

Special Issue

Catalysts for Structure-Functional Analysis and Enzyme Optimization

Message from the Guest Editors

The knowledge of an enzyme's catalytic mechanism can be of fundamental importance and a critical factor in the design and synthesis of compounds having biotechnological or therapeutic potential. The research is therefore multidisciplinary by its very nature and includes mechanistic enzymology, recombinant DNA (site-directed mutagenesis), as well as organic synthesis, medicinal/bioorganic chemistry, supramolecular chemistry, molecular modeling, and structural biology. Using the tools of chemo-organic synthesis, biochemistry, and computer modeling, this work aims to provide increased understanding of the chemical principles underlying mechanisms of action of natural catalysts with targeted activity. Structural models of the substrate enzyme complex are useful in order to investigate in detail the roles of the enzyme amino acid residues in its activity and the scope and limitation of substrates. We invite researchers to contribute into this Special Issue in order to share their up-to-date knowledge on structure-functional aspects of enzyme functionality and achievements in engineering enzymes with new catalytic activity.

Guest Editors

Dr. Anna A. Kulminskaya

Petersburg Nuclear Physics Institute named by B.P. Konstantinov of National Research Center "Kurchatov Institute", Mkr. Orlova Roshcha, 1, 188300 Gatchina, Russia

Dr. Vladimir V. Egorov

Department of Molecular and Radiation Biophysics, Petersburg Nuclear Physics Institute Named by B. P. Konstantinov of National Research Center "Kurchatov Institute", 188300 Gatchina, Russia

Deadline for manuscript submissions

closed (10 January 2022)



Catalysts

an Open Access Journal
by MDPI

Impact Factor 4.0
CiteScore 7.6



mdpi.com/si/52993

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

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





Catalysts

an Open Access Journal
by MDPI

Impact Factor 4.0
CiteScore 7.6



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



About the Journal

Message from the Editor-in-Chief

Editor-in-Chief

Prof. Dr. Keith Hohn

Carl R. Ice College of Engineering, Kansas State University, Manhattan,
KS, USA

Author Benefits

High Visibility:

indexed within Scopus, SCIE (Web of Science), Inspec, Ei Compendex, CAPlus / SciFinder, CAB Abstracts, and other databases.

Journal Rank:

JCR - Q2 (Chemistry, Physical) / CiteScore - Q1 (General Environmental Science)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 15.9 days after submission; acceptance to publication is undertaken in 3.5 days (median values for papers published in this journal in the second half of 2025).