

Predicting the stability of macromolecules at liquid/liquid interface

Tseden Taddese, David Cheung and Paola Carbone

*School of Chemical Engineering and Analytical Science, The University of Manchester, Oxford Road, M13 9PL,
United Kingdom*

paola.carbone@manchester.ac.uk

Department of Chemistry, University of Warwick, Coventry, CV4 7AL, UK and

*Department of Pure and Applied Chemistry,
University of Strathclyde, Glasgow, G1 1XL, UK*

Polymeric drug carriers are important for enhancing drug stability and solubility, and improving transport properties of pharmaceutical molecules.¹ For example, polyethylene oxide (PEO) based copolymers are of great interest for their applications in biotechnology and medicine. However, 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.

In this contribution we show free energy (FE) of desorption data obtained from a generic bead-and-spring polymer model at liquid-liquid interface between good and poor solvents.² This system was chosen because the aqueous exterior and the lipophilic bio-membrane can easily be mimicked using hydrophilic and hydrophobic solvents.

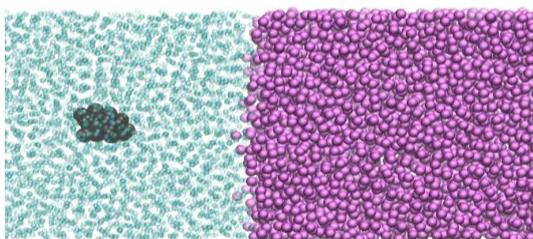


Figure 1. Polymer model (cyan bulky beads) in a poor solvent solution

The results reveal that especially in poor solvent the practice to associate to each monomer the same FE is not correct and that the FE of desorption is dependent on the topology of the macromolecule. We also show that the trend of the FE with the polymer molecular weight might be predicted from data available from the bulk phase.³

1. Zhang, L.; Gu, F.; Chan, J.; Wang, A.; Langer, R.; Farokhzad, O., *Clinical pharmacology and therapeutics* **2008**, 83 (5), 761

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