

## 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.

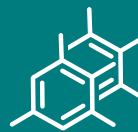
### Guest Editor

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### Deadline for manuscript submissions

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### Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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### Editor-in-Chief

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