

7th International Conference and Exhibition on**BIOPOLYMERS AND BIOPLASTICS****October 19-20, 2017 San Francisco, USA****Multiscale modeling of nanoengineered drug delivery systems based on smart nanofibers****Sergey Gusarov**

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Nanotechnology-based smart drug delivery systems becoming one of the most promising directions in the development of modern therapies which could dramatically improve drugs efficiency through targeted/precise delivery. However, despite the progress made during last years, there still remains an enormous potential for further development which could revolutionize the area. Unfortunately, in some cases, this potential is screened out by the complexity and multilevel character of systems and processes at the nanoscale. The success of future applications in high-tech medicine requires a deep understanding of fundamental mechanisms at different levels of description and their communication. That could be provided only by an appropriate combination of experimental study with predictive theoretical modeling. This study addresses the multiscale modeling of drug release (on/off states) in the smart nanofiber-based drug delivery systems to better understand the process and factors defining the mechanism, which could be efficiently used to deliver drugs. The properties (as well as the ratio) of monomers and temperature are becoming important variables that affect the drug release. So first, the constituent monomers and small copolymers were studied by quantum chemical methods. Next, the number of different copolymer systems was constructed and the molecular dynamics calculations were performed in water solvent with ions. The resulting trajectories were analyzed in detail (structure of radial distribution functions, a number of hydrogen bonds, etc.) to study the crosslinking between polymers. The MD calculations were also supported by statistical mechanical studies (3D-RISM) to get the solvation properties and thermodynamics of the equilibrium arrangements. Finally, the detailed structure of favorite relative orientations of copolymers was studied by quantum chemical methods to understand the factors affecting drug release process.

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