

## Special Issue

# Computer Simulation on Membrane Receptors

### Message from the Guest Editor

Cellular membranes contain membrane receptors which mediate signal transduction for cellular responses to extracellular stimuli. These receptors are transmembrane proteins, and are classified by structure and related function. They are associated with G-proteins, ion channels, and tyrosin-chinase receptors. The domain of the receptor exposed to the external medium often has a binding site for a ligand. The domain exposed to the cytoplasm activates intracellular proteins such as kinases, G-proteins, guanylate cyclase, ion transporters, among a myriad of other functions. In this Special Issue, we want to focus on various types of simulation aimed at elucidating the structure and the function of these receptors. In addition, studies related to a rational drug design approach with a membrane receptor as target are welcome. Potential topics include, without being limited to, the following:

- Molecular dynamics simulation of ion channels
- Computer aided drug design targeted at membrane receptors
- Ligand-receptor dynamics
- Function and structure of membrane receptors
- Coarse grained molecular dynamics of receptor association and oligomerization

---

### Guest Editor

Dr. Roberta Galeazzi

Department of Life and Environmental Sciences, Marche Polytechnic University, 60131 Ancona, Italy

---

### Deadline for manuscript submissions

closed (28 September 2019)



## International Journal of Molecular Sciences

---

an Open Access Journal  
by MDPI

---

Impact Factor 4.9  
CiteScore 9.0  
Indexed in PubMed



[mdpi.com/si/20480](https://mdpi.com/si/20480)

*International Journal of  
Molecular Sciences*  
Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[ijms@mdpi.com](mailto:ijms@mdpi.com)

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





# International Journal of Molecular Sciences

---

an Open Access Journal  
by MDPI

---

Impact Factor 4.9  
CiteScore 9.0  
Indexed in PubMed



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



## About the Journal

### Message from the Editor-in-Chief

The *International Journal of Molecular Sciences (IJMS)* 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, and molecular biophysics. *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.

---

### Editor-in-Chief

Prof. Dr. José L. Quiles  
Department of Physiology, Institute of Nutrition and Food Technology  
"Jose Mataix", Biomedical Research Center, University of Granada,  
Avda. Conocimiento s/n, 18100 Armilla, Granada, Spain

---

### 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, CAPus / SciFinder, and other databases.

#### Journal Rank:

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