Special Issue

Molecular Spectroscopy and Computations of Solvation Phenomena of Bioorganic Molecules: New Insights and Applications

Message from the Guest Editors

The structure and dynamics of ionic solvation are some of the most attractive subjects in chemistry, and numerous studies have been published since 1930s. Thus, a fairly large number of monographs summarizing results of various scattering and spectroscopic methods and quantum chemical calculations have been published. On the contrary, solvation phenomena of bioorganic compounds have received less attention, although they are of fundamental importance in a variety of chemical, physical, and biological processes. X-ray crystallography can provide high-resolution structural data of bioorganic molecules; however, the static structures obtained and the limited number of solvent molecules from crystalline samples do not provide sufficiently accurate descriptions of solvent binding and dynamics. We aims to underscore the recent advances of solvation phenomena in determining critical structural, thermodynamic, and dynamic properties of bioorganic molecules not only for specialists but also for neophytes in this exciting field.

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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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