2D assembly of helical rods: rhodopsin.

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Rhodopsin is part of the largest group of G-protein-coupled receptors (GPCR) named class A. It is made of seven transmembrane helices and a cofactor retinal linked via a Schiff base to Lys-296 which is in 7 TMD. Initiated by contact with light, retinal converts from 11-cis to 11-trans leading to conformational changes within the protein which ultimately trigger interaction of the protein with G-proteins. Upon conversion of the retinal it dissociates from the protein, leading to bleaching.

It is the goal to assemble rhodopsin in its bleached state following a bio-inspired pathway. Individual helices are taken from a reference crystal structure of rhodopsin and docked in a 2D approach to derive as best as possible the references structure. The docked poses are ranked using a force field based scoring function (AMBER96). Taking the first 2 helices are as an example, docking needs consequent multi nano second MD simulation of the two helices within a hydrated lipid bilayer to achieve an almost perfect match of the structural features with those of the crystal structure.

References: