Special Issue

Simulation and Artificial Intelligence Method Development for Complex Membrane Transport

Message from the Guest Editor

Recent advances in the field of molecular simulation and artificial intelligence have resulted in staggering advances in our understanding of drug delivery through complex membranes. Such discoveries have included the atomic-detail mechanisms of small-molecule permeation, the calculation of simulated permeabilities as a stand-alone value alongside experimental permeabilities, the prediction of transmembrane permeabilities, and the generation of novel findings about key drug delivery routes, among others. This Special Issue is dedicated to all aspects of molecular simulations and artificial intelligence developments related to membranes. When considering your submission, please note that *Membranes* is a journal that covers the broad aspects of the science and technology of both biological and non-biological membranes. This Special Issue will welcome submissions of any type of computational work on membranes.

Guest Editor

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Deadline for manuscript submissions

10 May 2026

Membranes

an Open Access Journal by MDPI

Impact Factor 3.6
CiteScore 7.9
Indexed in PubMed

mdpi.com/si/256086

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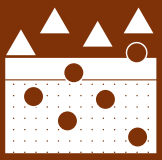

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Message from the Editor-in-Chief

You are cordially invited to contribute a research article or a comprehensive review for consideration and publication in *Membranes* (ISSN 2077-0375). *Membranes* is an international, peer-reviewed open accessjournal of membrane technology published monthly online by MDPI. The journal covers the broad aspects of the science and technology of both biological and non-biological membranes, including membrane dynamics and the preparation and characterization of membranes and their applications in water, environment, energy, and food industries. Articles contributing to better understanding of transport processes in all types of membranes are also welcome. The scientific community and the general public have unlimited and free access to the content as soon as it is published. We would be pleased to welcome you as one of our authors.

Editor-in-Chief

Prof. Dr. Spas D. Kolev
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