SABS Supervisor

Professor Garrett M. Morris, Co-Director, EPSRC & MRC Systems Approaches to Biomedical Science (SABS) Centre for Doctoral Training

Garrett's research interests are in methods development in computer-aided drug discovery, chiefly in high throughput docking, ligand-based virtual screening, network pharmacology, cheminformatics, bioinformatics, machine learning, and more recently protein engineering. He began as an Oxford undergraduate Chemist, completing his Part II and DPhil with W. Graham Richards. As an undergraduate, he developed Cameleon, the first ever graphical protein sequence analysis tool, which was one of the first academic software packages to be commercialized by Oxford Molecular plc, one of the first spinouts from the University of Oxford. In 1991 he moved to The Scripps Research Institute, California, USA, to work on protein-ligand docking and AutoDock, and in 2000 launched the first biomedical volunteer computing project, FightAIDS@Home, and later in 2005, using the open source BOINC platform helped IBM spawn other crowd-sourced biomedical projects with their World Community Grid. He moved back to the UK in 2008 to work in the University of Oxford spinout, InhibOx (now Oxford Drug Design), doing real-world drug discovery, where he spearheaded the use of cloud computing for high throughput cheminformatics, and developed software for ligand-based virtual screening, polypharmacological analysis, and side effect prediction; and then to Crysalin, another Oxford spinout, to develop novel protein engineering techniques for protein crystallization. He is now an Associate Professor and works closely with Prof. Deane in the Department of Statistics, and has been Co-Director of the EPSRC and MRC Systems Approaches to Biomedical Science (SABS) CDT since 2015.

Software Tools Developed

1. **AutoDock (http://autodock.scripps.edu)**
   AutoDock is a suite of automated docking tools, written in C++ and distributed under the Gnu GPL open source license. It is designed to predict how small molecules, such as substrates or potential drug candidates, bind to a receptor of known 3D structure. AutoDock is one of the most highly cited protein-ligand docking programs. Garrett worked with the Debian Med team to integrate it into the Linux operating system. AutoDock has had significant impact both in accelerating the development of other methods, and in identify lead compounds: see for example, the World Community Grid project, Help Fight Childhood Cancer and the discovery of a compound for the treatment of neuroblastoma. AutoDock has spawned new docking engines including AutoDock Vina and AutoDock FR.
2. **AutoDockTools (http://mgltools.scripps.edu)**
   AutoDockTools is graphical user interface for setting up protein-ligand docking experiments, launching AutoDock, and analyzing the results.
3. **WaterDock (http://sbcb.bioch.ox.ac.uk/waterdock/)**
   WaterDock is a fast and accurate method that predicts the location of water molecules in protein structures. The method's simplicity is the key to its speed; water molecules are docked into a structure using AutoDock Vina, low scoring sites are removed and the rest are clustered. The centroids of the clusters are the predicted water sites. WaterDock was developed by SABS IDC student, Greg Ross, and was co-supervised by Prof. Philip Biggin, and Garrett when he was at InhibOx.

SABS Students

Industrial SABS Supervisor

- Jean-Paul Ebejer (Marie Curie Fellow, SABS IDC)
- Greg Ross (SABS IDC)
- Sam Grayer (SABS IDC)
- Anthony Bradley (SABS IDC, Short Rotation Project)
- Saulo de Oliveira (SABS IDC, Short Rotation Project)

Academic Supervisor

- Hannah Patel (SABS CDT)
- Susan Leung (SABS CDT)
- Joseph Bluck (Systems Biology CDT)
- Fergus Boyles (SABS CDT)
- Anne Nierobisch (SABS CDT)
- Leung “Lucian” Sing Chan (Department of Statistics)

Software-related Contributions to the Research Community

- Secretary, Molecular Graphics and Modelling Society
- Advisory Board Member, **CCP-BioSim (Collaborative Computational Project for Biomolecular Simulation)**
- Advisor to **ELIXIR-UK**, at its Structural Bioinformatics Training Workshop, EMBL-European Bioinformatics Institute
- Scientific Advisory Board, EnzBond