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Design & Structural Characterization of Amphiphilic 4-Helix Bundle Peptides Vectorially-Oriented at Soft Interfaces

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Amphiphilic 4-helix bundle peptides have been designed to incorporate both biological and non-biological cofactors. An ensemble of these peptide-cofactor complexes, vectorially oriented at a soft interface between polar and non-polar media, can provide for the translation of their designed molecular function into a macroscopic material property of the interface. Such amphiphilic 4-helix bundle peptides can also serve as model integral membrane proteins for vectorial incorporation into a lipid bilayer providing a molecular laboratory for the detailed study of structure-function correlations. For example, the mechanism by which anesthetic binding to a designed cavity within its hydrophilic domain modulates the ion channel activity of its hydrophobic domain. Detailed structural studies of these amphiphilic peptides within such non-crystalline ensembles can be performed utilizing an essential combination of x-ray scattering, neutron scattering, and molecular dynamics simulation techniques.