Anthony Nash BSc MSc MSc PhD MRSC

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I'm a computational chemist with a background in translational and multidisciplinary science, combining expertise in molecular dynamics simulations, quantum chemistry, and cheminformatics across diverse biomedical fields. My recent work encompasses molecular simulations, theoretical biophysics, and machine learning for compound identification and hit optimisation, with a focus on protein targets relevant to age-related diseases and azole-resistant fungal infections.

I have significant experience in protein sciences, particularly in protein stability and degradation pathways, as well as in medical mycology. I regularly work at the interface between experimentalists and software developers, translating biological questions into computational approaches and scalable tools. Alongside this, I've developed software solutions to interrogate large-scale medical datasets, including NHS records, to support drug repurposing, particularly in the context of migraine. I've led cross-functional teams in both Agile and traditional environments, built full-stack software architectures, and have working knowledge of multiple programming languages.

Industrial Employment

Senior Scientist in Computational Chemistry and Structural Biology (Nov 2023 - Feb 2025)
Kuano AI Ltd (UK)

- Leading cheminformatics software development (Python and C), integrated with Conda, GitHub, and Docker, running SLURM from Google Cloud and AWS.
- Leading pipeline development of quantum chemistry calculations with Fragment Molecule Orbital analysis for compound hit optimisation with a team of medicinal chemists.
- Leading collaboration with CRO and university partner in next-generation machine learning force field for molecular dynamics to hit optimisation, and benchmark platform development for polarised pharmacophore protein-ligand analysis combined with a small-molecule generative AI model.

Senior Data Scientist and Epidemiologist (Jun 2022 - Sep 2023)
Human Centric Drug Discovery

- Leading the software development of the company's medical data analysis platform. Integrating Python, R, NHS data (Clinical Practice Resource Datalink), and UK Biobank clinical records and human genomes.
- Mouse-model RNA sequence analysis and cheminformatics analysis of drug-response data from ChEMBL.
- Designed and submitted clinical epidemiology studies for review, prepared documents for scientific advisory board review, and pitched to investors (Fujitsu, Lilli Plc, Oxford Science Enterprises).

Senior Software Engineer and Technical Lead (Jun 2005 - Feb 2009)
R&D Department, Motorola Mobile Devices (UK)

Software Engineer (Sep 2004 - Jun 2005)
R&D Department, Sendo UK (Mobile Devices)

Academic Employment

Computational Chemistry Consultant (Mar 2023 – June 2025)
School of Molecular Sciences, Arizona State University

- Pharmacophore modelling, ligand-protein docking, protein-protein interactions (HADDOCK) and Molecular Dynamics (Gromacs and OpenMM) of the matrix metalloprotease superfamily.

- High-throughput of membrane protein domain analysis, combining Quantum chemistry (PSI4), Fragment Molecular Orbital analysis (GAMESS), and Python with MDAnalysis.
- Working within an HPC (Linux and SLURM), with Jupyter Lab and Apptainer (Docker) environments.

Senior Postdoctoral Research Associate in Medical Statistics (Aug 2019 - Jun 2022)
Nuffield Department of Clinical Neurosciences, University of Oxford

Postdoctoral Research Associate in Bioinformatics and Medical Statistics (Jul 2017 - Jul 2019)
Department of Physiology, Anatomy and Genetics, University of Oxford

Visiting Research Fellow (Jan 2016 - Oct 2017)
Department of Infectious Disease Epidemiology, Imperial College London

Postdoctoral Research Associate in Computational Chemistry (Nov 2013 - Jul 2017)
Department of Chemistry and The Royal National Orthopaedic Hospital, University College London

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Education

PhD Computational Mathematical Biology and Biophysical Chemistry (Sep 2010 - Sep 2013)
Molecular Organisation and Assembly in Cells, Department of Chemistry, University of Warwick.

Understanding the "Rules of Engagement" for Membrane Protein Folding: Chemical Biology and Computational Approaches for Determination of Structure and Dynamics.

MSc Mathematical Biology and Biophysical Chemistry (Sep 2009 - Sep 2010)
Molecular Organisation and Assembly in Cells, Department of Chemistry, University of Warwick.

MSc Natural Computing (Sep 2003 - Sep 2004)
Department of Computer Science, Birmingham University.

BSc Hons Artificial Intelligence with Computer Science (Oct 1998 - Jun 2002)
Computer Science Department, Birmingham City University.

Skills

Computational Protein and Molecular Design

Structural biology, crystallography, PDB, ChEMBL, PubChem, ZINC, DrugBank, RDKit, AlphaFold, Rosetta, I-TASSER, Schrodinger.

Computational Chemistry

Quantum chemistry calculation including transition state modelling and fragment molecular orbital interaction analysis, density function theory (DFT), semi-empirical methods, effective core potentials, natural orbital analysis, and quantum theory of atoms in molecules. Software packages include GAMESS-US, Gaussian, ORCA, and PSI4.

Molecular Modelling

Molecular Dynamics (proteins, nanoparticles, drugs/small molecules) with advanced and enhanced methods, including GROMACS, OpenMM, and AMBER. Protein-ligand docking using Autodock and Autodock Vina. Protein-Protein and Ligand-Protein free energy calculations (Umbrella Sampling, Steered MD, Free Energy Perturbation), advanced force field parameterisation (including transition metals). Several pharmacophore modelling approaches and QSAR analysis.

Artificial Intelligence

Molecular modelling with deep learning neural network potential energy functions, small-molecule generation using generative AI, protein structure characterisation with self-organising neural network maps, disease prognosis with random forest and naïve classifiers, and data curation for large language modelling of medical records.

Software development

Software architecture design (pattern design and unified modelling language), version control (GitHub and ClearCase), Python (including Pandas and scikit-learn), R, C/C++, Java, Perl. Development in PyCharm and JetBrains IDEs. Integrated AI-assisted code development. Cloud experience: AWS and Google Cloud.

Management and administrative

Preparing investor pitch slide decks, processes for ISO 2001 and ISO 2004 qualifications, applications for medical data acquisition and grant submissions, Agile scrum, and traditional management tools.

Outreach

Science Outreach Servers 2020 - 2021

During the COVID-19 pandemic, I founded a small charitable initiative that provided remote HPC access and mentoring for postgraduate students in Nepal. This enabled them to run computationally intensive bioinformatics and chemistry projects, leading to two students securing PhD positions in France and Australia.

Licenses, Patents, and Publications

- University of Warwick & AstraZeneca - software license. A self-organising neural network that calculates protein secondary structure content based on Circular Dichroism spectra.
- University of Oxford & Human Centric Drug Discovery - software licence. A medical statistics software platform that detects drug efficacy in patient electronic healthcare records.
- University of Oxford & Human Centric Drug Discovery - patent. A mechanism for drug discovery using survival analysis in CPRD health records.
- 38 peer-reviewed publications in computational chemistry and protein sciences.
