Anastassia N. Rissanou

National Hellenic Research Foundation
Greece

A computational study on the affinity assessment of Self-Assembling dipeptides with the anticancer Peptide-Drug bortezomib

Abstract:

The investigation of potential self-assembled peptides as carriers for the delivery of the anticancer drug Bortezomib, using all-atom molecular dynamics simulations, is the topic of the present study. A series of dipeptides with a similar chemical formula to Bortezomib with hydrogel-forming ability are being investigated for their propensity to bind to the drug molecule. Dipeptides are divided into two classes, the protected FF (Fmoc-FF and Z-FF) and the LF-based (Cyclo-LF and LF) ones. The thermodynamic stability of the complexes formed in an aqueous environment, as well as key morphological features of the nanoassemblies are investigated at the molecular level. Binding enthalpy between Bortezomib and dipeptides follows the increasing order: LF < Cyclo-LF < Fmoc-FF < Z-FF under both van der Waals and electrostatic contributions. Protected FF dipeptides have higher affinity for the drug molecule, which will favor its entrapment, giving them an edge over the LF based dipeptides. By evaluating the various measures, regarding both the binding between the two components and the eventual ability of controlled drug release, we conclude that the protected FF class is more suitable for drug release of Bortezomib. The selection of the optimal candidates based on the present computational study will be a stepping stone for future detailed experimental studies, involving the encapsulation and controlled release of Bortezomib both in vitro and in vivo.

Biography

Anastassia Rissanou is Assistant Researcher at the Theoretical and Physical Chemistry Institute, of the National Hellenic Research Foundation, Athens, Greece. She has basic education in Physics and long expertise in modeling of soft materials. Systems of interest are polymers, colloids, biological molecules such as peptides, proteins, RNA/DNA, as well as hybrid nanostructured materials of the aforementioned matrices with organic or inorganic nanofillers. She is skilled in various simulation methods in atomistic and coarse-grained level, as well as multiscale simulation techniques. She has many publications in high-impact international journals and participations in many national and international conferences.