Special Issue

Simulational and Computational Approaches to Enhance Protein Inhibitor Designs

Message from the Guest Editors

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.

Guest Editors

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As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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