Special Issue

Antioxidant Discovery: Computational Modeling, Molecular Mechanisms and Therapeutic Applications

Message from the Guest Editor

The design of multifunctional antioxidants is a topic of great interest in the scientific community, mainly due to their therapeutic applications toward various disease types, including diabetes, different types of cancer, neurodegenerative diseases such as Alzheimer's (AD), Parkinson's (PD), and many others which affect the world's population. Regarding the latter, neuroprotective antioxidants that inhibit related enzymes, such as monoamine oxidase (MAO), catechol-o-methyl transferase (COMT), or acetyl choline esterase (AChE), have been proposed, and their design would be key to neurochemical research on the treatment of these types of illness. Even the elucidation of reaction mechanisms toward species that damage biomolecules and, therefore, cause diseases related to oxidative stress is of utmost importance, as well as their possible activities as repairers of damaged biomolecules. Thus, research related to the pharmaceutical industry is booming, as it will allow for the development of more effective, safe, and selective drugs.

Guest Editor

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