Potential Supervisors

Dr. Brian Marsden, PI (Research Informatics), Structural Genomics Consortium (SGC) and Kennedy Institute of Rheumatology

Brian has led the Research Informatics group at the SGC in Oxford since 2004 where he is responsible for data management, sharing and dissemination for all aspects of the SGC's structural and chemical biology platforms. At the Kennedy Institute, he spearheads the use of open source data warehousing platforms to facilitate the capture, sharing and efficient analysis of molecular and clinical data in the context of translational research. He has a particular interest in computational structural biology with a focus on novel methods for aggregating, summarising and interactive sharing of small molecule/protein complex structures.

Software Tools Developed

CCF – a suite of entirely open-source web-based tools for hypothesis generation and prioritisation of medicinal chemistry optimisation of small molecule binders. It includes the following discrete components:

1) WONKA, summarises the key interactions between ligands and protein including structural water molecules from a large set of crystal structure ensembles. This platform has been downloaded from over 300 unique IP addresses worldwide and has been used within pharmaceutical companies as a complementary tool to summarise internal data.
2) OOMMPPAA, uses 3D matched-molecular pair methodology to superimpose activity data of small molecules within the context of structural data, thereby assisting in the prioritisation of directed optimisation of small molecules. This platform has been downloaded over 400 times from unique IP addresses.

Involvement of DTC Students

The CCF platform was developed by Anthony Bradley, who went on to join the RCSB PDB at UCSD in San Diego. He has now returned to Oxford to manage the XChem fragment-screening platform with the SGC and Diamond Light Source.