



## Computer-Aided Screening and Action Mechanism of Bioactive Peptides

Guest Editor:

**Prof. Dr. Zhipeng Yu**

School of Food Science and  
Engineering, Hainan University,  
Haikou 570228, China

Deadline for manuscript  
submissions:

**closed (31 August 2023)**

### Message from the Guest Editor

Dear Colleagues,

Interest in research into bioactive peptides is growing because of their health-promoting ability. Several bioactivities have been ascribed to peptides, including antioxidant, antihypertensive, and antimicrobial properties. The implementation of a peptide's potential biological effect depends largely on its structure and bioavailability. The purpose of this Special Issue is to report the recent progress achieved in virtual screening and action mechanism of bioactive peptides. This includes, but is not limited to, isolation and identification of peptides, molecular docking, prediction, proteomics, metabolomics, bioavailability, permeability of peptides, and network pharmacology. The bioinformatics tools and databases assisting action mechanism are also welcomed.

Prof. Dr. Zhipeng Yu  
*Guest Editor*





an Open Access Journal by MDPI

## Editor-in-Chief

### Prof. Dr. Maurizio Battino

Department of  
Odontostomatologic and  
Specialized Clinical Sciences,  
Sez-Biochimica, Faculty of  
Medicine, Università Politecnica  
delle Marche, Via Ranieri 65,  
60100 Ancona, Italy

## Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

## 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), PubMed, PMC, MEDLINE, Embase, CAPlus / SciFinder, and other databases.

**Journal Rank:** JCR - Q1 (*Biochemistry & Molecular Biology*) / CiteScore - Q1 (*Inorganic Chemistry*)

## Contact Us

*International Journal of Molecular  
Sciences* Editorial Office  
MDPI, St. Alban-Anlage 66  
4052 Basel, Switzerland

Tel: +41 61 683 77 34  
www.mdpi.com

mdpi.com/journal/ijms  
ijms@mdpi.com  
X@IJMS\_MDPI