Special Issue

The Future of Force Fields in Computational Medicinal Chemistry

Message from the Guest Editors

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.

Guest Editors

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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.

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