Special Issue

Computational Approaches: Drug Discovery and Design in Medicinal Chemistry and Bioinformatics, 3rd Edition

Message from the Guest Editors

After the great success of the first two editions, we are pleased to inform you that *Molecules* will launch the third edition of the Special Issue "Computational Approaches: Drug Discovery and Design in Medicinal Chemistry and Bioinformatics".
https://www.mdpi.com/journal/molecules/special_issues/comput_appr_drug_dis_des_med_chem_bio
https://www.mdpi.com/journal/molecules/special_issues/comput_approach_drug_II In this latest Special Issue, we will continue to collect manuscripts concerning computational approaches that can improve the development of new drugs, or the repurposing of an old drug for the treatment of new diseases. This Special Issue welcomes submissions from researchers in the field of drug discovery and design, including original research and review articles related to pharmaceutical sciences, pharmacology, chemical biology, and bioinformatics. Papers combining both experimental and computational studies are encouraged.

Guest Editors

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Deadline for manuscript submissions

closed (31 January 2025)

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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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