

Special Issue

Computational Modelling at the Blood–Brain Barrier

Message from the Guest Editor

This Special Issue is dedicated to all aspects of the computational work of blood–brain barrier (BBB), including work on structural modeling, molecular dynamics simulations of the BBB, novel asymmetric BBB membranes, Bayesian CNS penetration models, drug discovery beyond the 'rule-of-five', neural networks for assessing CNS penetration, efflux pump in the BBB, the BBB glycocalyx, and in silico validation of experimental studies, among others. When considering your submission, please remember that IJMS is a journal of molecular science. However, this Special Issue will welcome submissions of any type of computational work on CNS drug delivery.

Guest Editor

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Deadline for manuscript submissions

20 November 2025



International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



mdpi.com/si/211668

*International Journal of
Molecular Sciences*
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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.

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