

Special Issue

Advances in Computational Spectroscopy

Message from the Guest Editors

It is my great pleasure to invite you to submit an article for a Special Issue of *Molecules* on the theme “Advances in Computational Spectroscopy”. The increasing sophistication of the experimental spectroscopic techniques makes the results increasingly difficult to interpret without the help of computational chemistry. Computational spectroscopy connecting quantum mechanics, molecular spectroscopy and computational chemistry is constantly developing as a tool to provide predictions of spectroscopic characteristics and properties. It is our hope that this Issue will highlight the achievements in the field of computational spectroscopy on topics such as single-molecule studies as well as simulations of clusters and the solid state, research on organic molecules and inorganic complexes, basic studies as well as different application areas. Manuscripts describing original research, perspectives, and reviews focusing on computational spectroscopy will be welcome in this Special Issue.

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Deadline for manuscript submissions

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About the Journal

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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