

## Special Issue

# Molecular Dynamics Simulations

### Message from the Guest Editors

Molecular Dynamics (MD) simulations, nowadays, allow to explore time-dependent changes occurring in molecular systems thus providing paramount information to understand a wide range of chemical and biological phenomena. In many cases, MD can be viewed as a counterpart to experiment as MD data frequently help interpret in vivo and in vitro results and are invaluable in proposing hypotheses and experiments. This Special Issue on “Molecular Dynamics Simulations” is open to researchers working with Molecular Dynamics at any level. Papers addressing methodological or computational developments on force field effects, full-atom/coarse grained calculations, explicit/implicit treatment of solvent, analyses of trajectories, etc., as well as papers reporting applications to diverse molecular systems, interactions, protein function, etc., are welcome. Submission of up-to-date review articles is also encouraged.

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### Guest Editors

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### Deadline for manuscript submissions

closed (31 December 2018)



## International Journal of Molecular Sciences

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### Message from the Editor-in-Chief

The *International Journal of Molecular Sciences (IJMS)* 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, and molecular biophysics. *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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