

# Curriculum Vitae

**Stewart Alan Adcock**, MChem *Sheffield*, D.Phil. *Oxford*, AMRSC

## *Personal Details*

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**Date of Birth:** 23<sup>rd</sup> September, 1975      **Nationality:** British

## *Education*

**October 1998 - October 2001:** Physical and Theoretical Chemistry, University of Oxford, UK  
D.Phil. "Computer simulation of membrane bound molecules"

Doctoral research under the supervision of Prof. W. G. Richards of the University of Oxford and Dr. F. E. Blaney of SmithKline Beecham Pharmaceuticals (now GlaxoSmithKline Pharmaceuticals). Supported by a CASE award from SmithKline Beecham Pharmaceuticals and the EPSRC.

Thesis abstract is attached.

Additionally performed the role of system administrator in this research group.

**September 1994 - May 1998:** Department of Chemistry, University of Sheffield, UK  
MChem Chemistry with Study in Industry

A four year Master's degree, including a one year industrial placement in the Computational Chemistry and Molecular Modelling group at SmithKline Beecham Pharmaceuticals. Final year project involved investigation of a novel representation of molecular shape, in collaboration with Zeneca Pharmaceuticals (now Astra Zeneca). Awarded a 2.1 degree with honours.

**September 1992 - June 1994:** Eaton (City of Norwich) Sixth Form Centre, UK

Three 'A' Levels (Chemistry, Maths, Physics) at grade A.  
Awarded the Thomas Grout memorial prize for Chemistry.  
Norfolk County Scholar.

**September 1988 - June 1992:** Hethersett High School, UK

9 GCSEs (including Mathematics, Double Award Science, English Language and English Literature).  
Awarded the school prize for Mathematics.

## *Relevant Work Experience*

**October 2001 – Present:** Department of Chemistry and Biochemistry,  
University of California, San Diego.  
UC Postdoctoral Research Scholar.

Postdoctoral research under the supervision of Prof. J. A. McCammon. Primary projects are modelling of the transmembrane domain of the nicotinic acetylcholine receptor and the development of novel protein modelling techniques. Highlights of research to date include development of a knowledge-based forcefield for protein structures, implementation of a protein threading toolkit, and conception of a novel approach to protein sidechain modelling using neural networks.

**Ongoing:** Occasional consultancy contracts to the Biotech industry.

Syrrx, Inc. - Implementation and support of an in-house protein-ligand scoring function.

Syrrx, Inc. - Training and custom code modification for use of genetic algorithms for optimisation problems.

Cerebus, Ltd. - Intranet development.

**June 1998 - August 1998:** Zeneca Pharmaceuticals, Alderley Park, UK.

Further development of the code and methodologies produced during final year project at Sheffield University. This related to use of ellipsoidal Gaussian functions for the representation of molecular shape and the potential applications of this technology.

**August 1996 - August 1997:** SmithKline Beecham Pharmaceuticals, Harlow, UK.

One year working in the Computational Chemistry and Molecular Modelling Group at SmithKline Beecham. Investigated the use of Locally Dense Basis Sets in *Ab Initio* calculations, an approach to reduce the computational expense of quantum mechanical studies of interactions. Implemented an intranet interface for clustering and diversity analysis of combinatorial libraries, including a method to predict the suitability of given compounds for drug development. Assisted in the installation of combinatorial library design and analysis technology for Takeda Pharmaceuticals, including a role in the provision of training and support. Developed a system for automated semi-empirical calculations on drug-like molecules for future data-mining initiatives, utilizing otherwise unused desktop CPU cycles. This required programming of a load balancing daemon and automated methods for analysis of the extensive output generated. Within six months approximately 200 000 compounds had been processed. Implemented log P prediction software based on the method of Moriguchi. Studied topological indices for applicability in diversity analysis, QSAR studies and database indexing. Besides the implementation of several topological indices described in the scientific literature, developed some novel indices. Produced a method to generate chemical structures with desirable structural fingerprints and physio-chemical properties. Importantly, gained an appreciation of the work undertaken by a computational chemistry department within the pharmaceutical industry.

### **Skills**

- **Molecular Modelling** Experience in protein modelling and biomolecular simulations. Proficient with several molecular modelling packages, and typical applications used in research environments. Have used Tripos, Inc.'s Sybyl modelling package extensively. Have undertaken two training courses for Accelrys, Inc.'s Insight II modelling package. Expert in use of CCG, Inc.'s MOE modelling package, including the SVL scripting language and the C API.
- **Computational Chemistry** Undertaken projects in industry and academia relating to QSAR, combinatorial library design and ligand docking. Proficient with several molecular modelling packages, and the typical applications and utilities used in computational chemistry research environments. Knowledge of development with standard computational chemistry and cheminformatics libraries such as the Daylight toolkit and the CEX toolkit.
- **Computing** Experience of using personal computers with Microsoft Windows and high-performance workstations using various UNIX operating systems. Expert in Linux use and administration. As system administrator in a research environment, had responsibility for a highly heterogeneous network, which included design and maintenance of a Beowulf-style cluster. Also gained experience in the maintainance of common molecular modelling and computational chemistry software.
- **Software development** Considerable programming experience with C, Perl, S-Lang and PHP. Knowledge of many standard programming libraries, including OpenGL, the GTK+ windowing toolkit and the MPI parallel programming interface. Past or present involvement in several Open Source software projects with a variety of roles. Lead developer of GAUL, the 14<sup>th</sup> highest rated project at openscience.org. Was an active member of the former Xandros Desktop Linux beta-test team.

## ***Society Memberships***

- Associate member of the Royal Society of Chemistry, since 1994.
- Member of the Molecular Graphics and Modelling Society, since 1999.
- Member of the American Chemical Society, since 2001.

## ***Interests***

- Water sports, surfing.
- Rock climbing.
- Open Source computing.

## ***Scientific Publications***

### **Papers:**

- S. A. Adcock, "BB: Accurate reconstruction of protein backbones", *Bioinformatics*, submitted.
- S. A. Adcock, "Peptide backbone reconstruction using dead-end elimination and a knowledge-based forcefield", *Journal of Computational Chemistry*, in press.
- S. A. Adcock, F. E. Blaney, and W. G. Richards, "Automated approach for construction of lipid bilayers for simulation", ready for submission.

### **Posters:**

- S. A. Adcock, J. A. McCammon, "Utilizing structural constraints in protein loop modelling", May 2003, UCSD Academia-Industry Interaction Day, San Diego, CA, USA.
- S. A. Adcock, J. A. McCammon, "Structural prediction and modelling of peptide loops with geometric constraints", March 2003, 225<sup>th</sup> ACS National Meeting, New Orleans, LA, USA.
- S. A. Adcock, "HelGA: A flexible software package for the analysis, modelling and prediction of TM proteins", August 2002, 16<sup>th</sup> Symposium of the Protein Society, San Diego, CA, USA.
- S. A. Adcock, P. D. Lyne, F. E. Blaney, and W. G. Richards, "Automated construction of lipid bilayers for simulation", June 2000, Computational Biophysics 2000, Nice, France.
- S. A. Adcock, P. D. Lyne, "Construction of lipid bilayers for simulation", April 2000, 18<sup>th</sup> International MGMS Conference, York, UK.
- S. A. Adcock, P. D. Lyne, "Helix docking for transmembrane protein structure prediction", August 1999, WATOC-99, London, UK.
- S. A. Adcock, P. D. Lyne, "Prediction of helix packing", March 1999, OSCAR poster session, Oxford, UK.
- S. A. Adcock, B. T. Pickup, "A Gaussian representation of molecular shape", April 1998, Final project poster session, Sheffield, UK.

### **Significant, Publicly Available, Software:**

- "GAUL: Genetic Algorithm Utility Library", a programming library for evolutionary computation and optimisation, <http://gaul.sourceforge.net/>
- "nn\_util", an efficient programming library and standalone neural network simulator, [http://mccammon.ucsd.edu/~adcock/nn\\_util.html](http://mccammon.ucsd.edu/~adcock/nn_util.html)
- "SWiM: Stewart's window manager", a lightweight window manager for the X windowing system, <http://mccammon.ucsd.edu/~adcock/swim.html>

## ***References***

Contact details for referees are available upon request.