**Bradley Anthony, Research Fellow, University of Oxford**

**Background**



I am a DPhil candidate in the Systems Approaches to Biomedical Sciences course at Oxford University. I graduated with an MChem in chemistry from Oxford University in 2010. I undertook a Part II under the supervision of Dr. Luet Wong in which I developed a novel biphasic system for the biotransformation of limonene to iso-piperitinol using a modified P450 enzyme. It was this early work with biological systems that lead me to want to work within biomedical research.

**Current work**

I am currently working at the Structural Genomics Consortium. My work is composed of a mixture of experimental and computational work. Experimentally I work within the Protein Crystallography group, developing fragment-soaking as a routine medium-throughput assay that can be used on novel protein-targets to gain an understanding of protein-ligand interactions and generate starting points for probe discovery. As part of my work I have developed a data-processing pipeline and result visualisation webapp to rapidly evaluate hundreds of datasets.

Computationally my work focusses on the development of knowledge-based methods to determine objective and efficient strategies for chemical probe development. I aim to combine structural data from X-ray crystallography with experimental activity data to produce predictive and descriptive models of protein-ligand binding. In this work I have developed a 3D Matched Molecular Pair tool, used to combine these two often disconnected data-sources. My work also aims to assess the extent to which current knowledge has efficiently tested available protein-ligand binding space and to suggest novel experimental work that might bridge current gaps. This work is carried out in collaboration with the Computational Chemistry department at GlaxoSmithKline in Stevenage under the supervision of Darren Green and Ian Wall.

**Research**

* Completed a Part II with Dr. Luet Wong in "Biotransformations of organic molecules involving engineered P450 enzymes"
* Completed a 10-week short project in: "Ab initio bromodomain Chemistry using fragment ensembles"
* Completed a 10-week short project in: "GPU accelerated ligand screening techniques"
* DPhil research project in: "The use of knowledge-based methods to understand protein-ligand interaction, towards improved inhibitor design" in the research group of Dr Brian Marsden at the Structural Genomics Consortium, co-supervised by Professor Charlotte Deane in the Department of Statistics.

**Talks, conferences and courses**

* Attended CUDA Programming on NVIDIA GPUs. From the e-infrastructure South Consortium, Oxford University.
* Spoke at the OeRC Many-Core Seminar Series on November 21st 2012 - "Accelerating Ligand-Based Virtual Screening Using a GPU
* Spoke at the second RDKit User Group Meeting on October 4th 2013 - "A 3D Matched Molecular Pair tool using the PDB, ChEMBL and RDKit"
* Winner of the poster prize at the DTC Final year conference, February 2014
* Winner of the Ludovico Award at Erice International School of Crystallography, May 2014
* Spoke at the SGC 10 Year Symposium, August 2014