

Special Issue

Protein Unfolding Induced by Chemical Agents

Message from the Guest Editors

Protein folding and unfolding has been an important research area since the Anfinsen dogma was established. We know that biologically important proteins work best around room temperature, atmospheric pressure, neutral pH, and in the absence of chemicals (e.g. small, organic molecules). However, the equilibrium that favours folded protein conformation can be shifted by changing any of the conditions mentioned above. Here, we aim at chemical unfolding as it has pharmaceutical importance. Importantly, folding and unfolding time scales are generally too fast for straight experimental (e.g. NMR, AFM, FRET) observations. Therefore, often the equilibria are studied by physical methods as shifted to irreversible „denatured” states. Sometimes even the unfolded states are interesting because they provide insight into the nature of disordered proteins (IDPs). In addition to experimental techniques, in-silico, molecular dynamics simulations may be of help for understanding the mechanism of chemical denaturation.

Guest Editors

Prof. Dr. Gyula Batta

Faculty of Science and Technology, Institute of Chemistry, Department of Organic Chemistry, University of Debrecen, H-4032 Debrecen, Hungary

Dr. Orsolya Tőke

Research Centre for Natural Sciences, Centre for Structural Science, H-1117 Budapest, Hungary

Deadline for manuscript submissions

20 March 2025



International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 8.1
Indexed in PubMed



mdpi.com/si/196442

*International Journal of
Molecular Sciences*
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
ijms@mdpi.com

mdpi.com/journal/

[ijms](https://www.mdpi.com/ijms)





International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 8.1
Indexed in PubMed



[mdpi.com/journal/](https://mdpi.com/journal/ijms)

ijms



About the Journal

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.

Editor-in-Chief

Prof. Dr. Maurizio Battino

Department of Odontostomatologic and Specialized Clinical Sciences,
Sez-Biochimica, Faculty of Medicine, Università Politecnica delle
Marche, Via Ranieri 65, 60100 Ancona, Italy

Author Benefits

Open Access:

free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, PMC, MEDLINE, Embase, CAPlus / SciFinder, and other databases.

Journal Rank:

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