Membrane Insertion of Peripheral Proteins on the BiophysJ Cover

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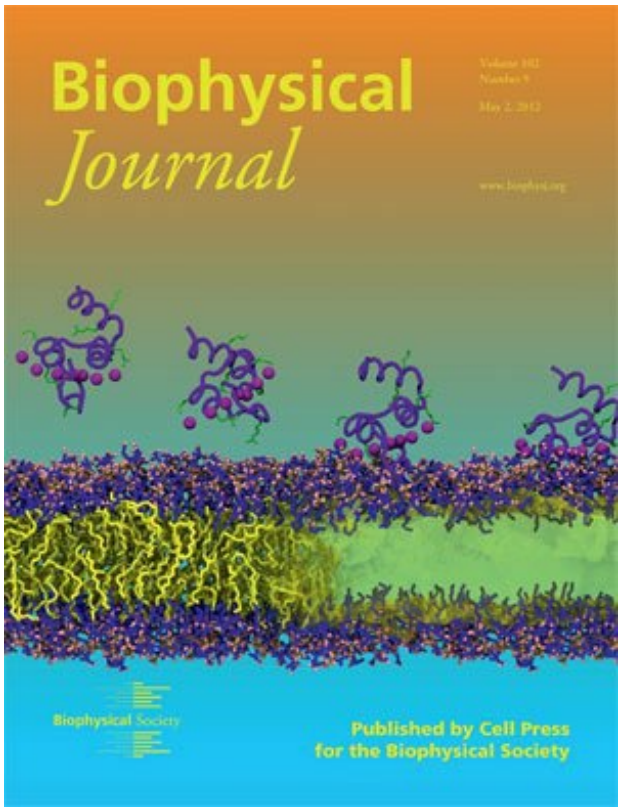
Authors Y. Zenmei Ohkubo, Taras V. Pogorelov, Mark J. Arcario, Geoff A. Christensen, and Emad Tajkhorshid discuss the science behind the cover image of the latest issue of Biophysical Journal. Binding to specific regions of the cellular membrane constitutes a key step in the biological function of peripheral membrane proteins. Describing this process at a sufficiently detailed level, however, continues to pose a challenge to both experimental and computational biophysical methodologies. While molecular simulation offers a sufficiently high resolution to investigate the process, its applicability has been severely hampered by the slow diffusion of membrane lipids on the timescales that are reachable by the method. The image describes the transformation of a conventional phospholipid bilayer model to a novel membrane representation, termed HMMM (**H**ighly **M**obile **M**embrane **M**imetic), in which a large fraction of the hydrophobic lipid tails has been replaced by a liquid organic solvent. The enhanced lateral diffusion of lipid molecules in an HMMM membrane permits one to capture membrane-associated phenomena much more efficiently. The HMMM model was realized as a result of a team effort between several graduate students and postdoctoral researchers at the Computational Structural Biology and Molecular Biophysics Group at the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign.



The image shows how the membrane-anchoring domain of coagulation factor VII binds and inserts into an HMMM membrane during unbiased molecular dynamics simulations. As computational scientists dealing with complex molecular systems, we make graphical representations of our simulated systems all the time. The main guidelines that we try to follow in order to make first-rate scientific figures are (1) highlighting the relevant feature clearly in the image, in such a way that “you shouldn’t even have to read the caption to understand it!”; (2) including as much relevant details (information) in the image without cluttering it; and (3) when possible capturing a dynamical process in a static image. Including all these aspects in a figure is non-trivial, but when optimally done it will result in a scientifically rich and visually appealing image. For example, in this image we are depicting the idea of representing a full membrane (left half) by the HMMM model (right half) by gradually transforming the long lipid tails into a liquid bulk-like phase, while highlighting the dynamic process of membrane insertion of a protein.

The image was created using VMD, a cutting-edge molecular visualization program allowing for sophisticated and detailed graphical manipulation of molecular representations. In particular, we have used the “ambient occlusion lighting” feature of the program, which allows one to create more realistic images of complex molecular systems. Making information-rich, yet nice and clear figures is not trivial, but it pays off! We are very pleased that our image was recognized and selected for the cover page of *Biophysical Journal*, as it attracts further attention to our novel membrane model which we believe is of great potential in simulation studies of diverse membrane-associated phenomena.