



Simulational and Computational Approaches to Enhance Protein Inhibitor Designs

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Deadline for manuscript
submissions:

closed (30 September 2022)

Message from the Guest Editors

Dear Colleagues,

Protein inhibitors' (which include small compounds, proteins, peptides, and antibodies) interactions with drug targets commonly involve the surface of the protein inhibitor or a complex of proteins that can potentially be disrupted or stabilized by small compounds, proteins, peptides, or antibodies that penetrate the cell. This is in contrast to small compounds, proteins, peptides, or antibodies' target proteins, whose activity can be measured in a biophysical, biochemical, or theoretical assay. Due to the growing interest in this field, this Special Issue aims to publish high-quality original research papers on the experimental and theoretical applications of protein-inhibitor interactions.

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Guest Editors





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Message from the Editor-in-Chief

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