

Special Issue

Conformations and Physicochemical Properties of Biological Ligands in Various Environments

Message from the Guest Editor

Understanding and describing the conformational landscape of druglike molecules is important in medicinal chemistry for the discovery of lead compounds and their optimization. The challenge of this quest is related to the fact that the conformational features of druglike molecules are strongly dependent on their environments. Furthermore, the biactive conformation of a ligand inside the target binding pocket is noticeably affected by induced fit. Therefore, the combination of experimental (from gas phase, solution to solid state environments) and theoretical approaches is a powerful means to decipher the effects underlying the conformational preferences observed. The invited papers will describe the conformational behavior of biological ligands, using a combination of experimental methods (for example either x-ray, NMR or gas phase studies) and quantum chemistry calculations, used to rationalize, through relevant descriptors, the observed preferences. Papers based on experimental observations in crystallographic databases compared with the results obtained through computational chemistry calculations are also welcome.

Guest Editor

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Deadline for manuscript submissions

closed (30 April 2021)



International Journal of Molecular Sciences

an Open Access Journal
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Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



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*International Journal of
Molecular Sciences*
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Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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