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Computational Chemical Biology

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Deadline for manuscript submissions:
closed (30 June 2019)

Message from the Guest Editors

Dear Colleagues,

The biological screening of compound collections continues to provide many new active chemical entities for further consideration. Large-magnitude screening campaigns typically require computational support for data analysis and the selection of preferred hits for follow-up studies. Here, the requirements for lead-like molecules in medicinal chemistry and probe-like compounds in chemical biology differ. Furthermore, the experimental studies must often be further extended through computational means. Computational chemical biology is tasked with delivering interpretation and prediction tools with significant potential to complement experimental investigations. This special issue aims to collect papers focusing on new computational methodologies, practical solutions, and perspectives with immediate relevance for chemical biology. Papers on diverse sub-topics, for example, molecular structure–selectivity analysis, single- and multi-target assay data exploration, or bioactivity modelling through artificial intelligence approaches including, but not limited to, machine learning are welcome.

Assoc. Prof. Dr. J. B. Brown
Prof. Dr. Jürgen Bajorath
Guest Editors

mdpi.com/si/16311

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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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Journal Rank: JCR - Q2 (*Chemistry, Multidisciplinary*) / CiteScore - Q1 (*Chemistry (miscellaneous)*)

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