



an Open Access Journal by MDPI

## Applications of Conceptual Density Functional Theory to the Chemistry and Discovery of Bioactive Compounds

Guest Editors:

**Prof. Dr. Chia Ming Chang**

Department of Soil and  
Environmental Sciences,  
National Chung Hsing University,  
Taichung 40227, Taiwan

**Prof. Dr. Pratim Kumar  
Chattaraj**

Indian Institute of Technology  
Kharagpur, Kharagpur, India

Deadline for manuscript  
submissions:

**closed (30 September 2022)**

### Message from the Guest Editors

It is well known that bioactive compounds are beneficial to human health and have therapeutic potential. It is necessary to understand the molecular mechanism to guide the rational design of synthetic analogues with improved biological activity and pharmacological properties. The significance of this Special Issue lies not only in the Conceptual DFT that can be used to explore the molecular mechanism of bioactive compounds, but also in providing a solid foundation for the design of new synthetic analogues. The structural characterization of bioactive compounds–biomacromolecule complexes is challenging to elucidate the structure–activity relationship. From a molecular point of view, the chemical reactivity and biological activity of bioactive compounds are correlated. Using Conceptual DFT, also known as chemical reactivity theory, we can predict their pKa values and biological activities. This Special Issue covers all types of bioactive compounds and collects original research and review articles on the mechanism of action and discovery from the perspective of conceptual DFT.



[mdpi.com/si/104332](https://mdpi.com/si/104332)

# 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 Estrutural (CQE), Institute of Molecular Sciences, Faculdade de Ciências, Universidade de Lisboa, 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, CAPus / SciFinder, and other databases.

**Journal Rank:** JCR - Q1 (Pharmacology and Pharmacy) / CiteScore - Q2 (*Pharmaceutical Science*)

## Contact Us

*Pharmaceuticals* Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland

Tel: +41 61 683 77 34  
[www.mdpi.com](http://www.mdpi.com)

[mdpi.com/journal/pharmaceuticals](http://mdpi.com/journal/pharmaceuticals)  
[pharmaceuticals@mdpi.com](mailto:pharmaceuticals@mdpi.com)