Stability of macromolecules at liquid-liquid interface

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Polymeric drug carriers are important for enhancing drug stability and solubility, and improving transport properties of pharmaceutical molecules.[1,2] For example, polyethylene oxide (PEO) based copolymers are of great interest for their applications in biotechnology and medicine. In order for these polymers to be applicable in the drug formulation it is important to understand their relative affinity towards living cells. Even though a great deal of experimental studies has been carried out on the structural characteristics and interactions of polymers with bio-membranes and lipid bilayers, the details of diffusion of polymers systems through lipid membrane itself are not well-known at the molecular level.

Due to this interest, the free energy profile of adsorption of a generic model of a polymer monomer at liquid-liquid interface is investigated using the Umbrella Sampling technique.[3] The two solvents are modeled as generic Lennard Jones particles with different affinity towards the polymer monomer.[4] This system was chosen because the aqueous exterior and the lipophilic bio-membrane can easily be mimicked using hydrophilic and hydrophobic solvents. This calculation gives us the understanding of how stable the monomer is at the liquid-liquid interface and the underlying energetics involved in the permeation of a monomer from the aqueous medium to the hydrophobic centre of a membrane. The results are then compared with the data gathered for polymers with varying topology (dendrimer, linear, and star-shaped). The final aim of this work is to understand how the polymer molecular weight and topology affect the free energy of absorption.

Reference:

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