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.

Guest Editors

Prof. Dr. Luis F. Pacios

Department of Biotechnology-Vegetal Biology, Universidad Politécnica de Madrid (UPM) and Center for Plant Biotechnology and Genomics (CBGP, UPM-INIA) Madrid, Spain

Dr. María Garrido-Arandia

Center for Plant Biotechnology and Genomics (CBGP, UPM-INIA), UPM Campus de Montegancedo, E28223 Pozuelo de Alarcón, Madrid, Spain

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Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
ijms@mdpi.com

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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.

Editor-in-Chief

Prof. Dr. Maurizio Battino
Department of Odontostomatologic and Specialized Clinical Sciences, Sez-Biochimica, Faculty of Medicine, Università Politecnica delle Marche, Via Ranieri 65, 60100 Ancona, Italy

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