DESIGN OF POLYMERIC DRUG CARRIERS

MACHÁČKOVÁ Miroslava, TOKARSKÝ Jonáš, ČAPKOVÁ Pavla

VSB – Technical University of Ostrava, Ostrava, Czech Republic, EU

Abstract

In recent years an increase of various medical publications is recorded. A large part of these works deals with the different uses of biodegradable polymers, eg. for targeted drug delivery, as carriers of anticancer drugs, prolonged circulation of drugs, for tissue engineering, etc. Biodegradable polymers due to their characteristics (eg. zero toxicity) are suitable substances for wide use not only in the medicine. The present work deals with the comparison of some properties of selected biodegradable polymers with different drug molecules in waterless and aqueous (60 wt.% of water) environment. Selected biodegradable polymers were: cellulose, chitosan, poly(glycolic acid), poly(ethylene glycol), poly(L-lactic acid) and poly(D-lactic acid). Drugs used were ibuprofen and cyclosporine A. All simulations were performed in Forcite and Blends modules in Materials Studio modeling environment. The relevant energy and charge were assigned using pcff (Polymer Consistent Force Field). The mutual interactions between the polymer and drug molecules were characterized using the Flory – Huggins theory. The aim of this work was to compare the stability, miscibility, cohesive energy, concentration profiles and radius of gyration of selected polymer chains with drug molecule in a given environment in order to prepare the molecular system with non-bond polymer-drug interactions and further to estimate the most suitable candidate as a drug carrier.

Keywords: Molecular modeling, biodegradable polymers, drug carriers, structure.

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