Special Issue

Molecular Advances in Computational Chemistry for Drug Design

Message from the Guest Editor

The impressive recent progress made advancing the richness of scientific data and enhancing commonly available computational power is supporting the development of innovative computational approaches for drug design. Overall, the field has benefited from the power of the artificial intelligence (AI) algorithms implemented in countless applications, including ligand- and structure-based methods. Innovative AI-based methods have been reported for rational de novo design of promising compounds, property prediction, ADME/Tox profiling, docking simulations, and MM/MD calculations and analysis. In parallel, enhanced computational power has allowed the development of targeted MD/MM approaches capable of extensively simulating the molecular recognition processes, thus gaining information concerning the complex stability and free energy from the corresponding interaction. Overall, this Special Issue aims to publish manuscripts dealing with novel computational approaches in drug design by considering both methodological and applicative studies, with a view to offering a picture of the fields in which computational chemistry can impact the drug discovery process.

Guest Editor

Prof. Dr. Giulio Vistoli
Department of Pharmaceutical Sciences, Università degli Studi di Milano, via Mangiagalli 25, 20133 Milano, Italy

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International Journal of Molecular Sciences
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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