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Theoretical and Computational Chemistry in Antioxidant Research

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Message from the Guest Editors

The main aim of this Special Issue is to offer an overview of the potentiality of modern theoretical and computational methods to elucidate structural, electronic, spectroscopic, kinetic, and biomolecular properties of natural and newly synthetized antioxidant systems and their interactions with radicals. Contributions on acid-base equilibria in water, reaction mechanisms, metal chelation, Fenton reaction behaviors, enzyme inhibition, dynamical behaviors, new methods and computational procedures, de novo drug design, and reactivity indices are welcome, as well as other theoretical and computational aspects on the properties and antioxidant working mechanisms.

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Message from the Editor-in-Chief

It has been recognized in medical sciences that in order to prevent adverse effects of "oxidative stress" a balance exists between prooxidants and antioxidants in living systems. Imbalances are found in a variety of diseases and chronic health situations. Our journal *Antioxidants* serves as an authoritative source of information on current topics of research in the area of oxidative stress and antioxidant defense systems. The future is bright for antioxidant research and since 2012, *Antioxidants* has become a key forum for researchers to bring their findings to the forefront.

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