Anthony Nash BSc MSc MSc PhD MRSC

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Academic Employment

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

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

Honorary positions

Research Member of Common Room (Jun 2018 – Jun 2022)
Kellogg College, University of Oxford

Researcher (Jul 2017 - Jul 2018)
Department of Infectious Disease Epidemiology, Imperial College London

Consultancy

School of Molecular Sciences, Arizona State University (*Mar 2023 - on-going)*

Physics Department, Colorado School of Mines (*Nov 2022 - Mar 2023)*

Industrial and Start-up Employment

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

Senior Scientist (Jun 2022 - Sept 2023)
Human Centric Drug Discovery (University of Oxford Spin Out)

Company Director and bioinformatician (Jan 2018 - Oct 2018)
Helix Scientific Consulting Ltd

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

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

Consultancy

Crystal Health Ltd (Jun 2019 - Feb 2020)
University of Oxford (Start-up)

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.

Supervisors: Dr Ann Dixon and Dr Rebecca Notman.

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.

Publications

Summary (see attached Publication document)

Number of journal publications: 33

Number of conference proceedings: 6

Number of manuscripts in review (June 2025): 2

Total citations: 532

H-index: 16

Highest impact factor: Matrix Biology 11.58

Grants and Data Acquisition

Grant – NIH R01 ($1.14 million grant funds)

NIH R01 $1.14 million. "Allosteric control of collagen fibril degradation by matrix metalloprotease-1". Colorado School of Mines, US. Contributed preliminary works to the grant submission. I have been consulting, part-time, on this grant.

Grant – NIH R35 (submitted May 2025)

NIH R35 Research Strategy "Substrate-specific allosteric control of matrix metalloprotease". Arizona State University. Contributed preliminary works, study designs, concept, and write-up.

Microsoft equipment grant (received $25,000 in credit)

A Microsoft Research Foundation equipment grant (2015) of $25,000 to be spent on Microsoft Azure compute services. 2015, University College London.

CPRD Data Acquisition (value of £90,000)

Identifying coincident drugs that alter headache progression and remission (20_000279). 06-01-2022. For Human Centric Drug Discovery. I designed, contributed to preliminary works, and submitted the medical protocol.

CPRD Data Acquisition (value of £30,000)

Identifying coincident drugs that alter headache progression and remission (17_255). 05-03-2018. For the University of Oxford. I designed, contributed to preliminary works, and submitted the medical protocol.

UK Biobank Data Acquisition (value of £9,000)

Identifying coincident drugs that alter headache progression and remission (41284). 12-12-2018. For the University of Oxford. I designed, contributed to preliminary works, and submitted the medical protocol.

Skills

Computational chemistry and theoretical biophysics

- **Protein and Membrane Modelling:** Expertise in all-atom and coarse-grained simulations of proteins and multi-component lipid bilayers using conventional and enhanced MD (e.g., REMD, GaMD) across classical and machine learning-based force fields (e.g., AMBER, OPLS, neural network potentials).
- **Biophysical Method Development:** Developed custom analysis tools integrating MDAnalysis with GROMACS, AMBER, and OpenMM for advanced biophysical property calculations; supported by 20+ years of programming experience.
- **Computational Drug Discovery:** End-to-end pipeline development including generative ML for small-molecule libraries, pharmacophore mapping, virtual screening (orthosteric/allosteric), MM-PBSA rescoring, and alchemical/pathway free energy methods.
- **Quantum Interaction Analysis:** Quantum chemical analysis of molecular interactions using FMO, PSI4, GAMESS, and Gaussian to compute fragment-based energetic contributions.

Computational biology

- **RNA-Seq and GO Analysis:** Conducted RNA sequencing and downstream gene ontology analysis in mouse models for migraine research and drug discovery.
- **Drug-Induced Gene Expression Profiling:** Parsed LINCS whole-genome datasets to extract gene expression signatures under specific drug conditions.
- **Genome-Wide Association Studies:** Performed whole-genome analysis using UK Biobank data to identify genetic factors linked to disease phenotypes.

Medical statistics

- **Design and analysis of clinical epidemiology studies:** Including cross-sectional and longitudinal analyses of electronic health records, applying survival analysis to assess drug efficacy and disease outcomes, and statistical methods to investigate population health trends.
- **Preparation of clinical research protocols:** Collaborating with clinicians to develop study designs and documentation for submission to institutional ethics review boards.

Experimental

- **Experimental biophysics of soluble proteins:** PhD-level expertise in protein expression and purification, with application of circular dichroism, linear dichroism, and dynamic light scattering to characterize protein conformation and secondary structure.
- **Molecular biology techniques:** Proficient in plasmid design, cloning, and E. coli transformation for protein expression, with application of membrane-focused two-hybrid assays to quantify transmembrane domain interactions.

Administration/Business

- **Business and administration:** Trained in ISO 9001, ISO 27001, and the NHS Digital Protection Toolkit. Experienced in delivering investment pitches for university-affiliated startups, including Human Centric Drug Discovery. Skilled in project management methodologies, including Agile and Waterfall. Competent in conducting interviews and managing disciplinary procedures.

Teaching

Undergraduate lecture programs

Molecular Dynamics in Protein Sciences - Department of Physics, School of Mines, Colorado. Remote lecturing. Jan 2023 – March 2023

Theoretical approaches to studying the extracellular matrix - The Royal National Orthopaedic Hospital (UCL). In-person lecturing, setting exam questions, and marking. Mar 2016 – May 2016

Supervisory roles

MSc Digital Public Health - University of Oxford, Kellogg College and Green Templeton College. 2018 - 2022

MSc Digital Public Health and Pharmacology - Nuffield Department of Neurology, University of Oxford. 2021

MSc Clinical Neuroscience - Nuffield Department of Neurology, University of Oxford. 2021

PhD Single Molecule Biophysics - Department of Physics, School of Mines, Colorado. 2021 - 2023

Outreach

Science Outreach Servers 2020 - 2021

During the COVID-19 pandemic, I founded a small charity that provided online computational resources for post-graduate students from Nepal to run computationally intensive bioinformatic and computational chemistry experiments. Two postgraduates went on to undertake PhD studies abroad, in France and Australia.

Licenses and Patents

- 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.
