Nicholas J. Fowler

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I am a research associate in biophysics working at interface of computational and experimental structural biology. My current research involves applying mathematical rigidity theory to validate the accuracy of NMR protein structures. I am also investigating how rigidity theory can be used in model refinement and ensemble generation. I am looking to develop my skills in computational modelling and in the lab to solve problems in integrative structural biology.

Education

PhD Biophysics, University of Manchester   2014–2018
  Thesis: Investigating the role of electrostatic interactions in modulating protein function
  Supervisors: Jim Warwicker, Sam de Visser and Chris Blanford

MSc Physics, University of Manchester   2012–2014
  Thesis: Experimental confirmation of a Kibble-Zurek scaling law in a nematic liquid crystal
  Supervisors: Ingo Dierking and Tobias Galla

PGCE Physics Secondary, University of Manchester   2011–2012
  Dissertation: Teaching strategies enabling pupils with moderate learning difficulties to learn more effectively

BSc Physics, University of Manchester   2007–2010
  Dissertation: The physics of traffic jams

Research Experience

Research Associate, Molecular Biology and Biotechnology, University of Sheffield   2018–2021
  I developed a method, Accuracy of NMR Structures using Random Coil Index and Rigidity (ANSURR), to validate the accuracy NMR protein structures. It works by comparing local flexibility (i.e. per residue) as measured from chemical shifts to that computed from a structure using mathematical rigidity theory. The method is freely available here: github.com/nickjf/ANSURR. I am now working on a comprehensive analysis of the quality of all NMR structures published in the PDB. I am also investigating how rigidity theory might be applied in model refinement and ensemble generation.

PhD Biophysics, School of Chemistry, University of Manchester   2014–2018
  I used different levels of theory (e.g. QM/DFT, molecular dynamics and continuum electrostatics) to computationally model metal proteins with potential biotechnological applications. I developed a method to predict the reduction potential of copper protein mutants and experimentally tested these predictions using techniques in molecular biology and electrochemistry. I also used computational methods to investigate conformational change in an iron protein to complement an experimental investigation using double electron-electron resonance (DEER).

MSc Physics, School of Physics, University of Manchester   2012–2014
  I used nematic liquid crystals to validate a scaling relation for topological defect formation in symmetry-breaking phase transitions.

Publications

NJ Fowler, A Sljoka, MP Williamson. A method for validating the accuracy of NMR protein structures. *Nature Communications* 11, 6321 (2020).

N Iwakawa, NJ Baxter, DCC Wai, **NJ Fowler**, RAV Morales, K Sugase, RS Norton, MP Williamson. Conformational exchange in the potassium channel blocker ShK. *Scientific Reports* 9(1), 1-8 (2019).

E Fournier, S Tachon, **NJ Fowler**, G Gerbaud, P Mansuelle, P Dorlet, SP de Visser, V Belle, AJ Simaan, M Martinho. The Hunt for the Closed Conformation of the Fruit-Ripening Enzyme 1-Aminocyclopropane-1-carboxylic Oxidase: A Combined Electron Paramagnetic Resonance and Molecular Dynamics Study, *Chemistry–A European Journal* 25(60), 13766-13776 (2019). **(A 'Hot Paper' as chosen by editors)**

A Timmins, **NJ Fowler**, J Warwicker, GD Straganz, SP de Visser. Does substrate positioning affect the selectivity and reactivity in the hectochlorin biosynthesis halogenase? *Frontiers in chemistry* 6, 513 (2018).

NJ Fowler, CF Blanford, SP de Visser, J Warwicker. Features of reactive cysteines discovered through computation: from kinase inhibition to enrichment around protein degrons. *Scientific Reports* 7(1), 1-12 (2017).

NJ Fowler, CF Blanford, J Warwicker, SP de Visser. Prediction of reduction potentials of copper proteins with continuum electrostatics and density functional theory. *Chemistry–A European Journal* 23(61), 15436-15445 (2017).

NJ Fowler, I Dierking. Kibble–Zurek scaling during defect formation in a nematic liquid crystal. *ChemPhysChem* 18(7), 812-816 (2017).

Prizes and Awards

Summer Student Bursary (£2080), Physics of Life Network 2	2019
Biomedical Vacation Scholarship (£1600), Wellcome Trust (awarded but I declined)	2019
Travel Award, NMR in Biophysics and Molecular Biology, Uni. of Leeds	2019
Talk Prize and Travel Award, MGMS Young Modellers Forum, Uni. of Greenwich	2017
Talk Prize, School of Chemistry PhD Conference, Uni. of Manchester	2017
Talk Prize, BBSRC/MRC DTP PhD Conference, Uni. of Manchester	2017
Poster Prize, Reson8 2nd Biophysical and Biochemical Symposium, Uni. of Leeds	2017
Outstanding Contribution to Public Engagement, Better World Awards, Uni. of Manchester	2016
Talk Prize, Computational and Evolutionary Biology Symposium, Uni. of Manchester	2015
BBSRC DTP PhD Studentship	2014–2018

Research Activity

Poster/Flash Talk at Reson8 5th Biophysics and Biochemistry Symposium, Uni. of York Title: Is your NMR protein structure accurate? We have the ANSURR!	2020
Attended/Summer student Poster presented at Physics of Life Town meeting, The Royal Society	2019
Poster presented at the European Conference on Computational Biology, Uni. of Basel Title: Validating NMR protein structures using structural rigidity theory and random coil index	2019
Invited Seminar given at the European Bioinformatics Institute (EMBL-EBI), Cambridge Title: Validation of NMR protein structures using structural rigidity theory and random coil index	2019
Poster presented at NMR in biophysics and molecular biology conference, Uni. of Leeds	2019

Title: Validation of NMR protein structures using structural rigidity theory and random coil index

Talk given at Reson8 4th Biophysics and Biochemistry Symposium, Uni. of Sheffield   2019
  Title: Validation of NMR protein structures using structural rigidity theory and random coil index

Attended ICMRBS 2018, University College Dublin   2018

Academic Visit Kwansei Gakuin University and Osaka University, Japan   2018
  2 week visit to discuss project with collaborators and PDBj

Poster/Flash Talk at Reson8 3rd Biophysics and Biochemistry Symposium, Uni. of Manchester   2018
  Title: Features of reactive cysteines discovered from computation

Talk given at MGMS Young Modellers Forum, Uni. of Greenwich   2017
  Title: Prediction of reduction potentials of copper proteins with continuum electrostatics and
  density functional theory

Poster presented at QM/MM Methods and Applications, Uni. of Manchester   2017
  Title: Prediction of reduction potentials of copper proteins with continuum electrostatics and
  density functional theory

Talk given at BBRSC/MRC DTP PhD Conference, Uni. of Manchester   2017
  Title: Biophysical correlates of lysine acetylation

Talk given at School of Chemistry PhD Conference, Uni. of Manchester   2017
  Title: Prediction of reduction potentials of copper proteins with continuum electrostatics and
  density functional theory

Poster presented at Reson8 2nd Biophysics and Biochemistry Symposium, Uni. of Leeds   2017
  Title: Modulating the reduction potential of copper proteins

Poster presented at Protein Electrostatics Berlin, Freie Universität Berlin   2016
  Title: Modulating the reduction potential of copper proteins

Poster presented at Dalton 2016: Inorganic Reaction Mechanisms Discussion Group, Uni. of Oxford   2016
  Title: Modulating the reduction potential of copper proteins

Attended Reson8 Biophysics and Biochemistry Symposium, Uni. of Liverpool   2016

Talk given at Computational and Evolutionary Biology Symposium, Uni. of Manchester   2015
  Title: Modulating the reduction potential of copper protein mutants

Poster presented at British Liquid Crystal Society Annual Conference, Durham University   2014
  Title: Experimental confirmation of the Kibble-Zurek mechanism in a nematic liquid crystal

Teaching Experience

Level 1/level 2 tutor, Molecular Biology and Biotechnology, Uni. of Sheffield   2018–present
- Six six-student tutorials per year
- Mark essays, give feedback and facilitate discussion on how to write a scientific essay

Student supervision, Uni. of Manchester and Uni. of Sheffield   2015–present
- Devised and ran an 8 week project for an undergraduate Summer student
- Day-to-day supervision of two PhD, two MSc and three undergraduate students

Teaching assistant, Uni. of Manchester   2015-2017
- Helped deliver maths workshops for BBSRC PhD students
- Facilitated "Introduction to reaction mechanisms" tutorials for first year students
- Demonstrated how to run and analyse computational chemistry simulations in a workshop for final year students

Teacher of science, Loreto High School, Chorlton, Manchester   2012-2014
- Taught physics, chemistry and biology to pupils aged 11-16
- Graded 'Outstanding' according to Ofsted criteria

Private tutor   2012-2014
- Taught maths and physics at A level and maths, physics and chemistry at GCSE level

Administration Experience

ICMRBS Early Career Researcher Webinars   2020–present
- I jointly organise the monthly ICMRBS Early Career Researcher Webinars. Details can be found here: njfowler.com/icmrbs

Maintenance of Linux cluster   2018-present
- I maintain a cluster of 12 Linux computers used by the bioNMR group at the University of Sheffield

PhD and postdoc seminars   2019–2020
- I organised a monthly seminar for PhD students and postdocs department of Molecular Biology and Biotechnology.

Manchester Energy PhD conference   2017
- Organised and chaired the inaugural Manchester Energy PhD conference
- Secured funding from the University for printing, catering and prizes

Outreach and Public Engagement

Widening participation fellow, Uni. of Manchester   2014–2018
- Created and delivered workshops, talks and tutorials for University events, schools and science festivals aimed at children less likely to be considering higher education. Topics included astrobiology, protein synthesis, computational population dynamics, rocket building and electrochemical cells

Outreach events, Uni. of Manchester   2014–2018
- Participated in numerous outreach activities outside of my role as a widening participation fellow including training and managing science busking teams, presenting my research to the public at SciBAR events and judging a national science competition at the Big Bang Fair

Other Experience

Motivational speaker, various schools and colleges in Manchester   2017–2018
- Wrote and delivered interactive lectures talking about my experience of higher education and why students should consider going to University

Internship at Manchester Energy, Uni. of Manchester   2015
- Developed a 'Sim City' style computer game where the player controls the National Grid while trying to meet 2050 environmental targets