS

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

Team Leader at BioHackathon Edinburgh 2026 - Led a team focused on computer vision challenge.

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.