

MRB NEWS

Featured Faculty: Yang Zhang, Assistant Professor Bioinformatics, with a joint appt in the Dept of Molecular Biosciences



Academic Areas:

Physics

Research Interests

Bioinformatics; Protein structure prediction; Protein-protein & protein-ligand docking; New drug design; Single molecule mechanics

Educational

Background:

Ph.D., 1996, Central China Normal University
B.S.

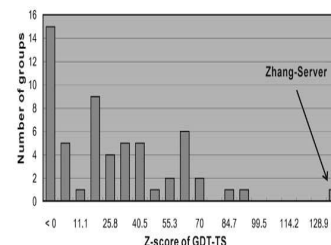
Dr. Zhang spent two years as the Alexander von Humboldt research fellow at Free University of Berlin, Germany. After a subsequent postdoctoral research in the Chinese Academy of Sciences, he joined the group of Jeffrey Skolnick at the Danforth Center. Prior to coming to the University of Kansas, Dr. Zhang had been on the faculty of the Center of Excellence in Bioinformatics at the University of Buffalo.

The Zhang laboratory is developing various novel computational algorithms to generate large-scale, high throughput predictions of tertiary protein structures and protein-protein interactions from amino acid sequences. The goal is to annotate the function of proteins based on the sequence-to-structure-to-function paradigm and therefore enhance the impact of genome sequencing on biology and medicine.

Critical Assessment of Structure Prediction (CASP) is a biennial worldwide competition in protein structure prediction, which is also called Olympic games of protein structure prediction. The organizer releases a number of amino acid sequences whose structure is unknown to the predictors. The 3-dimensional models predicted by the participants have to be submitted before a deadline. Finally, the models are compared with the structures solved by X-ray or NMR experiments. This blind experiment helps to obtain a fair and objective assessment of the most efficient algorithms in the field of protein structure prediction.

The 7th CASP competition was held in 2006, which included two sections. The Human section included 207 worldwide laboratories; the automated server section included 98 server predictors. Depending on modeling difficulty, the targets were split into 3 categories: HA (easy), TBM (medium), and FM (hard) targets. The Zhang lab participated in the CASP7 experiment as "Zhang" in the human section and as "Zhang-Server" in the server section; both were ranked as the No 1

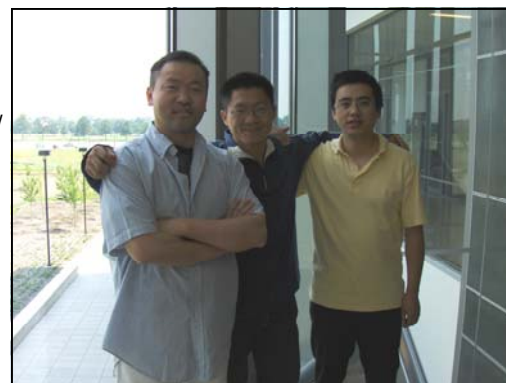
predictors based on the official accumulative GDT-TS score.



Details focusing on the Zhang lab include: **(1)**, developing computational algorithms to generate large-scale, high-throughput, and reliable predictions of 3-dimensional protein structures from amino acid sequences. The functional insights can therefore be obtained by matching the global topology and active site of the predicted high-resolution structures to the known structure/function databases. **(2)**, modeling the specificities of the protein-protein and protein-ligand interactions. These include docking the predicted/solved monomer structures into multimer structures, and/or generate multimer conformations directly from amino acid sequences by extending the current successful monomer-simulation approaches. **(3)**, studies of the reverse process of protein structure prediction, i.e. designing new sequences to create novel proteins of desired structure and function. Protein design is on its own of great biological interest

because it provides opportunities for developing new drugs and therapeutics. It will also provide helpful insights and stringent tests of our current understanding of fundamental principles underlying sequence, structure and function. **(4)**, constructing new dynamic models for the understanding of the mechanics of spider capture silk. Spider silk is a natural material produced by orb-web weaving spiders that has a high tensile strength comparable to steel; but unlike steel, it is also extremely resilient with the ability to be stretched to 10 times without breaking. Our purpose is to simulate in real time the dynamic process and the elastic response of the spider silk molecules under external stretching forces. This effort will provide a route to solving the puzzle of what mechanism underlies the high tenacity and extensibility of the spider capture silk, which will also lend insights to the genetic design of special proteins like spider silk molecules. Dr. Zhang is the author/co-author of numerous publications.

Pictured below: Dr. Yang Zhang and post docs Yunqi Li and Sitao Wu



MEET THE GRA



Name: Pradyot Nandi
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Field of Study:
Pharmaceutical Chemistry
Time at KU: 4 years
Hobbies: Technology,
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Pictured above: Another snapping turtle takes a break on the front sidewalk of MRB.

IMPORTANT BUILDING INFORMATION

CONGRATULATIONS TO WONPIL IM! KU BIOINFORMATICS RESEARCHER RECEIVES PRESTIGIOUS ALFRED P. SLOAN FELLOWSHIP (REPRINTED FROM THE KU WEBSITE)

LAWRENCE — Because the good news arrived by letter, Wonpil Im, assistant professor of molecular biosciences at the University of Kansas, was surprised to find that he was the recipient of a 2007 Alfred P. Sloan fellowship. “A letter usually means rejection,” said Im. “I got the Sloan fellowship news by mail, so when I opened it up I was quite shocked to read that first sentence, ‘It is a great pleasure ...’ ”

Im is one of only 12 molecular biologists in the nation to receive the fellowship this year. Sloan Research Fellowships are designed to boost the careers of the most promising university faculty members involved in scientific investigation. In the past, 35 Sloan fellows have gone on to win Nobel Prizes.

For Im’s colleagues, news of his fellowship came as no surprise at all.

“Im is fast becoming a leader in bioinformatics on the KU campus and in the country,” said Kathy A. Suprenant, chair and professor of molecular biosciences at KU. “His research is at the cutting edge and we don’t know where it’s going, but we’re hopeful it will allow us to predict new drugs. This Sloan fellowship is a fantastic honor for him. They’re very competitive awards.”

The \$45,000 fellowship will continue for two years, with a possible two-year extension. Sloan Research Fellowship funds may be used for equipment purchases, technical help, business travel, trainee support and other costs directly related to Im’s research.

“These are funds I can utilize to support the people in my research group,” said Im.

Im leads a team of KU students and postdoctoral researchers who study protein interactions in biological membranes and determine the structure of biological macromolecules. They also are developing a Web site dubbed CHARMM-GUI to provide a useful resource for the biomolecular simulation community.

“Computer models are useful in the lab, but to use a computer you need an algorithm or a method,” said Im. “We develop the method or algorithm if they are not available.”

Im’s research could have applications in nanotechnology and pharmaceuticals.

“The aim of our work is to understand human disease at the molecular level,” said Im. “If you look at the drugs that we’re using now, about 50 percent of commercial drugs are targeting membrane proteins. As our research progresses, we hope to help make a map to develop the drugs of the future.”

A committee of researchers reviews more than 500 nominations each year to determine a final selection of 116 Sloan fellows in seven scientific fields.



Pictured above: Wonpil Im, Alfred P. Sloan Fellowship recipient.

EHS has a website of surplus items that are FREE to researchers. Check to see what’s available at :

http://www.ehs.ku.edu/documents/ehs_forms/surplus_chemical_requests.aspx

Security Reminder:

When entering the building using your KU ID, be sure the door shuts completely behind you. Please also try to be aware of those who try to enter with you without using a card. It is good practice to only allow those in your lab group to enter with you.