Special Issue

Computational Modelling of Biological Processes with Peptides and Proteins

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.

Guest Editor

Dr. Sergio Madurga

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Deadline for manuscript submissions

closed (30 September 2020)

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Message from the Editor-in-Chief

Since its foundation in 2009, *Polymers* has developed into an internationally renowned, extremely successful open access journal. The editorial team and the editorial board dedicatedly combine open-access publishing and high-quality rigorous peer reviewing. The performance of the journal has proven this strategy to be well-suited and highly successful. This is reflected in the increasing impact factor of *Polymers*, the most recent one being 4.7.

I would like to invite you to contribute to the success of the journal by sending us your high quality research papers. We would be pleased to welcome you as one of our authors.

Editor-in-Chief

Prof. Dr. Alexander Böker
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