



an Open Access Journal by MDPI

The Role of Molecular Docking in the Design of Targeted Therapeutic Entities and Nanomaterials

Guest Editors:

Prof. Mahmoud Elsabahy

1. Department of Chemistry,
Texas A&M University, College
Station, TX, USA
2. Science Academy, Badr
University in Cairo, Badr City,
Egypt

Dr. Noura G. Eissa

1. Department of Pharmaceutics,
Faculty of Pharmacy, Zagazig
University, Zagazig 44519, Egypt
2. Science Academy, Badr
University in Cairo, Badr City,
Cairo 11829, Egypt

Deadline for manuscript
submissions:

25 March 2024

Message from the Guest Editors

Molecular docking has become a useful computational technique for aiding in drug design by providing insights on interactions and dynamics of molecules and nanomaterials within biological systems. The docking of therapeutic entities and/or nanomaterials enables the prediction of preferred orientations and binding capacities of the developed therapeutics and nanostructures with the target site, thus, providing the capability to predict and achieve superior pharmacological activities. Given the wide variety of pharmacological targets and biomedical applications of nanoconstructs, this research area has received considerable interest.

Accordingly, authors are invited to submit high-quality research articles regarding topics such as, but not limited to, molecular docking studies for designing novel compounds and/or nanomaterials for various biomedical applications. Review submissions highlighting the latest advances in the study of the design and biological interactions of novel active entities (i.e., active molecules and nanomaterials) with pharmacological targets are also encouraged.



mdpi.com/si/146571

Special Issue



an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Amélia Pilar Rauter

Departamento de Química e Bioquímica (DQB) e Centro de Química e Bioquímica (CQB), Faculdade de Ciências, Universidade de Lisboa (FCUL), Rua Ernesto de Vasconcelos, Campo Grande, Edifício C8, 5º Piso, 1749-016 Lisboa, Portugal

Message from the Editor-in-Chief

Because of your expertise in the field of drug sciences, I kindly invite you to consider publishing your current work, in the form of a research article or a review, in the open access electronic journal *Pharmaceuticals*.

Pharmaceuticals is characterized by an active editorial board and a dynamic editorial staff. Manuscripts are peer-reviewed and a final decision is provided to authors within 4–6 weeks after submission. Papers are published on the web immediately after acceptance. For details on the submission process or any other matter, please do not hesitate to contact us.

We hope to handle your contribution to *Pharmaceuticals* soon.

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, Embase, CAPlus / SciFinder, and other databases.

Journal Rank: JCR - Q2 (*Pharmacology & Pharmacy*) / CiteScore - Q2 (*Pharmaceutical Science*)

Contact Us

Pharmaceuticals
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

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

mdpi.com/journal/pharmaceuticals
pharmaceuticals@mdpi.com