Special Issue

Recent Advance in QSAR Modelling and Related Methods for Rapid Screening of Pandemics Agents

Message from the Guest Editors

QSAR modeling is an integral part of rational drug design (RDD). Despite the prediction of biological activities, QSAR models help to identify the parameters responsible for biological response that is essential for lead compound optimization. In addition, recent developments in molecular docking have been successful in providing information such as relative orientation of drug molecule binding to their targeted receptor, leading to the optimization of lead compounds to achieve more potent and selective analogs. With the recent global pandemic of COVID-19, there is an immediate urge for rapid development and screening of pandemic agents against SARS-CoV-2 (anti-SARS-CoV-2 agents). QSAR-based screening can be successfully employed to screen and develop anti-SARS-CoV-2 agents from the existing drug database. This Special Issue of *Molecules* will consider submissions related to recent development of rapid predication of pandemic agents using QSAR and related methods. Assoc. Prof. Dr. Kok Hwa Lim

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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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