## **Special Issue**

## From Electronic Structure to Application: Computational Insights into Bioactive and Functional Molecules

## Message from the Guest Editor

The search for new compounds with biological potential and the study of existing structures as drug candidates have become some of the most important tasks in modern chemistry. Currently, the fastest screening methods for evaluating the biological potential of molecules are techniques based on computational chemistry. Among these, the most popular and widely used include rule-based filtering, virtual high-throughput screening, similarity searching, molecular docking, and quantitative structure-activity relationships (QSAR).

Therefore, this Special Issue will focus on research concerning the structural properties of molecules based on reactivity descriptors, as well as their potential applications as biological agents and functional materials in various industries. In particular, we invite researchers to submit research and review articles on recent advances in this area.

## **Guest Editor**

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#### Deadline for manuscript submissions

15 January 2026



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## Message from the Editor-in-Chief

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#### **Editor-in-Chief**

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