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Spectroscopic, Thermodynamic and Molecular Docking Studies on Molecular Mechanisms of Drug Binding to Proteins

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Deadline for manuscript submissions:
closed (31 May 2022)

Message from the Guest Editors

Dear Colleagues,

Biological macromolecules interact with each other or ligands to form complexes. Quantifying the binding of chemical entities to a protein is an important early screening step during drug discovery and is of fundamental interest for estimating safety margins during drug development. Since recognition of their importance at the beginning of the 20th century, investigations into binding parameters have received significant attention. Spectroscopy has emerged as an invaluable tool for such studies, proving to be more efficient and cost-effective. A detailed understanding of protein–ligand interactions is therefore central to understanding biology at a molecular level. Moreover, knowledge of the mechanisms responsible for protein–ligand recognition and binding will also facilitate the discovery, design, and development of drugs.

It is a pleasure to invite you to contribute to this Special Issue. We aim to collect contributions in the form of original research articles and review articles to add new insights into the role of spectroscopic, thermodynamic and molecular docking studies in drug–protein interactions in biological processes.

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Message from the Editor-in-Chief

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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