

Special Issue

Computer Modeling in Molecular Biophysics and Nanomedical Applications

Message from the Guest Editor

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.

Guest Editor

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Deadline for manuscript submissions

closed (31 May 2023)



International Journal of Molecular Sciences

an Open Access Journal
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Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



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*International Journal of
Molecular Sciences*
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Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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