International Journal of
Molecular Sciences

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How Are Predicted Protein Structures Advancing the Development of New Drugs?

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Deadline for manuscript submissions:
20 February 2025

Message from the Guest Editor

Dear Colleagues,

Structural drug development has relied on having access to the three-dimensional structure of the protein or nucleic acid targets. This approach has been effective at enabling computational screening of molecular libraries containing as many as a billion small molecules and prioritizing those that can be utilized in experimental validation. However, given the available DNA and amino acid sequence data sets, the number of known high-resolution target structures is limited. There have been significant advances in the ability to predict the three-dimensional structure of proteins from their amino acid sequence. This Special Issue is soliciting articles that address:

1. How accurate is structure-based drug design in producing drugs that go on to be approved for clinical use?
2. Are there new generalizable approaches/methods that are proving to be more effective?
3. What is the effectiveness of using the newly predicted protein structures, i.e., are they accurate enough to supply the critically needed targets and lead to new drugs?

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Message from the Editor-in-Chief

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Journal Rank: JCR - Q1 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Inorganic Chemistry)

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