Special Issue

After AlphaFold2: Exploring beyond Its Limits

Message from the Guest Editor

AlphaFold2(AF2) has an enormous impact on the scientific and medical fields. AF2 can predict the three-dimensional structures of proteins from their primary amino acid sequence at high accuracy. Despite the achievement of significant breakthroughs, there is still room for development. Researchers have recognized the limitations of AF2, reporting that the prediction of the effect of missense mutations on proteins and conformational changes of proteins upon binding ions (or ligands) is challenged. The accuracy of their structural information is important for drug discovery and development. However, the prediction of conformational changes of kinases by AF2, so-called open and closed conformations, need to be approached in a cautious manner. In this Special Issue, we aim to collect new research and reviews that highlight any efforts to overcome AF2's limitations and the next generation of algorithms. In addition, the application of AF2 in predicting membrane proteins, kinases, and intrinsically disordered proteins (IDPs), and designing de novo proteins is encouraged.

Guest Editor

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Deadline for manuscript submissions

closed (20 August 2023)

International Journal of Molecular Sciences

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an Open Access Journal by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed

mdpi.com/si/158563

International Journal of Molecular Sciences
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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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