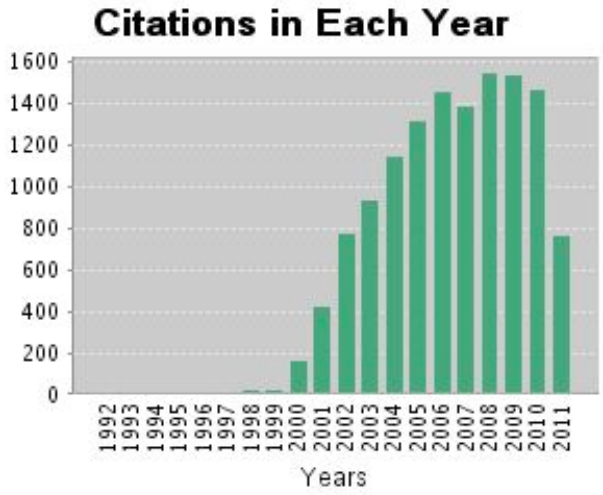
Lab Accomplishments 2008 - 2011

- Published **46** peer reviewed papers (**9** additional under review or accepted).
- Published an additional **9** editorials, commentaries and articles on professional development. The latter have been downloaded over **300,000** times from PLoS.
- Received **4556** citations (data from Web of Science) in the last 3 years – more than many UC science professors accumulate in their whole careers.
- Currently hold grants worth **$16.4** million with 3 RO1's and 1 SBIR pending.
- Received four major career awards in four different disciplines:
    - Fellow of the American Association for the Advancement of Science (2011) for contributions to pharmacology.
    - Fellow of the International Society for Computational Biology (2011) for contributions to computational biology and bioinformatics.
    - The Jim Gray eScience Award from Microsoft (2010) for contributions to information and computer science.
    - The Benjamin Franklin Award (2009) for contributions to open science.
- Developed and supported web sites (PDB, SciVee, IEDB) used by over 225,000 scientists every month who collectively download data equivalent to one quarter of the US Library of Congress.
- Saw the journal PLoS Computational Biology maintain number one ranking in the field of computational biology with an impact factor of ~6.
- Co-edited and published several chapters in the book *Pharmacy Informatics* from Taylor & Francis that is the textbook for our course SPPS205.
- Co-edited and published several chapters in a second edition of the book *Structural Bioinformatics* from Wiley which is used in my course PHAR201.
- Directed **3** courses each year (Phar201, SPPS205, Phar221).
- Delivered **37** invited lectures (**12** internationally).
- Graduated 2 PhD and 4 Masters students (the latter through York University, UK).
- Organized a workshop *Beyond the PDF* in early 2011 attended by 100 people and which was considered a very important event in changing scholarly communication in the digital age.
- Took over as on-going Scientific Chair for 3Dsig, considered the premier international conference in structural bioinformatics.
- Chaired or co-chaired two UCSD Senate committees and participated in a number of others.

More detail is provided on a few of these points.

Research



Results found:	159
Sum of the Times Cited [?] :	13,131
View Citing Articles View without self-citations	
Average Citations per Item [?] :	82.58
h-index [?] :	30

Our work has consistently achieved approximately 1,500 citations per year (see Fig. source Thomson Reuters) over the past 3 years. While many of the citations come from the data resources maintained by the laboratory, we have impacted five distinct fields in the past three years with fundamental contributions as follows.

Drug Discovery – In the prior period we established a methodology for determining off-targets for existing drugs and lead compounds which may explain side effects or suggest possible drug repositioning strategies. We have applied this methodology in ~ 15 papers over the past 3 years. Notable are our landmark efforts in explaining polypharmacology at a systems level (with Bernhard Palsson *Plos Comp. Biol.* 2010 6(9): e1000938), computation of the complete TB drugome (*PLoS Comp. Biol.* 2010 6(11): e1000976), a hypothesis concerning drug action through broad based low affinity binding to kinases (featured in *Science* 2011 332(6030) 648-649) and an improved docking strategy (*J. Chem. Info. Model*. 2011 51(2), 408-419).

Evolution – In the prior period we established protein structure as a fundamental tool in the study of evolution. We have now integrated other type of on-line data into our study including functional and cellular location information. With these tools we have contributed to a further understanding of the impact of environmental change on evolution (*PNAS*, 2011 doi: 10.1073/pnas.0912491107), the major divisions of life and when they emerged (*Biology Direct* 2011 6:16; *Biology Direct*, 2010 5:44) including the rooting of the tree of life (*Biology Direct*. 2009 4(1) 30).

Scholarly Communication – We have been very active in supporting the belief that the dissemination and comprehension of science could be much improved in the Internet era beyond the traditional printed and PDF form. We have shown this in our work on integrating literature into the PDB **(***BMC Bioinformatics* 2010 11:220) and developing tools that allow new discoveries from open access literature *NAR* 2010 36(S2) W385-389). This led to the Benjamin Franklin award in 2009, for trying to live up to the philosophies of Franklin (he is assumed responsible for the first public library in the United States). We have also written widely on the subject of new modes of publishing (e.g., *PLoS Comp Biol* 6(5): e1000787; *Serials 2011, accepted)*.

Immunology – Aside from contributions to the Immune Epitope Database (*NAR*. 2011, 39 D1164-70), which is attempting to catalogue all reported B and T cell epitopes, we have reviewed our ability and that of others to predict peptide binding to MHC class II molecules **(***PLoS ONE* 2010 5(2): e9272).

Allostery, protein-protein interactions, protein-ligand interactions protein classification, protein fold space –Areas in which we continue to have impact with ~ 10 new papers. For example algorithms to detect circular permutations in proteins (*Bioinformatics* 2010 10.1093/bioinformatics/btq572), algorithms to resolve mixtures of cross-linked peptides in mixture tandem mass spectrometry data (2011, under review) and determination of domains in 3D structures (*BMC Bioinformatics*, 2010 11:310).

Teaching

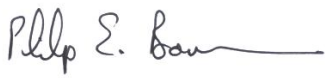
We have continued to direct and teach three courses:

1. PHAR201 (Biological Data and Analysis Tools) in the fall quarter is one of the four core courses in the Systems Biology and Bioinformatics graduate program and I teach 85% of the lectures.
2. SPPS205 (Pharmacy Informatics) is a required course in the spring quarter for all first year PharmD students and I teach 20% of the lectures.
3. BIOM221 Professional Development is an elective that I taught in the winter quarter of 2009 and 2011 to BMS and bioinformatics graduate students.

We have given guest lectures in MED260, BIOM202 and PHAR202. We push the students towards original thinking, which is not always popular relative to rote learning, but teaching evaluations are usually excellent.

University/Public

We have co-chaired or chaired two senate committees in this period, The Joint Senate Administration Task Force on University Industry Relations and the Senate Library Committee. Both have been challenging in this time of budget cuts and changing perceptions by faculty and by the public.. Outside of the University we continue the role as inaugural Editor in Chief of PLoS Computational Biology now in its seventh year. We also participate in a number of Advisory Boards, most notably Microsoft Research and the National Library of Medicines, PubMed Central.



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