

## Special Issue

# Molecular Spectroscopy and Computations of Solvation Phenomena of Bioorganic Molecules: New Insights and Applications

### Message from the Guest Editors

The structure and dynamics of ionic solvation are some of the most attractive subjects in chemistry, and numerous studies have been published since 1930s. Thus, a fairly large number of monographs summarizing results of various scattering and spectroscopic methods and quantum chemical calculations have been published. On the contrary, solvation phenomena of bioorganic compounds have received less attention, although they are of fundamental importance in a variety of chemical, physical, and biological processes. X-ray crystallography can provide high-resolution structural data of bioorganic molecules; however, the static structures obtained and the limited number of solvent molecules from crystalline samples do not provide sufficiently accurate descriptions of solvent binding and dynamics. We aim to underscore the recent advances of solvation phenomena in determining critical structural, thermodynamic, and dynamic properties of bioorganic molecules not only for specialists but also for neophytes in this exciting field.

### Guest Editors

Prof. Dr. Teobald Kupka

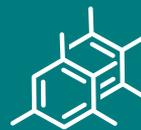
Institute of Chemistry, University of Opole, 48, Oleska Street, 45-052 Opole, Poland

Prof. Dr. Ioannis P. Gerotheranassis

Section of Organic Chemistry & Biochemistry, Department of Chemistry, University of Ioannina, GR-45110 Ioannina, Greece

### Deadline for manuscript submissions

30 May 2026



## Molecules

an Open Access Journal  
by MDPI

Impact Factor 4.6  
CiteScore 8.6  
Indexed in PubMed



[mdpi.com/si/229738](https://mdpi.com/si/229738)

*Molecules*  
Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[molecules@mdpi.com](mailto: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 30th 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 15.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the second half of 2025).