Special Issue

Drug Design

Message from the Guest Editor

The treatment of diseases requires the design of drug molecules with defined properties in order to modulate the associated therapeutic targets. Drug design is therefore a key component of the drug discovery and development process to provide pharmacologically active substances with a particular function. Different approaches have been developed for the rational design of drug molecules with targeted properties: Structure-based, ligand-based, fragment-based, computer-aided, and de novo approaches, to name a few, have emerged over time and demonstrated their value. The design of drug molecules with tailored biological activity is a very creative process, which includes traditional small molecules as well as antibodies and biologics but also conjugates of these molecular entities. As this multidisciplinary field is rapidly progressing, the intention of this Special Issue is to cover current developments on all aspects related to drug design by original research and review articles.

Guest Editor

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As the premier open access journal dedicated to molecular chemistry, now in its 30th 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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