

Special Issue

Organocatalysis: Mechanistic Investigations, Design, and Applications

Message from the Guest Editor

Catalysis remains one of the most challenging topics in contemporary organic chemistry. Because of the absence of transition metals, organocatalytic methods are attractive for the preparation of pharmaceutical compounds where levels of certain metal-ion contamination are tightly controlled. While the asymmetric organocatalysis field is currently growing exponentially, an understanding of the mechanistic details involved in most of these reactions has often lagged far behind the pace of catalyst development, which retards catalyst design. However, over the last two decades, computational methods have become a cost-effective treatment of large chemical systems with reasonable accuracy. Remarkably, density functional theory (DFT) has been especially useful in the field of organic chemistry in order to elucidate the mechanisms behind chemical reactions. This Special Issue focuses on synthetic and computational organic chemistry and their contributions to enlarge and enhance our understanding of organocatalysis. This will include studying, predicting, understanding, and validating chemical reactivity in catalytic systems.

Guest Editor

Dr. Cristina Trujillo

Trinity Biomedical Sciences Institute, School of Chemistry, Trinity Dublin College, D02 R590 Dublin 2, Ireland

Deadline for manuscript submissions

closed (30 June 2022)



Catalysts

an Open Access Journal
by MDPI

Impact Factor 4.0
CiteScore 7.6



mdpi.com/si/58790

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).