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

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Message from the Guest Editors

Dear Colleagues,

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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Guest Editors



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Special Issue



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Message from the Editor-in-Chief

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