Amphiphilic triblock copolymers as membrane-active agents: Monte-Carlo simulations

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Abstract

Interactions between amphiphilic block copolymers and lipid bilayer membranes have been attracting much scientific interest for many years. This is due to the many possible applications of this type of polymer, e.g. in pharmaceutical or biochemical contexts.[1,2]

In particular, ABA triblock copolymers composed of poly(etylene oxide) as hydrophilic block (A), and poly(propylene oxide) as hydrophobic block(B), known under the generic name Poloxamer, are promising candidates for use in anti-cancer treatments.

Despite the many studies on the interaction of lipid membranes with Poloxamer that have been carried out, several questions regarding the molecular mechanism of these interactions remain unresolved.

Here, we show results of Monte-Carlo simulations of ABA-triblock copolymers interacting with lipid bilayer membranes as a function of block-lengths and -hydrophobicity. The coarse-grained Monte-Carlo model[3] has been used to study the induced membrane permeability, as well as the conformations of the copolymers with respect to the membrane.

The results indicate that the surface active behaviour of amphiphilic ABA triblock copolymers can be understood by their hydrophilic-lipophilic balance, as supported by recent experimental findings[4].

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