

## Special Issue

# In Silico Methods Applied in Drug and Pesticide Discovery, 2nd Edition

### Message from the Guest Editors

Nowadays, there is a successful large-scale application of computational techniques (in silico methods) in the area of drug discovery, while a smaller involvement of these techniques has been noted in the field of agrochemistry. In silico methods are especially applied in the early stages of the research process, when basic studies aim to decipher the biology associated with the desired pharmacological/agrochemical response, prioritizing drug/pesticide targets, and identifying or optimizing new active chemical entities. The great advantages of computational methods consist of rapidity and cost-effectiveness compared with in vitro/vivo tests.

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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 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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