The Bourne Laboratory – A Review of 2012

This past year, we submitted 21 papers and 17 have been published already. We accrued about 2400 citations in 2012 according to Google Scholar; while many of these relate to PDB activities and our methods work with CE, SMAP and our collaborations with **Robert Preissner**, our systems pharmacology work is gaining traction and our work on the role of structure in studying evolution continues to have increasing impact.

It is fitting to start with our students. **John Bell** joined us as an exchange student from Monash University in the early part of the year and worked on SciVee interface developments. **Yann Heuber** came from the University of Nice and worked with **Lilia Lacoucheva** on autism-related SNP mapping to protein structures. His work also continued on as part of a grant led by **Lilia,** which included **Andreas Prlic** and **Spencer Bliven. Andreas** and **Spencer** also published the first PLOS Topic Page, which is a static version (the copy of record) of an identical dynamic version that is entered into Wikipedia. In this way, scientists get credit for their work (publication, PubMed entry) and Wikipedia is expanded in the much-needed area of computational biology. Over the summer, **Jenny Liang** joined us as an undergraduate prime student and went to work in Indonesia with **Habibah Wahab** on the role of natural products in treating Chagas disease. Other talented undergraduates, **Chirag Krishna** and **Douglas Myers-Turnbull,** worked with us all year and are both close to having their first papers written. **Chirag** on repositioning opportunities in the treatment of Chagas Disease; **Douglas** on domain-domain comparison in proteins. **Yinliag Zhang** continues her work with us, initially on the malaria drugome and now protein kinase binding pocket comparison; she too is close to her first paper with us. **Kieran Alden** returned to the lab for a period late in the year prior to starting a postdoc at Birmingham University to update and improve the pDomains resource that he developed with **Stella Veretnik**. **Roger Chang** completed his thesis on pioneering studies combining structural bioinformatics and systems biology and has gone off to a postdoc at Harvard. The paper we wrote together with **Lei Xie**, **Li Xie** and **Bernard Palsson** on the use of flux balance analysis to understand the off-target effects of Torcetrapib is gaining citations fast. Last and certainly not least among the students, **Jian Wang** continues his work with **Nuno Bandeira** on computational approaches, with a new paper under review, to unravel mass spectrometry data. This will have enormous impact on the field of proteomics in years to come.

The dynamic Xie[2] team of **Li Xie** and **Lei Xie** continues with 6 papers this year; including work with **Gabriel Haddad** on hypoxia and **Fiona Brinkman** on the role of Raloxifene attenuation on *Pseudomonas aeruginosa.* There was also an important review on polypharmacology with **Sarah Kinnings** who has now moved to Sequenon after a postdoc at UCSD.

The PDB's impact continues to rise and a recent survey of users shows a very diverse audience. **Peter Rose** led the way with a paper in NAR; **Cole Christie** has redesigned and implemented a completely new hardware/software system using virtual machines; **Dimitris Dimitropoulos** left us for Google after improving our search capability and contributing to an underlying architecture redesign. He will be missed. **Wolfgang Bluhm** continues to take major responsibility for our incredible PDB speed and reliability; **Alex Ramos** has provided us with improved usability, new timeline displays and the beginnings of a simplified user interface. **Andreas Prlic** and **Chunxaio Bi** have added lots of important features including new sequence feature displays and domain based structure comparison as well as new result displays. **Greg Quinn** has developed mobile apps for the iPhone and iPad and led the PDB to be the only biological resource to have a presence in the App Store.

Willy Suwanto and **Alex Ramos** continue their work on SciVee, this year releasing a new podium capture feature called TeachU. SciVee now has 28,000 subscribers.

Let us not forget our valuable collaborators. **Michael Baker,** who continues to be a valuable colleague. Congratulations on his Academic Senate grant that was awarded this past spring. Also to another valuable colleague, **Philippe Youkharibache** who, from afar, continues to teach us so much about symmetry in proteins which we will publish soon! Closer to home, **Julia Ponomarenko** who now charts here own course as an independent investigator and continues to work on the Immune Epitope Database among other projects.

We continued our work in scholarly communication with a grant from the Alfred P. Sloan Foundation in support of developing FORCE11, a community of like-minded folks interested in improving how we learn. **Marianne Martone** has been spear-heading that initiative and a second *Beyond the PDF* workshop will be held in Amsterdam early in 2013. Speaking of grants, we were awarded a NSF planning grant for a major new initiative *"Toward the 3D Virtual Cell".* The initial conference, with the objective of building a community supporting the structural and simulation of a cellular environment, took place in December and was deemed highly successful. Kudos to **Stephanie Hagstrom** for all her hard work; it is great to have her working with us again after so many years. (We worked on the ISMB conference in 2000). Also to **Sharon Franks,** who is helping with the 3DVC, and is a great new colleague from the Vice Chancellor for Research's office.

A major change for me this year was taking on the role of Associate Vice Chancellor for Innovation and Industrial Alliances. In balancing this, I reduced my role with PLOS to that of an advisor and a selective number of new projects. There are aspects of this change that are positive for the lab. For example, we will be leading an institutional response to a call from the Gordon and Betty Moore Foundation and the Sloan Foundation for a data science initiative, hopefully leading to a Data Sciences Department or Center. There are other initiatives in 2013 to look forward to: In collaboration with **Yolanada Gil** from USC, we submitted an NSF grant for work in discovery informatics, and in collaboration with **Shuchi Dutta** from

Rutgers, we submitted a training grant for a summer program in structural and computational biology.

This past year was also a year of premature loss. We lost our collaborator (and my squash partner) **Virgil Woods** to brain cancer at the age of 64, and **Lee Dirks** of Microsoft and his wife, were tragically lost in a car crash in Peru.

On a positive note, we welcome our Norwegian colleagues **Tor Gjoen** and **Anne Simonsen,** who have added vitality to our laboratory.

Last but never least, **Ann Kagehiro**, who has suffered through my new role as AVC, and continues to hold us all together.

With some good science in the works, the PDB having a non-competitive renewal, and with the 3D Virtual Cell project starting to take off, I am sure that 2013 will be another good year for the lab. Thank you for all your hard work.

Phil Bourne, December 29, 2012