Special Issue

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

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.

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

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Pharmaceuticals
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
pharmaceuticals@mdpi.com

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

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

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