Christopher Michael Baker

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Postdoctoral Research Experience

2008-present School of Pharmacy, University of Maryland Baltimore

Postdoctoral fellow in the research group of Prof. Alexander MacKerell Jr., working primarily on the development of the Drude oscillator based CHARMM polarizable force field, with a particular interest in the development of parameters for the modelling of nucleic acids. A secondary project, in collaboration with the group of Dr. Jing Chen (Emory University) focuses on the computationally-assisted discovery of novel inhibitors of protein-protein interactions involving 14-3-3, a potential drug target for the treatment of human 8p11 myeloproliferative syndrome.

April-May 2008 CAS-MPG Partner Institute for Computational Biology, Shanghai
Institutes for Biological Sciences, Shanghai, China

Visiting researcher, Protein Mechanics and Evolution Group. Month-long research project employing statistical coupling analysis to investigate the correlation between evolutionary coupling of protein residues and protein function in von Willebrand Factor A-like proteins.

Education

2005-2006 Unilever Centre for Molecular Science Informatics, University of Cambridge

Visiting student; continuing my DPhil work in the research group of Dr. Guy Grant.

2003-2007 Physical and Theoretical Chemistry Laboratory, University of Oxford

DPhil (Oxford equivalent of PhD)

Working within the research group of Dr. Guy Grant and Prof. Graham Richards, and funded by the National Foundation for Cancer Research, my main research interest was the development of new force fields incorporating effects arising from non atom-centred charge distribution within molecules, with a particular view to improving the representation of aromatic interactions. A second area of research was in determining the role that aromatic interactions play in situations of biological importance, including the conformational behaviour of small molecule neurotransmitters and the recognition of nucleic acids by proteins.

1999-2003 Balliol College, University of Oxford

MChem (undergraduate masters in chemistry); 2.i

Included a year-long research project in computational chemistry, investigating secondary structure in carbohydrate based peptide mimetics using a combination of *ab initio* techniques and molecular dynamics.

Undergraduate Research Experience

June-September 2002 GlaxoSmithKline Medicines Research Centre, Stevenage, UK

Summer student, computational chemistry. Working in the computational chemistry department evaluating new techniques for the rational development of drugs, with a specific interest in the treatment of Alzheimer's disease (full details subject to confidentiality agreement).

Peer Reviewed Publications

13. Baker, C. M.; Anisimov, V. M.; MacKerell Jr., A. D. "Development of CHARMM Polarizable Force Field for Nucleic Acid Bases Based on the Classical Drude Oscillator Model" *J. Phys. Chem. B*, **2011**, *115*, 580-596.
12. Baker, C. M.; Lopes, P. E. M.; Zhu, X.; Roux, B.; MacKerell Jr., A. D. "Accurate Calculation of Hydration Free Energies using Pair-Specific Lennard-Jones Parameters in the CHARMM Drude Polarizable Force Field" *J. Chem. Theory Comput.*, **2010**, *6*, 1181-1198. *** Cover Article ***
11. Baker, C. M.; MacKerell Jr., A. D. "Polarizability Rescaling and atom-based Thole Scaling in the CHARMM Drude Polarizable Force Field for Ethers" *J. Mol. Model.*, **2010**, *16*, 567-576.
10. Banham, J. E.; Baker, C. M.; Ceola, S.; Day, I. J.; Grant, G. H.; Groenen, E. J. J.; Rodgers, C. T.; Jeschke, G.; Timmel, C. R. "Distance measurements in the borderline region of applicability of CW EPR and DEER: A model study on a homologous series of spin-labelled peptides" *J. Mag. Res.*, **2008**, *191*, 202-218.
9. Baker, C. M.; Grant, G. H. "The Effect of Solvation on Biomolecular Conformation: 2-Amino-1-phenylethanol" *J. Phys. Chem. B*, **2007**, *111*, 9940-9954.
8. Baker, C. M.; Grant, G. H. "Role of Aromatic Amino Acids in Protein-Nucleic Acid Recognition" *Biopolymers*, **2007**, *85*, 456-470.
7. Baker, C. M.; Grant, G. H. "Modeling Aromatic Liquids: Toluene, Phenol, and Pyridine" *J. Chem. Theory Comput.*, **2007**, *3*, 530-548.
6. Comméiras, L.; Moses, J. E.; Adlington, R. M.; Baldwin, J. E.; Cowley, A. R.; Baker, C. M.; Albrecht, B.; Grant, G. H. "Total synthesis of the epoxyquinol dimer (+)-panepophenanthrin: application of a diastereospecific biomimetic Diels-Alder dimerisation" *Tetrahedron*, **2006**, *62*, 9892-9901.
5. Baker, C. M.; Grant, G. H. "The Structure of Liquid Benzene" *J. Chem. Theory Comput.*, **2006**, *2*, 947-955.
4. Baker, C. M.; Grant, G. H. "A solvent induced mechanism for conformational change" *Chem. Commun.* **2006**, 1387-1389.
3. Macleod, N. A.; Butz, P.; Simons, J. P.; Grant, G. H.; Baker, C. M.; Tranter, G. E. "Structure, electronic circular dichroism and Raman optical activity in the gas phase and in solution: a computational and experimental investigation" *Phys. Chem. Chem. Phys.*, **2005**, *7*, 1432-1440.

2. Claridge, T. D. W.; Long, D. D.; Baker, C. M.; Odell, B.; Grant, G. H.; Edwards, A. A.; Tranter, G. E.; Fleet, G. W. J.; Smith, M. D. "Helix-Forming Carbohydrate Amino Acids" *J. Org. Chem.*, **2005**, *70*, 2082-2090.
1. Macleod, N. A.; Putz, P.; Simons, J. P.; Grant, G. H.; Baker, C. M.; Tranter, G. E. "Electronic Circular Dichroism Spectroscopy of 1-(R) Phenylethanol: The "Sector Rule" Revisited and an Exploration of Solvent Effects" *Isr. J. Chem.*, **2004**, *44*, 27-36.

Selected Conference Presentations

"Building a CHARMM polarizable force field for nucleic acids" a poster at "Frontiers in the Simulation of Macromolecules, Los Angeles, USA, November 2010.

"Building a CHARMM polarizable force field for nucleic acids" an oral presentation at the 238th ACS National Meeting, Washington DC, USA, August 2009

"The Moment of Truth? A New Model for Aromatic Interactions" an oral presentation at the MGMS international conference "Quantum Pharmacology – 30 years on" Oxford, UK, September 2006

"Modelling Aromatic Interactions" an oral presentation at the SCI conference "Modelling the Properties and Behaviour of Molecules" London, UK, September 2006

"The Role of the Aromatic Amino Acids in Protein-Nucleic Acid Recognition" a poster at the EMBO course "Proteins: Structure, Dynamics, Energetics…" Shanghai, China, May 2006

"Modelling Aromatic Interactions via Molecular Mechanics Simulation" a poster at the Keystone Symposium "Structure Based Drug Discovery" Whistler, Canada, April 2006

"Modelling Aromatic Interactions via Molecular Mechanics Simulation" an oral presentation at the MGMS "Young Modellers' Forum" London, UK, December 2005

"Computational Modelling of Aromatic Interactions" a poster at the GDCh-JCF "Frühjahrsymposium" Berlin, Germany, April 2005

Awards

- InhibOx Student Bursary: Quantum Pharmaology – 30 years on, September, 2006
- EMBO 2006 travel award
- Scholarship to attend Frühjahrsymposium 2005, Berlin
- Frühjahrsymposium 2005 poster prize

Hobbies/Interests

Mandarin. After completing a month long intensive course in Mandarin at the Beijing Language and Culture University, I continue to study at Baltimore Chinese School.

Travel. From October 2008 to July 2009, I spent nine months travelling around the world, an experience which I regard as an important, if less formal, part of my education.