2009

In many respects this was an excellent year for the laboratory. Twenty-eight publications either published, in press or submitted. This included several chapters in two books: the second edition of *Structural Bioinformatics* for which former laboratory member **Jenny Gu** contributed greatly; and *Pharmacy Informatics* with **Phil Anderson** and **Sue McGuinness** which is the textbook for the course of the same name we offer to first year pharmacy students in the spring quarter. Conversely, it was a poor year for funding. We submitted eight grants, none of which were funded. Five were part of the recovery act initiative. This mirrors what other laboratories have reported and may be a sign of hard times ahead. We have two grants pending now, **Apostol Gramada's** multi-scale modeling proposal building on multipole analysis and **Lei Xie's** application to the Gates Foundation for work on TB. Other grants are in the pipeline to see us through these hard times. On a more positive note the journal we co-founded, *PLoS Computational Biology,* continues to be the highest impact journal in our field. The new year will see the start of a "Roots in" series in the journal which traces the beginnings of our field and will be interesting reading for us all.

Equally positive is our work on the PDB. We started a new five-year award at the beginning of this year and have already accomplished a significant number of the five-year deliverables under **Peter Rose's** management. Most recently **Dimitris Dimitropoulos** from EBI and **Chunxaio Bi** from Rutgers joined the PDB group and are already making significant contributions. **Andreas Prlic** has contributed two papers, including extensions to BioLit for database-literature integration, a project that was so well done by **Lynn Fink** and **Marco Martinez**, who both left the lab this past year. Lynn continues to work with us through early morning skype calls from Australia. **Boki Beran** has reworked the PDB interface to great acclaim and **Greg Quinn** has converted all web content to a content management system for ease of management and adding new content. **Ben Yukich** and **Rika Yatchak** have kept everything running and last, but not least in the PDB world, **Wolfgang Bluhm** has contributed important code developments (finally fulfilling his wish thanks to team support) as well as keeping the PDB production systems running. The new year will

see new views on the PDB data, including a drug view that is important to our other endeavors and the resurrection of CE as a structure comparison tool.

Stella Veretnik also left us this year, albeit only physically, but not before publishing an important paper on the Sm/Lsm gene family. She continues to work with us remotely and mentored **Kieren Alden** one of our trusty York students this summer in a consensus 3-D protein domain analysis that will be published in 2010. Our other York students **Qian Ye** and **Natalie Dawson** as well as Kieran all graduated and are pursuing PhDs. **Jian Wang** successfully defended his minor proposition on using cross-linking and mass spectrometry and judging by the enthusiasm of the committee is expected to do great things. **Ruben Valas** continued his battle with the old men of evolutionary biology in his quest to save the tree of life, first with a paper questioning Lake's work on polarizing indels in *Biology Direct* and with a soon to be submitted paper arguing that the consideration of functional evolution is as important, if not more so, than a purely genomic analysis. The role that structure has to play in understanding evolution was further enforced with a book chapter, a review and a research paper by the dynamic duo of Ruben and **Song Yang**. Song is now a postdoctoral fellow in systems biology with Herbert Sauro at the University of Washington, Seattle. Structure also has a role in further work, currently under review at PNAS, led by **Chris Dupont** using data from **Andy Butcher** on the interplay between evolution and the environment.

SciVee continues to evolve thanks to Lynn, **Alex Ramos** and **Willy Suwanto** on the academic side and **Marc Friedmann** and **Ken Liu** on the business side and now has about 60,000 unique users per month and growing. We have learnt a lot about running academic websites by trying to commercialize a site through contracts with companies in the STM publishing market. It is much easier with grant funding!

Our immunology research continues to do well in the capable hands of **Julia Ponomarenko** and **Zhanyang Zu.** Aside from joint papers and a book chapter this year, Julia also had a paper in PNAS, a tribute to her independent success. Speaking of independence, first, **Nikitas Papangelopoulos** left the Immune Epitope Database project and is now part of the bioinformatics graduate program at UCSD where we expect great things. Second, **Michael Baker** and **Betty Shih** have their own independent work, but share time and experience with us and are great assets to the lab.

Our work in network pharmacology is regarded as pioneering and has gained considerable attention in the both the literature, with six papers this year, and the blogosphere. Thanks to **Lei Xie** and **Li Xie** for the foundation that has made all this possible. **Sarah Kinnings**, an ex-Yorkie, was kind enough to leave the comfort of her PhD in Leeds to spend six months with us and, aside from the TB paper from her Yorkie days, has contributed to at least two forthcoming publications on developing drug-receptor interaction networks, a protocol we will be pushing this year for the treatment of pathogenic neglected diseases. A theme we also have followed in collaboration with Jabob Durrant and Andy McCammon in determining the side effects of an NCE against sleeping sickness. **Thomas Evangelidis** another ex-Yorkie worked on a drug repositioning project and **Roger Chang** a bioinformatics rotation student took our work

to the next level through the construction of a metabolic kidney model for the dynamic examination of off-targeting.

All in all not a bad year! One last acknowledgement to the person who always gets mentioned last but in many ways should be first, **Ann Kagehiro** who holds it all together.