Membrane Curvature Induced by Transmembrane Proteins

Christoph Kluge[1] and Rainer A. Böckmann[1]

[1]*Computational Biology, Friedrich-Alexander University of Erlangen-Nürnberg, Erlangen, Germany*

The (local) curvature of cellular membranes can function as a sorting mechanism for membrane proteins, e.g. by accumulation of membrane proteins in regions of specific curvature, as shown recently for potassium channel KvAP and water-pore AQP0 [1]. Until now, the direction of the induced curvature for these proteins, as well as the molecular driving forces for the curvature induced by transmembrane proteins could not be resolved.

Here, using both coarse-grained and atomistic molecular dynamics (MD) simulations, we addressed the curvature induced by KvAP, AQP0, and different transmembrane peptides. KvAP induces a strong negative curvature of -0.036nm^{-1} while AQP0 hardly affected the spontaneous membrane curvature when embedded in a POPC lipid bilayer, in excellent agreement with experiment [1]. The dominant contribution to membrane curvature is attributed to electrostatic interactions between lipid headgroups and protein charges at the membrane interface.

[1] S. Aimon *et al.* De-velopmental Cell 28, 212 (2014).