

2010

"It was the best of times, it was the worst of times, it was the age of wisdom, it was the age of foolishness, it was the epoch of belief, it was the epoch of incredulity, it was the season of Light, it was the season of Darkness, it was the spring of hope, it was the winter of despair, we had everything before us, we had nothing before us ..."

Charles Dickens A Tale of Two Cities

Loosely translated papers and you are the light; grants are the darkness. Consider the year in numbers and more:

- Papers 31 (highest ever) – 20 papers actually out and 11 submitted or under revision all of which will be published. That's without papers published separate from the lab by **JianWang** and **Julia Ponomarenko**.
- Our work received over 1500 citations this year.
- Our resources (PDB, IEDB, SciVee, pDomains etc.) are accessed by over 250,000 unique users every month and those users download the equivalent of ¼ of the US Library of Congress each month.
- Thanks to the hard work of **Ann Kagehiro** (not to mention everything else she does for us), at least six grants were submitted; unfortunately none were funded.
- There were a couple of press releases around our work, notably the TB drugome.
- **Lei Xie** got an Assistant Professorship at CUNY and will leave us next June.
- **Ruben Valas PhD** graduated with ten papers and got a position at the J. Craig Venter Institute.
- **Sarah Kinnings PhD** graduated and joined Wei Wang's lab at UCSD.
- **Satnam Surae MS** graduated and started his PhD with Jens Neilsen in Ireland.
- **Spencer Bliven** did a rotation and joins the lab in Jan. 2011 as a PhD student to work on practical applications of protein fold space.
- **Robert Preissner** visited us for several months on sabbatical from Charite in Berlin and we published a paper together.
- **Ricky Lozano** did a PRIME project with us while in Melbourne, Australia.
- SciVee signed a contract with Thompson Reuters and a whole new white label website was developed.
- **Zhangyang Zhu** left the lab to join Teradata.
- **Rika Yatchak** left to pursue graduate studies in the Bay area.
- The PDB had a very successful mid-cycle review.
- **Teddy O'Brien** rotated with us.
- We submitted two papers that I believe are the first between clinical faculty (**Grace Kuo, Joseph Ma** and **Grace Kelly**) and basic science faculty at SSPPS.

Looking beyond the bullets to the focus of our efforts lets start with the PDB, which is the foundation for much of our research. **Peter Rose, Wolfgang Bluhm, Greg Quinn** and **Andreas Prlic** (2) led the writing of some important papers on PDB developments, including mobile support, and reviewers confirmed our belief that the PDB team (in Rutgers and San Diego) has done an outstanding job in making us the biological database that others look too. **Chunxiao Bi** contributed new ways at looking at query results, **Dimitris Dimitropoulos** contributed important revisions to the underlying architecture, **Ben Yukich** kept everything running smoothly and **Boki Beran** continues to add amazing interface developments. Most importantly the PDB is a great team and assigning developments to any one person is a bit silly as everyone contributes to all that is done.

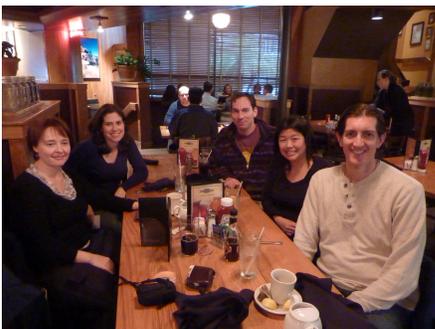
Since 2005 our work in evolution through the lineage of **Song Yang**, **Chris Dupont** and finally **Ruben Valas** has made some important contributions. Song's original 2005 PNAS paper has been cited over 100 times. This year Ruben made a plea for the tree of life and later for the origins of Archaea both based on a variety of data analyzed with bioinformatics tools in a way rarely used by evolutionary biologists. A lasting memory will be the perception that **Russ Doolittle**, **Bill Loomis** and **Milton Saier** were all at his feet during the closed thesis defense. The scene only lacked one thing **Thomas Cavalier-Smith**. I am hopeful that with Chris and Ruben both at JCVI and new students coming in, we can continue work in this area.

Our leadership role in polypharmacology and the application of systems biology to drug discovery is exemplified by the four papers published and four under review in work led by **Lei Xie**, **Li Xie** and **Sarah Kinnings** and including **Roger Chang** and **Josh Lerman** from **Bernard Palsson's** laboratory, and **Jacob Durrant** from **Andy McCammon's** Lab, as well as a variety of other collaborators. This says nothing of the four reviews we are also working on in areas of off-targeting, side-effects and drug repositioning. Lei's leadership here is exemplary and we already have a collaborative grant under review for when he starts at CUNY.

In the more fundamental aspects of protein structure, **Apostol Gramada** has turned his attention to the application of multipole techniques in course graining large macromolecular systems in a paper under review and **Kieran Alden** and **Stella Veretnik** made available their pDomains server for the important task of determining the number and boundaries of 3D domains in proteins.

In the world of immunology **Julia Ponomarenko** and **Nikitas Papangelopoulos** continued to contribute to the IEDB database as well as Julia contributing to an analysis of methods for prediction peptide binding to MHC class II molecules. We will continue with our collaboration with LIAI as we prepare the IEDB renewal grant.

In our work in scholarly communication the journal *PLoS Comp Biol* continues to thrive with a 17% increase in number of submissions over 2009. It is nice to know the laboratory is strongly identified with the highest impact journal in our field. Under the guidance or **Marc Friedmann** and with the work of **Alex Gramos** and **Willy Suwanto**, SciVee continued to grow in 2010 with about a 5% increase in number of users and content per month. Four of the five major science publishers are currently doing trials with SciVee to determine whether they will use it as a video resource in support of publications. **Lynn Fink** and **Greg Quinn** had significant impact with their Word plug-in for semantic tagging and we are hosting what we hope will be a seminal workshop in January 2011 titled Beyond the PDF. The goal of the workshop is to be thinking about comprehending science in ways beyond the traditional research article.



Lastly let us take a look at how a few of the former lab members are doing. **Kristine Breidis** (2nd from left) is a software engineer at Accelrys; **Jenny Gu** (2nd from right) is a Humboldt Fellow in Munster Germany and Eric Scheeff is a postdoc at the Salk Institute. The photo (also on the [labs Facebook page](#)) was taken at Rock Bottom on December 29, 2010 illustrating that the lab is like the Hotel California "you can check-out anytime you like, but you can never leave."