Special Issue

Molecular Dynamics Simulations of Protein Structures

Message from the Guest Editor

The International Journal of Molecular Sciences can announce a Special Issue dedicated to advancing the frontiers of molecular dynamics simulations in protein structure research. This Special Issue will highlight cutting-edge methodologies and breakthrough insights that are transforming our understanding of protein dynamics at an atomic level. As the of this Special Issue, I invite researchers to contribute original research articles, reviews that showcase pioneering computational methodologies, innovative simulation techniques, and novel theoretical frameworks to deepen our understanding of protein structure, folding, and function.

Areas of interest could include, but are not limited to, the following:

- Molecular dynamics simulations of protein structures;
- Advancements in computational methods for protein analysis;
- Drug discovery and target identification through molecular simulations;
- Machine learning and AI for protein folding and stability studies;
- Hybrid methods combining experimental and computational techniques;
- Enhanced sampling techniques in molecular dynamics.

Guest Editor

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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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