International Journal of
Molecular Sciences

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Molecular Dynamics Simulations

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Deadline for manuscript submissions:
closed (31 December 2018)

Message from the Guest Editors

Dear Colleagues,

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.

Prof. Dr. Luis F. Pacios
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Guest Editors

mdpi.com/si/16035

Special Issue

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Message from the Editor-in-Chief

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