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***Mechanisms and Energetics of
Protein/Peptide Interactions in Biological Membranes***

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Understanding the delicate balance of forces governing helix/ β -hairpin interactions in transmembrane proteins is central to understanding membrane structure and function. These membrane constituent interactions play an essential role in determining the structure and function of membrane proteins, and protein interactions in membranes, and thus form the basis for many vital processes, including transmembrane signaling, transport of ions and small molecules, energy transduction, and cell-cell recognition. "Why does a single transmembrane helix or β -hairpin have specific orientations in membranes?" "What are the roles of hydrogen bonds, close packing, and helix-lipid or β -hairpin-lipid interactions in helix or β -hairpin associations in membranes?" "How do these interactions change the membrane structures?" "How do transmembrane domains transmit signals across membranes?" These are fundamentally important biophysical questions that can be addressed by understanding the delicate balance of forces governing helix/ β -hairpin interactions in membranes. Recently, we have published novel methods and their applications that begin to address the complicated energetics and molecular mechanisms of these interactions at the atomic level by calculating the potentials of mean force (PMFs) along reaction coordinates relevant to helix/ β -hairpin motions in membranes, and dissecting the total PMF into the contributions arising from physically important microscopic forces [1-5]. In this work, I will summarize our research accomplishment so far, and present recent research activities to elucidate the influence of helix tilting on ion channel gating and the molecular basis of transmembrane signaling.

[1] Lee, J. and W. Im, *J. Comput. Chem.*, **28**: 669-680 (2007); [2] Lee, J. and W. Im, *Chem. Phys. Lett.*, **441**:132-135 (2007); [3] Lee, J. and W. Im, *Phys. Rev. Lett.*, **100**:018103 (2008); [4] Lee, J. and W. Im, *J. Am. Chem. Soc.*, **130**:6456-6462 (2008); [5] Lee, J., S. Ham, and W. Im, *J. Comput. Chem.*, in press (2008).



Wonpil Im received his B.Sc. in Chemistry, at Hanyang University, Seoul. He pursued his graduate studies under the direction of Professor Won and received his M.Sc. degree in 1996. Moving to Montreal, Canada in February 1997, he started Ph.D. studies in Chemistry at University of Montreal under the supervision of Professor Benoit Roux. Following Professor Roux, he moved to Weill Medical College of Cornell University in New York in June 2000, where he received his Ph.D. in 2002. In June 2002, he pursued postdoctoral studies with the group of Professor Charles L. Brooks, III at the Scripps Research Institute, La Jolla, where he was the recipient of a CTBP (Center for Theoretical Biological Physics) fellowship. He joined the Faculty in Department of Molecular Biosciences and Center for Bioinformatics at the University of Kansas in August 2005.