Special Issue

Computational Chemical Biology

Message from the Guest Editors

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.

Guest Editors

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Message from the Editor-in-Chief

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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