

## EDITORIAL

### ***Protein Science* Best Paper Awards to Yu-ming Huang and Abhay Thakur**

Warmest congratulations to Yu-ming “Mindy” Huang<sup>1</sup> and Abhay Thakur<sup>2</sup> (Figure 1), recipients of the Protein Society’s Year 2018 “Best Paper” awards.

At the beginning of each year, two “best papers” are selected from articles published in *Protein Science* during the preceding 12 months. A junior author (typically the first author) is designated as the award winner and invited to give a talk at the following Annual Protein Society Symposium.

Mindy Huang completed her undergraduate education in both chemistry and physics at the National Taiwan University. Her Ph.D. in computational chemistry was at UC-Riverside under the guidance of Chia-en Chang. She is currently a postdoctoral fellow with Andrew McCammon at UC-San Diego where her work focuses on the development and application of advanced simulation tools to better understand biomolecular diffusion.

As noted by Dr. McCammon, “Mindy is a remarkably versatile young theoretician of protein science. She has successfully developed new computer simulation methods and applied these in studies of protein dynamics and of biomolecular diffusion. The work recognized here is in an important area of cell biology, namely, how co-localization of enzymes and other macromolecules lead to efficiency in metabolism, signaling and other processes. The importance of diffusional channeling of intermediates from one enzyme to another is increasingly recognized in such processes. Beyond its fundamental significance, targeting channeling in signaling or metabolic arrays represents a novel opportunity for drug discovery. In addition to her outstanding research, Mindy has been active in mentorship of students in the groups she has been associated with, and she brims with enthusiasm for all her projects. She is on her way to a productive career as a professor of molecular biophysics!”

One of Mindy’s earlier projects, for which she received considerable recognition, used extended MD simulations and enhanced sampling methods to model drug binding to the HIV protease. As she notes “Molecular diffusion, a main mechanism of transport of materials within cells, plays a fundamental role in a vast array of biological processes. A deep understanding of the processes can directly improve rational drug design and protein engineering with therapeutic applications to diverse diseases.” The long-term goal of her research is to develop theoretical and computational methods to unravel the detailed role of biomolecular diffusion and recognition at the atomistic level. Mindy will be starting as Assistant Professor of Physics at Wayne State University this coming fall.

Abhay Thakur received his initial training in India, including his Ph.D. with Mohan Rao at the Center for Cellular and Molecular Biology in Hyderabad. The work for which he received the Best Paper Award was carried out as a postdoctoral associate in the group of Lila Gierasch at the University of Massachusetts. He is currently a Senior Scientist with Pall Corporation.

Abhay summarizes his career path in the following way. “When I started my career I was fascinated with protein folding, misfolding and aggregation. I joined Dr. Mohan Rao's Lab at the Centre for Cellular and Molecular Biology (CCMB, India) to investigate the conformational changes of prion protein in the presence of copper. I was fortunate to explore multiple biophysical techniques in his lab. Utilizing multiple techniques we proposed a novel long-range interaction between N- and C-terminal of prion protein in the presence of copper. During my graduate tenure, I attended Lila's seminar on protein folding. Her research work on folding of the beta-barrel protein, CRABP1 is inspiring and extensive. I felt it was a logical route for me to understand the folding of the complex protein. In her lab, I learned a lot about protein folding and used NMR to understand the denatured ensemble of CRABP1. Her mentoring has significantly helped in refining my thoughts and approaches to tackle scientific problems.”

Dr. Gierasch comments that “I am delighted that the paper by Abhay Thakur based on work he did in my lab while he was a postdoc, in collaboration with his co-author Wenli Meng, another postdoc, was selected as a best paper in *Protein Science* in 2018. Abhay did a virtuoso job of extracting information from the NMR parameters for the denatured state ensemble of cellular retinoid acid binding protein including developing powerful computational approaches to compare information from many mutant versions of this protein. The resulting picture fills in gaps in our understanding of the folding landscape of this beta-rich protein and raises new questions for us to pursue. Abhay showed a great combination of perseverance and innovation to complete this study.”

## **Background Information**

All articles published in *Protein Science* are candidates for the “Best Paper” awards. No nomination statement is required. At the same time, if authors submitting a manuscript feel that it will be a strong candidate for a “best paper” award, they are very welcome to include a brief note in the submission letter explaining why the contribution is especially worthy of consideration.

Brian W. Matthews  
Editor

## **References**

1. Huang Y-mH, Huber GA, Wang N, Minter SD, McCammon JA (2018) Brownian dynamic study of an enzyme metabolon in the TCA cycle: Substrate kinetics and channeling. *Protein Sci* 27:463-471.
2. Thakur AK, Meng W, Gierasch LM (2018) Local and non-local topological information in the denatured state ensemble of a  $\beta$ -barrel protein. *Protein Sci* 27:2062-2072.

## **Figure Caption**

Figure 1. Award winners. (A) Yu-ming Huang. (B) Abhay Thakur