New Arrivals

Kihara Lab: Muyi Liu, joined from the PULSe program

Dr. Hyungrae Kim, postdoc, joined from September 1st. Hyungrae received his PhD from Korea Advanced Institute of Science and Technology (KAIST) and formerly was associate scientist at Academy of Sciences of the Czech Republic.

Mario Messih, summer intern student from King Abdullah University of Science and Technology, Saudi Arabia. He worked from July 1st to August 30th.

Gribskov Lab: Biaobin Jiang and Junhui Wang joined the Lab.

Rossmann Lab: Ju Sheng joined the Rossmann lab in March and is managing the Rossmann BSL-2 area as well as training for BSL-3 level work. Ju has M.S. degrees from both the University of Windsor (Canada) and Ocean University of Qingdao (P.R. China). She comes to Purdue from Henry Ford Hospital (Detroit, MI) where she was a senior research assistant and laboratory manager.

Kuhn Lab: Crysta Colangelo and Devika Sirohi (PULSe) joined our lab in April 2011.

We presently have three students, Andrea Ray, Nicole Davis and Renee Wenig as PULSe Fall rotations in the lab. Renee Wenig is collaborating with our lab and Jason Lanman’s lab on some projects.

Departures

Kihara Lab: Mateusz Kurcinski, he is now back in Warsaw, Poland.

Dr. Sael Lee, she starts her new position at Samsung Bioinformatics Institute in Korea.

Satwica Yersini, intern student from Vellore Institute of Technology, India. She worked in Kihara group from December 2010 to May 2011. She is now in the Bioinformatics program at Indiana University, Bloomington, IN, from Fall 2011 semester.

Kuhn Lab: Visiting faculty member Young-Min Lee and post-doctoral fellow Byung-HaK Song have returned back to Chungbuk National Laboratory, Laboratory of Molecular Virology, Department of Microbiology, Cheongju, South Korea, and will be moving to University of Utah in the fall.

Mansoora Khaliq left in February to join ImQuest Biosciences in Frederick, MD as a post-doctoral fellow.

Visitors

Rossmann Lab: Alasdair Steven, NIAMS, National Institutes of Health, Bethesda, MD

New PhD's

Rossmann Lab: Anthony J. ("TJ") Battisti. (July 2011) After completing his Ph.D. requirements this summer, Anthony J. ("TJ") Battisti joined the Rossmann lab as a postdoc. He will be continuing his investigation into the structures of rubella and Newcastle disease virus.

Gribskov Lab: Kejie Li graduated this Summer and is now a postdoc at The Broad Institute of MIT and Harvard. Congratulations Dr. Li!
Kuhn Lab

Congratulations to Jon Snyder who received the 2011-2012 Biophysics Training Grant!

Jiraphan Junjhon presented an oral presentation at the Gordon Research Conference in Barga, Italy, May 28-June 3, 2011. Title of presentation “Molecular and Ultrastructural Characterization of Dengue Virus Replication in Mosquito Cells”

Rushika Perera, Joyce Jose, Ranjan Sengupta, Hongsheng Dai and Jon Snyder all attended and presented oral presentations at the 2011 American Society of Virology Conference in Minneapolis, MN July 16-20, 2011.

Cramer Lab:


Seminar: “Travels on and Within Membrane Proteins,” at the Department of Chemistry, University of Missouri, September 29, - October 1, 2011.

Kihara Lab

Sael Lee and Daisuke Kihara attended the 55st Annual meeting of Biophysical Society, Baltimore MD, on March 5-9, 2011 and presented two posters:

- "Novel methods for rapid comparison and multimeric protein complex fitting for low-resolution electron microscopy data", L. Sael, J. Esquivel-Rodriguez, D. Kihara
- "Local protein surface patch method for protein-ligand binding prediction", L. Sael, D. Kihara

Oral presentations:

- Binding ligand prediction by comparing local surface patches of potential pocket regions. Computational Biology Research Center, Tokyo, Japan, September 2, 2011
- Next generation protein structure analysis for structure comparison and interaction prediction. Fukushima Medical University, Fukushima, Japan, September 1, 2011.
- Binding ligand prediction by comparing local surface patches of potential pocket regions. RIKEN, Yokohama, Japan, August 30, 2011
- Unified molecular representation for protein shape comparison and interaction. ICR Symposium to Celebrate the Bioinformatics Center’s 10 Year Anniversary and New Restructuring, Institute for Chemical Research, Kyoto University, Uji, Kyoto, Japan, August 29, 2011
- Next generation protein 3D structure analysis: rapid global/local surface comparison and low-resolution data. Seoul National University, Dept. of Computer Science and Engineering, August 22, 2011
- 4 lectures, Faculty of Chemistry, Warsaw University, Poland, May 23-27, 2011

- Template-based structure prediction and quality assessment using suboptimal alignments
- Sequence-based function prediction: from prediction of single genes to functional coherence for protein groups
- Protein-protein docking prediction: from pairwise docking, docking using docking interface information, and multiple protein docking
- Binding ligand prediction by Comparing Local Surface Patches of Potential Pocket Regions

- Surface Representation for Molecular Global and Local Shape Comparison and Docking. International Institute of Molecular and Cell Biology, Warsaw, Poland, May 25, 2011
- 6 selected oral presentations at Great Lakes Bioinformatics Conference 2011, May 2-4, 2011, Ohio University, Athens, Ohio
  Protein-protein Interaction Sites Prediction using Phylogenetic Substitution Models, D. La, & D.Kihara
  Protein Docking Prediction Using Predicted Protein-Protein Interface, B. Li, & D. Kihara
  Multi-LZerD: Multiple Protein Docking for Asymmetric Complexes, J. Esquivel-Rodriguez, & D. Kihara
  Rapid Comparison and Multimeric Protein Complex Fitting for Low-Resolution Electron Microscopy Data*, J. Esquivel Rodriguez, L. Sael, & D. Kihara
  Patch-Surfer: Alignment Free Surface Patch-Based Ligand Binding Pocket Comparison, L. Sael, & D. Kihara
  Functional Coherence Assessment for Protein Groups and its Application to Pathway Assignment, M. Chitale, & D. Kihara
Kihara Lab Continued…….

Poster presentations:

- 3 poster presentations at International Conference on Intelligent Systems for Molecular Biology (ISMB), Vienna, July 17-19, 2011:
  
  Binding ligand prediction by comparing local surface patches of potential pocket regions. L. Sael & D. Kihara.
  
  

- 3 poster presentations at 3D-SIG, ISMG, Vienna, July 15-16, 2011. Kihara has also served as a session chair in this meeting.
  
  MULTI-LZERD: Multiple protein docking for asymmetric complexes. J. Esquivel-Rodriguez & D. Kihara
  
  
  Binding ligand prediction by comparing local surface patches of potential pocket regions. L. Sael & D. Kihara

- 2 poster presentations at International Conference on Structural Genomics, May 10-14, 2011, Toronto, Canada.
  
  Binding ligand prediction by comparing local surface patches of potential pocket regions. L. Sael & D. Kihara. (won the poster award)
  
  Rapid comparison and multimeric protein complex fitting for low-resolution electron microscopy data. J. Esquivel-Rodriguez, L. Sael & D. Kihara

Sael Lee and Daisuke Kihara received the International Structural Genomics Organization Poster Prize, International Conference on Structural Genomics 2011, Toronto, Canada, May 10-14, 2011. The title of the poster was “Binding ligand prediction by comparing local surface patches of potential pocket regions.”

Rosssmann Lab

- Michael attended the 2011 National Academy of Sciences annual meeting in Washington, DC on May 1st and 2nd.
  
- May 22-26 Michael attended the IX European Symposium of the Protein Society in Stockholm, Sweden and presented a talk on “Virus Host Entry”.
  
- May 26 & 27 Michael attended a symposium in honor of the 75th birthday of Dr. Eckard Wimmer (Stony Brook University) and presented a talk on “Picornavirus Receptors”.
  
- Michael attended the Gordon Research Conference on Three-Dimensional Electron Microscopy held June 26 – July 1 in New London, NH.
  
- July 24-31 Pavel Plevka participated in the 5th International UVM Practical Course on Three-dimensional Cryo-electron Microscopy of Single Particles in Burlington, VT.
  
- July 27-August 3 the Chinese Biological Investigator Society (CBIS) invited Michael to attend a memorial symposium honoring Hsien Wu and Ray Wu and to join them at their 9th biannual meeting. July 27 was spent at Tsinghua University (Beijing) where Michael visited with faculty and presented a talk entitled “Conformational changes in enveloped viruses during maturation and fusion”. July 28 he toured various Institute of Biophysics (Beijing) facilities before resuming his visit at Tsinghua. July 29 was the Hsien and Ray Wu Symposium at Peking Union Medical College (Beijing) where Michael gave a talk on “Virus Host Entry”. July 31-August 3 the CBIS meeting was held in Zhang Jia Jie in the Chinese National Forest Park where Michael presented a talk on “Structural changes in alphavirus envelope glycoproteins during maturation and fusion”.

Michael will be going to the XXII Congress and General Assembly of the International Union of Crystallography from August 22-29 in Madrid.

Gribskov Lab

Patrick Doland has joined the Gribskov (BIOL) and LaCount Labs (MCMP).

He recently attended the American Society of Virology Meeting in Minneapolis, MN and the Midwestern Neglected Infectious Diseases (MNID) conference where I won 1st place in the poster competition and $100. I'm headed to the Hepatitis C Virus meeting in Seattle, WA from Sept. 8-12. At all of these meetings I presented a poster entitled “The Hepatitis C Virus - Human Interaction Network”.

(Daisuke, Sael Lee)

Rossmann Lab


Kihara Lab

Quantification of protein group coherence and pathway assignment using functional association. M. Chitale, S. Palakodety, & D. Kihara BMC Bioinformatics, accepted. (2011)


A Book “Protein function prediction for omics era” edited by D. Kihara is now published from Springer Verlag. It includes 3 chapters from Kihara group:

- Computational protein function prediction: framework and challenges., Meghana Chitale & Daisuke Kihara, Chap. 1, pp. 1-17
- Enhanced sequence-based function prediction methods and application to functional similarity networks. Meghana Chitale & Daisuke Kihara, Chap. 2, pp. 19-34
- Protein binding ligand prediction using moment-based methods., Rayan Chikhi, Lee Sael & Daisuke Kihara, Chap. 8, pp. 145-163.

Cramer Lab


PUBLICATIONS cont.....

Kuhn Lab


Chen Lab


RESEARCH HIGHLIGHTS

Kihara Lab


We developed a new method for predicting protein-protein interaction sites in protein surface. The method, named BindML, identifies protein surface regions which have specific mutation patterns of protein-protein interaction sites. Input of BindML: multiple sequence alignment, and the tertiary structure of the protein. Output: A list of amino acid residues of the protein that are predicted to be at protein interaction sites.

(David La)
Steve Wilson with his new grandson, Reed Alexander Hoagland.

Chen Lab

Birth Announcement !!!!!
Sara Zhang and her husband, Ping Chen, announce the birth of their little boy, Ben. He was born on Aug 23, 2011 at 11:11 am. He was 6.5 lbs and 19 inch-long. The picture was taken on Aug. 26th (3 days old). The entire family are having a wonderful time taking care of little Ben, especially his sister, Lyra.

Kihara Lab

Muyi Liu, joined Dr. Kihara’s Lab from the PULSe program.
Congratulations to Pavel Plevka and Zuzana Ringlerova on their June wedding in the Czech Republic! The lab celebrated and wished them well after their return with a potluck dinner at Michael’s home on July 22.

TJ’s graduation party in July.

TJ Battisti was the 2011 recipient of the Umbarger Outstanding Graduate Student Award and also received a Bilsland Dissertation Fellowship which provided him with funding while he was preparing his thesis.

Seated on the left is Dongcai Liang, the first protein crystallographer in China, student of Dorothy Hodgkin and leader of the famous Chinese insulin group. Seated on the right is Xiaocheng Gu of Peking University and of the CUSBEA program that brought the first Chinese students (including Ming Luo) to the US after the end of the cultural revolution.
The Terracotta Warriors (located in Xi’an) represent only a small portion of the eight thousand strong underground army buried in front of the Emperor Qinshihuang’s tomb (r. 221-207 BC) to defend him in the afterlife.

The Great Wall (Beijing) one of the greatest wonders of the world.

Alter of Heaven (Beijing), was used to worship heaven at the winter solstice. The center stone (which is what David is standing on) is called the Heavenly Center Stone.
Gribskov Lab

Kejie Li graduated this Summer and is now a postdoc at The Broad Institute of MIT and Harvard. Congratulations Dr. Li!


Biaobin Jiang (below) and Junhui Wang (right) joined the Lab. Welcome!
Carol Post and Jeff Bolin vacationing in the Bear Tooth Mountains at the Montana/Wyoming border.