Special Issue

Application of Computational Methods in Drug Design

Message from the Guest Editors

The proposed workshop, entitled "*DesignIT-TO-LEAD: 1st Computational Medicinal Chemistry WorkShop*" is intended as a first trial to establish regular workshops in drug design on a biennual based frequency. The *DesignIT-TO-LEAD* will be organized at the Faculty of Science, University of Kragujevac, Republic of Serbia, from June 11 to June 15, 2018. The contribution of computational methodologies to drug discovery is no longer a matter of dispute, and all major world pharmaceutical and biotechnology companies use computational design tools. Computer-aided drug design encompasses computational methods and resources that are used to facilitate the design and discovery of new bioactive chemical entities. This workshop "*DesignIT-TO-LEAD: 1st Computational Medicinal Chemistry WorkShop*" will cover the main computational techniques currently used in the drug discovery process, supplying a basic level of knowledge of this field.
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As the premier open access journal dedicated to molecular chemistry, now in its 29th 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 all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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