# Transmembrane Protein-Induced Membrane Curvature

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The local curvature of cellular membranes can function as a sorting mechanism for transmembrane proteins, e.g. by accumulation in regions of matching spontaneous curvature (SC), as shown recently for potassium channel KvAP and water-pore AQP0 by Aimon et al. [Aimon (2008), Dev. Cell, 28(2), 212-218]. However, the direction of the reported SC as well as the molecular background could not be addressed experimentally yet. Using coarse-grained and atomistic molecular dynamics simulations, we analyzed the levels of spontaneously induced curvature for the homologous potassium channel Kv 1.2/2.1 Chimera (KvChim) and AQP0 when embedded in unrestrained POPC lipid nano-discs. Coarse-grained results are in excellent agreement with the experiments, at values of 0.036 $nm^{-1}$ and -0.019 $nm^{-1}$ induced by KvChim and AQP0, respectively. Furthermore, the direction of curvature can be retrieved directly from the simulations. Atomistic simulations of both systems show a SC comparable to the coarse-grained results, and allow for detailed investigation of its origin, especially in terms of protein-lipid interactions. Here, uneven distribution and organization of POPC lipids at the interface of KvChim establishes a basal positive curvature, which is then further modified by the dynamics of the protein.