



Computational Modelling of Biological Processes with Peptides and Proteins

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Message from the Guest Editor

This Special Issue focused on the current state-of-the-art of modeling of important biological phenomena of peptides and proteins, including protein folding/misfolding, aggregation, diffusion, and enzyme catalysis from all-atom to coarse-grained simulations.

Papers are sought that discuss the latest research in the area or summarize selected areas of the field. The scope of the Special Issue encompasses the modeling, simulation, and characterization of processes of peptides and proteins, especially with enhanced sampling methods such as replica-exchange molecular dynamics, metadynamics, simulated annealing, enhanced Monte Carlo methods or Brownian dynamics.

Of particular interest are the characterization of intrinsic disordered proteins (IDPs), the simulation of the effect of pH, and the importance of charge regulation in macromolecular interactions, diffusion, and recognition.





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Message from the Editor-in-Chief

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