Special Issue

Computational Chemistry of Pharmaceutical and Biomolecules

Message from the Guest Editor

We promote publications that combine theoretical and experimental approaches. The structural insights gained from the studies should be related to the properties, function and reactivity of the molecule under investigation and the interactions of this molecule and its implications should be discussed. Drug discovery is a critical issue in pharmaceutical research as it is a very cost-effective and time-consuming process for producing a new drug candidate. There are a number of computational advances which have significant impact in the field of computer-aided drug design over the last several years. These advances can be grouped into three basic areas: conformational modeling (of small molecules, macromolecules and their complexes), property modeling (of physical, biological and chemical properties) and molecular design (to optimize physical, biological or chemical properties). Hence, computational approaches have provided a tremendous opportunity to pharmaceutical companies to identify new potential drug targets, which in turn affect the success and time of performing clinical trials for discovering new drug targets.

Guest Editor

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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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