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The Future of Force Fields in Computational Medicinal Chemistry

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Deadline for manuscript submissions:
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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.

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Message from the Editor-in-Chief

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