



Computer Modeling in Molecular Biophysics and Nanomedical Applications

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Message from the Guest Editor

Dear Colleagues,

With this Special Issue, we would like to celebrate the 50th anniversary of the molecular dynamics of polymer and biopolymer systems by publishing new articles devoted to both the general problems and results of modeling the structure, mobility, and self-organization of macromolecular systems (including protein folding), and the results of modeling intended for solving applied biomedical problems (for example, the development of novel carriers for the delivery of drugs and genetic material, for the creation of new biocompatible scaffolds and biocomposites).

We would like to see in this issue not only reviews and articles on the elaboration and application of the classical molecular dynamics method, but also on the elaboration and use of its variants (Rahman–Parinello MD, non-equilibrium MD (NEMD), controlled molecular dynamics (SMD), etc.) as well as papers on other numerical methods for studying the structure, mobility, and self-organization of various polymer and biopolymer molecular systems.

Prof. Dr. Igor Neelov
Guest Editor





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Message from the Editor-in-Chief

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