Special Issue

Recent Advances in Artificial Intelligence-Based Drug Discovery

Message from the Guest Editors

Drug discovery is the process through which potential new compounds are identified by means of biology, chemistry, and pharmacology. Billions of dollars are invested annually in research aimed at discovering, designing, and developing new drugs for a wide range of diseases. However, the research and development of novel drugs are still time-consuming and sometimes difficult to accomplish. With the development of new experimental techniques, vast amounts of datasets now flow through the different stages of drug development. Biomedical research, especially for the field of drug discovery, is currently experiencing a global paradigm shift with artificial intelligence (AI) technologies and their application to “Big Data”. Therefore, a key challenge for future drug discovery research is the development of powerful AI-based computational tools that can capture multiple dimensions of biomedical insights. We invite investigators to contribute research articles and reviews describing recent findings which use AI-based computational techniques for research in computer-aided drug discovery.

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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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