Special Issue

Research on Biological Characteristics of Macromolecular Crystals

Message from the Guest Editors

With increasing demands for faster and more effective drug development, structure-based drug design (SBDD) has gained increasing attention. By investigating macromolecular crystals, particularly protein and nucleic acid crystals, researchers can uncover the precise three-dimensional arrangements of these macromolecules, which allows for the identification of potential binding sites that are critical for their biological function and the design of molecules that can specifically interact with these sites to modulate their activity. This Special Issue aims to present an update on the advancements and emerging trends in the biological characteristics of macromolecular crystals, including drug target identification, post-translational modifications, synthetic biology and artificial macromolecules, computational structural biology, etc. Keywords:

- protein/peptide crystals
- DNA/RNA crystals
- biological functions of macromolecules
- drug target identification
- computational structural biology
- high-resolution microscopy
- synthetic macromolecules

Guest Editors

Dr. Jingxiang Yang

State Key Laboratory of Elemento-Organic Chemistry, College of Chemistry, Nankai University, Tianjin 300071, China

Dr. Wenchao Yang

College of Chemistry, Nankai University, Tianjin 300071, China

Deadline for manuscript submissions

20 August 2025



Applied Sciences

an Open Access Journal by MDPI

Impact Factor 2.5 CiteScore 5.5



mdpi.com/si/226697

Applied Sciences
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
applisci@mdpi.com

mdpi.com/journal/applsci





Applied Sciences

an Open Access Journal by MDPI

Impact Factor 2.5 CiteScore 5.5



About the Journal

Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal Applied Sciences has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multidimensional network.

Editor-in-Chief

Prof. Dr. Giulio Nicola Cerullo

Dipartimento di Fisica, Politecnico di Milano, Piazza L. da Vinci 32, 20133 Milano, 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), Ei Compendex, Inspec, CAPlus / SciFinder, and other databases.

Journal Rank:

JCR - Q2 (Engineering, Multidisciplinary) / CiteScore - Q1 (General Engineering)

