Interaction of polymers with lipid bilayers studied with Single Chain Mean Field theory

YACHONG GUO[1], VLADIMIR BAULIN[1]

[1]*Departament d'Enginyeria Química, Universitat Rovira i Virgili, Tarragona, Spain*

Abstract

Single Chain Mean Field (SCMF) theory is a fast numerical tool that provides microscopic details of the structure and equilibrium properties of lipid bilayers[1,2]. It can give detailed information about the structure and physical properties of lipid membranes when interacting with biological macromolecules that can be difficult to achieve in direct experiments. This theory can also reveal the molecular mechanisms of these interactions, and the conformational changes that biomolecules undergo while transferring from water to the quasi two-dimensional geometry of the membrane.

The structural changes in the bilayers induced by the presence of the polymers of different composition are shown in the example of interaction of hydrophobic homopolymers and block copolymers with lipid bilayers. Rearrangements of hydrophobic and hydrophilic regions due to polymers result in volume fractions of components and significant changes in the elasticity of the bilayers.

This microscopic information can be validated against neutron and X-ray scattering and will elucidate the fundamental mechanisms of membrane activity and selectivity of biomolecules and the key parameters that control self-assembled membrane structures.

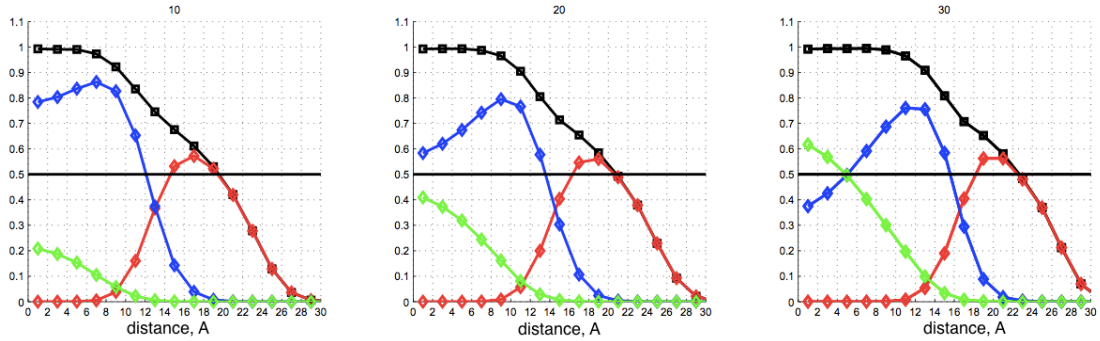

Fig. Structural changes in the lipid bilayer upon addition of hydrophobic polymer T8 into the lipid bilayer. The concentration of the polymer (green) is increased from left to right. Hydrophobic tails (blue) and hydrophilic heads (red) rearrange in order to accommodate the polymer.

[1] Pogodin, S.; Baulin, V. A. Coarse-Grained Models of Phospholipid Membranes Within the Single Chain Mean Field Theory. *Soft Matter* **2010**, *6*, 2216–2226.

[2] Pogodin, S.; Baulin, V. Equilibrium Insertion of Nanoscale Objects into Phospholipid Bilayers. *Current Nanoscience* **2011**, *7*, 721–726.