Special Issue

Halogen Bonding: Insights from Computational Tools

Message from the Guest Editor

The distinctive features of halogen bonds have prompted their widespread application in many areas such as supramolecular chemistry, crystal engineering, catalysis, medicinal chemistry, and chemical biology, among others. Given their relevance, computational and molecular modeling methods are extremely helpful in the quest for further understanding the phenomenon or to guide new experimental work. Indeed, theoretical studies are in the frontline of quarrels concerning the nature of the halogen bond, and the study of solvent and substituent effects. This Special Issue aims to highlight the role of computational methodologies in the study of halogen bonds, ranging from the most common quantum mechanics calculations to force field-based methods. Therefore, original manuscripts reporting the application of computational tools in the study of halogen-bonded systems are encouraged. In addition, perspectives and reviews are also welcome.

Guest Editor

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Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th 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 multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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