

Special Issue

Research on Crystal Structures of Metal Complexes

Message from the Guest Editor

In the field of coordination chemistry, clarifying the 3D structure of metal complexes is as important as promoting science that utilizes this information, for example, proving that a compound has been synthesized correctly; determining the stereochemistry and isomers of a compound beyond the composition and atomic bonds obtained in identification analysis; elucidating the possibility of intermolecular interactions and supramolecular formation; and combining three-dimensional structures, such as docking with complex functional materials (porous materials and guest molecules) and nucleic acids and proteins (biomolecules, pharmaceuticals, etc.) including metal complexes. We welcome original research papers and reviews on the following topics: the principles of and equipment used for crystal structure analysis (devices, quantum beams, crystallization, and sample preparation), analysis programs, mathematical algorithms, compound structure reports, computational chemistry, data derived from crystal databases, etc., for metal complex studies.

Guest Editor

Prof. Dr. Takashiro Akitsu

Department of Chemistry, Faculty of Science, Tokyo University of Science, Tokyo, Japan

Deadline for manuscript submissions

30 April 2026



Molecules

an Open Access Journal
by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed



mdpi.com/si/252123

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

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





Molecules

an Open Access Journal
by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed



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



About the Journal

Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

Author Benefits

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, MEDLINE, PMC, Reaxys, CaPlus / SciFinder, MarInLit, AGRIS, and other databases.

Journal Rank:

JCR - Q2 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the first half of 2025).