





an Open Access Journal by MDPI

The Future of Force Fields in Computational Medicinal Chemistry

Guest Editors:

Dr. Agnieszka Bronowska

Chemistry – School of Natural and Environmental Sciences, Newcastle University, Newcastle, UK

Dr. Dominik Gront

Department of Chemistry, University of Warsaw, Warsaw, Poland

Deadline for manuscript submissions:

closed (29 June 2021)

Message from the Guest Editors

Dear Colleagues,

Molecular force fields are the cornerstone of modern biomolecular simulations, enabling structure-guided drug design; multiscale molecular modeling; molecular dynamics simulations of macromolecular complexes; studies of protein folding, misfolding, and aggregation; and the discovery of novel "druggable" sites. Empirical force fields, traditionally used in atomistic MD simulations and molecular docking algorithms, are undergoing continuing improvements. However, existing limitations and inaccuracies of contemporary force fields limit their applicability.

This Special Issue will focus on the approaches crucial for the successful design of next-generation force fields. Recent improvements in protein force fields will be overviewed, including polarizable and reactive force fields, and scoring functions suitable for ensemble, adaptive, and covalent docking. Improved parameters, electrostatics, and solvation modelling will be included, regarding their accuracy in modeling challenging systems. Studies involving theoretical underpinning, applications of these new force fields, and some recent benchmarks will be covered













an Open Access Journal by MDPI

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

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.

Author Benefits

Open Access: free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility: indexed within Scopus, SCIE (Web of Science), PubMed, PMC, MEDLINE, Embase, CAPlus / SciFinder, and other databases.

Journal Rank: JCR - Q1 (*Biochemistry & Molecular Biology*) / CiteScore - Q1 (*Inorganic Chemistry*)

Contact Us