Structural Studies of Model Membrane Systems by Surface X-ray and Neutron Scattering

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Abstract

Integral α-helical membrane proteins play a fundamental role in cell membrane structures and functions. It is estimated that roughly 15~30% of the proteins in currently known genomes are integral membranes proteins. Given their relevance to cellular physiology, membrane proteins are of great significance for a wide variety of therapeutics, with ~60% of currently available drugs having a membrane proteins as a target. Due to challenges in working with membrane proteins, we designed artificial peptides to possess 4-helical bundle motifs with well-defined hydrophilic and hydrophobic domains via *de novo* computational methods. Surface X-ray scattering techniques, i.e., X-ray reflectivity and grazing incidence X-ray scattering, have been employed to measure the bundle orientation and four-helix assembled structure, respectively. These *de novo* designed peptide bundles were utilized for model ion channel proteins for anesthetic halothane binding and photosynthetic light harvesting peptide for photovoltaic applications via incorporation of the PZnPI chromophore.