



Computational Chemistry of Pharmaceutical and Biomolecules

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Message from the Guest Editor

Dear Colleagues,

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.





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Message from the Editor-in-Chief

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