



Computational Diagnostics and Therapeutics for COVID-19 and Other Associated Viral Infections

Guest Editors:

**Prof. Dr. Natarajan Arul
Murugan**

Department of Computational
Biology, Indraprastha Institute of
Information Technology, New
Delhi, India - 110020 Theoretical
Photochemistry and
Photophysics Group, Faculty of
Chemistry, Wrocław University of
Science and Technology,
Wrocław PL-50370, Poland

Prof. Dr. G. Narahari Sastry

CSIR - North East Institute of
Science & Technology (CSIR-
NEIST), Jorhat, Assam, India

Deadline for manuscript
submissions:

closed (30 September 2022)

Message from the Guest Editors

Dear Colleagues,

COVID-19, caused by the SARS-CoV-2 virus, has become the most devastating health care challenge of this century. The outbreaks caused by SARS and MERS coronaviruses, swine- and avian-origin influenza, and Ebola and Zika viruses cannot be overlooked. This Special Issue is devoted to promoting research in the area of the computational development of diagnostics and therapeutics for COVID-19 and other associated viral infections. We recommend the submission of articles where the results from computational screening (molecular docking) or de novo design are validated using either experimental techniques or by employing more accurate and reliable approaches with superior ranking potential. In particular, we encourage authors to submit articles based on computational approaches for identifying lead compounds which employ scoring functions based on electronic structure theory, machine learning, or deep learning. Regarding the design of diagnostic compounds, the coverage is not limited to optical or infrared probes, but studies devoted to diagnostic platforms using biosensors and bioelectronics will also be considered.





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

Contact Us

International Journal of Molecular
Sciences Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

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

mdpi.com/journal/ijms
ijms@mdpi.com
X@IJMS_MDPI