

## Special Issue

# Molecular Dynamics Simulations in Structural Biology: From Proteins to Complex Biomolecular Systems

### Message from the Guest Editor

This Special Issue The purpose of this is to gain insights into the atomic structures and the temporal evolution of proteins, including experimental techniques, as well as mathematical and computational modeling approaches for the comprehension of biological function. There is also interest in molecular interactions involved in the protein function and molecular docking. It is known that the role biological of new proteins is usually very complicated to determine. For this reason, dynamic simulations are extraordinary tool for predicting the behavior in the binding side. Therefore, the objective of this Special Issue is to publish high-quality articles, including original research, reviews, short communications, and clinical reports on diagnosis, investigation, and treatment, where the proteins and their biocomplexes are participants at the molecular level.

### Guest Editor

Dr. Ana E. Ledesma

1. Centro de Investigación en Biofísica Aplicada y Alimentos (CIBAAL-UNSE-CONICET), Universidad Nacional de Santiago del Estero, Santiago del Estero 4206, Argentina
2. Facultad de Ciencias Exactas y Tecnologías, Departamento Académico de Química, Universidad Nacional de Santiago del Estero, Santiago del Estero 4200, Argentina

### Deadline for manuscript submissions

31 July 2026



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Impact Factor 3.0  
CiteScore 3.7  
Indexed in PubMed



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Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[cimb@mdpi.com](mailto:cimb@mdpi.com)

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## About the Journal

### Message from the Editor-in-Chief

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#### Editor-in-Chief

Prof. Dr. Madhav Bhatia

Department of Pathology and Molecular Medicine, University of Otago,  
Christchurch 8140, New Zealand

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