Callum Dickson

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WORK EXPERIENCE

2017 – Present, Investigator II, Computer Aided Drug Discovery, Novartis Institutes for Biomedical Research, Cambridge, MA, USA

Computational Chemist

- Working with project teams to understand and steer small molecule design.
- Application of chemoinformatics and molecular modelling tools, including docking, molecular dynamics, homology modelling.
- Particular focus on GPCRs, ion channels and other membrane protein targets.

2007 – 2008, Lead Discovery Department, Pfizer, Sandwich, UK

Computational Chemist (Industrial Trainee)

- Learned and applied different computational methods employed in drug discovery.
- Worked as part of a team, giving regular presentations to update the team on progress. Evaluated docking software for the virtual screening of fragment libraries and developed a Pipeline Pilot tool for the combinatorial growing of fragment hits.

EDUCATION

2014 – 2017, Presidential Postdoctoral Research Fellow, Computer Aided Drug Discovery, Novartis Institutes for Biomedical Research, Cambridge, MA, USA

Molecular dynamics simulation of GPCRs & small molecule permeation, waters in drug discovery, pharmacokinetic-pharmacodynamic models in drug discovery.

- Exploring ligand binding to GPCRs using molecular dynamics, developing structure-kinetic relationships of small molecule membrane permeation.
- Mechanistic PK/PD modelling, Markov models of ion channel gating.
- Supervisor: Dr Viktor Hornak.

2010 – 2014, Institute of Chemical Biology, *Imperial College London, UK*

PhD thesis: In silico prediction of non-specific binding.

- Simulating lipid bilayers as model cell membranes and studying the interaction of medical imaging pharmaceuticals with such membranes.
- Supervisors: Dr Ian R. Gould, Prof Antony Gee.
- Collaboration with the Ross Walker Lab at University of California San Diego/San Diego Supercomputer Center.
- Funded by Biotechnology and Biological Sciences Research Council and GlaxoSmithKline.

2009 – 2010, Imperial College London, UK

Masters of Research in Bioimaging Science (distinction)

- Gained in-depth knowledge concerning numerous medical imaging techniques; including positron emission tomography, MRI, ultrasound and CT scanning.
- Masters research project: Quantum chemical drug-lipid interaction energy as a predictor for non-specific binding.
- Supervisors: Dr Lula Rosso, Dr Ian R. Gould, Prof Antony Gee.

2004 – 2009, University of Edinburgh, Scotland, UK

Masters of Chemical Physics with Honours with Industrial Experience (first class)

- Masters research project: Modelling water movement through membrane-bound proteins.
- Supervisor: Dr Carole Morrison.

1998 – 2004, Balerno High School, Edinburgh, Scotland, UK

Five 'A' grades at Higher level: Maths, Chemistry, Physics, Geography and English.

RESEARCH EXPERIENCE AND TECHNICAL SKILLS

- Experience in python, MATLAB, C and Fortran99 programming and shell scripting.
- Advancing the molecular dynamics simulation of lipid bilayers using AMBER by developing robust parameters as part of academic research. Modifying the source code of AMBER to allow free energy of transfer calculations to be performed.
- Use of many different computational chemistry applications while at Novartis and previously Pfizer: Schrödinger software, OpenEye, MOE and Accelrys Pipeline Pilot.

PUBLICATIONS

Callum J. Dickson, Camilo Velez-Vega, Jose S. Duca, Revealing molecular determinants of hERG blocker and activator binding, *JCIM*, 2020, **60** (1), 192-203.

Clément Ghiazza, Thierry Billard, Callum J. Dickson, Anis Tlili, Christian Gampe, Chalcogen OCF3-isosteres Modulate Drug Properties without Introducing Inherent Liabilities, *ChemMedChem,* 2019, **14** (17), 1586-1589.

Lieyang Chen, Anthony Cruz, Steven Ramsey, Callum J. Dickson, Jose S. Duca, Viktor Hornak, David R. Koes, Tom Kurtzman, Hidden Bias in the DUD-E Dataset Leads to Misleading Performance of Deep Learning in Structure-Based Virtual Screening, *PLoS One*, 2019, **14** (8), e0220113.

Callum J. Dickson, Viktor Hornak, Dallas Bednarczyk, Jose S. Duca, Using membrane partitioning simulations to predict permeability of forty-nine drug-like molecules, *JCIM*, 2019, **59** (1), 236–244.

Magd Badaoui, Adam Kells, Carla Molteni, Callum J. Dickson, Viktor Hornak, Edina Rosta, Calculating Kinetic Rates and Membrane Permeability from Biased Simulations, *J. Phys. Chem. B*, 2018, **122** (49), 11571–11578.

Callum J. Dickson, Viktor Hornak, Robert A. Pearlstein, Jose S. Duca, Structure-kinetic relationships of passive membrane permeation from multiscale modelling, *J. Am. Chem. Soc.,* 2017, **139** (1), 442–452.

Robert A. Pearlstein, Callum J. Dickson, Viktor Hornak, Contributions of the membrane dipole potential to the function of voltage-gated cation channels and modulation by small molecule potentiators, *BBA Biomembranes,* 2017, **1859** (2), 177-194.

Michael R. Dent, Ismael Lopez Duarte, Callum J. Dickson, Phoom Chairatana, Harry Laurence Anderson, Ian R. Gould, Douglas Wylie, Aurimas Vysniauskas, Nicholas Jan Brooks and Marina Konstantinovna Kuimova, Imaging plasma membrane phase behaviour in live cells using a thiophene-based molecular rotor, *Chemical Communications*, 2016, **52**, 13269-13272.

Callum J. Dickson, Viktor Hornak, Camilo Velez-Vega, Daniel J. J. McKay, John Reilly, David A. Sandham, Duncan Shaw, Robin A. Fairhurst, Steven J. Charlton, David A. Sykes, Robert A. Pearlstein, Jose S. Duca, Uncoupling the structure-activity relationships of β2 adrenergic receptor ligands from membrane binding, J*ournal of Medicinal Chemistry,* 2016, **59** (12), 5780-5789.

- Highlighted on the Novartis "nerd blog": *https://www.nibr.com/stories/nerd-blog/tuning-drugs-succeed-cells-surface*

Åge A. Skjevik, Benjamin D. Madej, Callum J. Dickson, Charles Lin, Knut Teigen, Ross C. Walker, Ian R. Gould, Simulation of lipid bilayer self-assembly using all-atom lipid force fields, *Physical Chemistry Chemical Physics*, 2016, **18** (15), 10573-10584.
Michael R. Dent, Ismael López-Duarte, Callum J. Dickson, Niall D. Geoghegan, Jonathan M. Cooper, Ian R. Gould, Rob Krams, James A. Bull, Nicholas J. Brooks and Marina K. Kuimova, Imaging phase separation in model lipid membranes through the use of BODIPY based molecular rotors, *Physical Chemistry Chemical Physics,* 2015, **17**, 18393-18402.

Åge A. Skjevik, Benjamin D. Madej, Callum J. Dickson, Knut Teigen, Ross C. Walker and Ian R. Gould, All-atom lipid bilayer self-assembly with the AMBER and CHARMM lipid force fields, *Chemical Communications*, 2015, **51**, 4402-4405.

Callum J. Dickson, Benjamin D. Madej, Åge A. Skjevik, Robin M. Betz, Knut Teigen, Ian R. Gould and Ross C. Walker, Lipid14: The Amber Lipid Force Field, *Journal of Chemical Theory and Computation*, 2014, **10**, 865-879.

- 400+ citations, JCTC top 10 Most Read Article of 2014.

Callum J. Dickson, Lula Rosso, Robin M. Betz, Ross C. Walker and Ian R. Gould, GAFFlipid: a General Amber Force Field for the accurate molecular dynamics simulation of phospholipid, *Soft Matter*, 2012, **8**, 9617-9627.

- 100+ citations.

Callum J. Dickson, Antony D. Gee, Idriss Bennacef, Ian R. Gould and Lula Rosso, Further evaluation of quantum chemical methods for the prediction of non-specific binding of positron emission tomography tracers, *Physical Chemistry Chemical Physics*, 2011, **13**, 21552-21557.

CONFERENCES ATTENDED

Talks

Understanding passive membrane permeation with microscecond molecular dynamics, *255th American Chemical Society National Meeting & Exposition*, New Orleans, March 2018.

Structure-kinetic relationships of passive membrane permeation from multiscale modelling, *253rd American Chemical Society National Meeting & Exposition*, San Francisco, April 2017.

Uncoupling the structure-activity relationship of β2 adrenergic receptor ligands from membrane binding, *3rd NovAliX Conference: Biophysics in Drug Discovery*, Strasbourg, June 2016.

Uncoupling the structure-activity relationship of β2 adrenergic receptor ligands from membrane binding, *250th American Chemical Society National Meeting & Exposition*, Boston, August 2015.

Molecular dynamics simulation of lipid membranes with AMBER and application to the study of radioimaging pharmaceuticals, *27th Molecular Modelling Workshop,* Erlangen, February 2013.

- Awarded a €350 travel grant.

Posters

Callum Dickson, Viktor Hornak, Uncoupling the structure-activity relationship of β2 adrenergic receptor ligands from membrane binding. *GRC Molecular Pharmacology*, Ventura, February 2019.

Callum Dickson, Viktor Hornak, Camilo Velez-Vega, Dan McKay, Robert Pearlstein, Jose Duca, Uncoupling the structure-activity relationship of β2 adrenergic receptor ligands from membrane binding, *Computer Aided Drug Design Gordon Research Conference: New Frontiers in Computer-Aided Drug Design,* Vermont, July 2015.

- Selected for one of five highlight flash talks.

Callum Dickson, Viktor Hornak, Camilo Velez-Vega, Dan McKay, Robert Pearlstein, Jose Duca, Uncoupling the structure-activity relationship of β2 adrenergic receptor ligands from membrane binding, *CCG UGM & Conference*, Montreal, June 2015.

Callum Dickson, Antony Gee, Ian Gould, Molecular dynamics simulation of lipid membranes with AMBER and application to the study of radioimaging pharmaceuticals, *3rd Annual CCP-BioSim Conference, Frontiers of Biomolecular Simulation*, Edinburgh, May 2014.

Callum Dickson, Antony Gee, Ian Gould, Molecular dynamics simulation of lipid membranes with AMBER and application to the study of radioimaging pharmaceuticals, *Multiscale Modelling of Condensed Phase and Biological Systems*, Manchester, January 2014.

Callum J. Dickson, Lula Rosso, Ian R. Gould, Recent developments in the molecular dynamics simulation of lipid membranes using AMBER, *Faraday Discussions 161: Lipids and Membrane Biophysics*, London, September 2012.

- Awarded a £150 bursary to assist with attendance.

Callum J. Dickson, Lula Rosso, Ross Walker, Ian R. Gould, Lipid bilayer simulations: Expanding time and space with the General Amber Force Field, *243rd ACS National Meeting & Exposition*, San Diego, March 2012.

- Awarded a £400 travel grant to assist with attendance.

Callum Dickson, Ian R. Gould, Lula Rosso, Antony Gee, The relationship between drug-lipid interaction energy and non-specific binding, *19th International Symposium on Radiopharmaceutical Sciences,* Amsterdam, August 2011.

AWARDS

- Selected for the Imperial College Singapore summer school placement (2011): one week International Research Skills workshop at the National University of Singapore, followed by a three week research placement at the Bioinformatics Institute, Agency for Science, Technology and Research (A*STAR), Singapore.
- Awarded a Personal Achievement award by Pfizer for implementing a desktop docking tool which aided a department's drug discovery programme.