

The Bourne Laboratory – A Review of 2011

This year saw us publish 22 papers with 4 additional submitted and 2 more in the draft stage. This equals our record for one year and is something we should all be proud of. Stepping back from the last year to look at all years, the laboratory is approaching 20,000 Google Scholar citations (19,750 currently), which means we are having a very significant impact. Much of what we published this past year was a reconciliation of previous achievements. For example, for the PDB **Wolfgang Bluhm** led a paper on PDB quality assurance, **Peter Rose** a paper on PDB functionality as well as a paper on the evolution of the PDB. Our work in polypharmacology was characterized by three reviews led by **Lei Xie** and **Li Xie**. Similarly, **Julia Ponomarenko** and **Nikitas Papangelopoulos** published a paper on the structural aspects of the Immune Epitope Database (IEDB). As for original research **Jian Wang** published a proteomics paper on identifying peptides from mixture tandem mass spectra, **Ruben Valas** published a paper on the derivation of the superkingdoms, **Sarah Kinnings** published a paper on improving docking scores, **Apostol Gramada** a paper on course graining the electrostatic potential for large scale structure representation and **Thomas Evangelidis** a paper on the anti-cancer effects of Nelfinavir.

As usual it was an active year with a number of folks coming and going. **Spencer Bliven** joined the lab in January to work on the characterization of fold space and has already made an impact through collaborations, namely with **Andreas Prlic** with work on circular permutations and with **Philippe Youharabache** with work on characterizing pseudo symmetry. Spencer passed his qualifying exam in June. **Ruben Valas** left the lab early in the year after a very successful thesis comprising ten papers to take up a position at the J Craig Venter Institute and we are pleased he still drops by from time to time. **Boki Beran** and **Ben Yukich** left us in March and later in the year **Cole Christy** joined us and went to work on immediately fixing a number of systems issues that appeared in Boki and Ben's absence as well as define a new architecture for the PDB. **Apostol Gramada** left us this year after over ten wonderful years of service to the laboratory. His physics background and his alternative ways of thinking about protein structure are sorely missed.

Crystal Ku and **Hiruy Sibhatu** rotated with us in spring quarter and Crystal joined the lab to look at drug interactions with targets other than proteins. **Nan Zhang** also visited to experimentally validate our findings around new drug targets in *Mycobacterium tuberculosis*. We had a number of students this past summer, **Glorimar Castro Noriega** from Puerto Rico worked on our continued exploration of fold space, **Kunal Dhir** came from York University, UK and developed a new visualization application for exploring the PDB, **Alexander Hsieh** a UCSD undergraduate worked on a carbohydrate remediation project for the PDB and **Xiaolong Qiu** was a PRIME student working in Australia on looking at possible drug repurposing in the treatment of spinal muscular atrophy (SMA). In addition we had

two Google of summer codes students, **Jianjiong Gao** and **Dong Xu** who worked on the automatic assignment of post translational modifications with **Peter Rose** and **Andreas Prlic**. **Andrey Karney** and **Yinliang Zhang** joined the lab as a volunteer and as part of her PhD, respectively to work on drugome related studies.

Alex Gramos joined the PDB group to work on user interface issues and along with **Willy Suwato** continues to develop for SciVee. The latest product for 2012 is a podium capture technology using only a smart phone and Powerpoint presentation and having a direct upload to SciVee of a synchronized Podcast and slide presentation.

We were responsible for two important meetings in 2011 and contributed to a third. *Beyond the PDF* was held at UCSD in January and it was generally agreed that it had a very significant impact on how we think about scholarly communication. A follow-up meeting is likely in 2012. We took over a major organizational role for *3Dsig* which is held in conjunction with ISMB, this year in Vienna. We will continue this in 2012 in Long Beach CA. Finally the PDB celebrated 40 years with a *PDB40 Symposium* held where the PDB originated at Cold Spring Harbor laboratory on Long Island in NY. We should be very proud of our ever-increasing user base – now about 270,000 unique scientists per month. This past year has seen some every important PDB innovations under **Peter Rose's** scientific management and **Wolfgang Bluhm's** production management. A few are **Chunxiao Bi's** work on tabular reporting, **Greg Quinn's** work on supporting mobile devices, **Dimitris Dimitropoulos's** autocomplete search feature and ligand searching and **Andreas Prlic's** structure and sequence comparison and display.

On a less positive note this is our second year without a new grant. Fortunately, and because of the efforts of **Lei Xie** and **Li Xie** we have been able to secure contracts with Optima Pharmaceuticals, Limerick Pharmaceuticals and Johnson & Johnson (pending lawyer approval). We have also submitted and will continue to submit grants in broader areas that previously to secure funds. So all-in-all another fabulous effort and I thank everyone for their contributions, especially **Ann Kagehiro** who has worked so hard and efficiently to keep the ball moving forward.

Phil Bourne January 2, 2012