Special Issue

Computational Strategy for Drug Design

Message from the Guest Editor

Rational drug discovery is one of the “holy grails” for modern medicine, and the marching developments in computational strategies have greatly revolutionized this area. Trans-omics analyses accelerate the elucidation of novel drug targets as well as facilitate the mechanistic characterization of drug resistance; ever-developing computational structural bioinformatic tools such as molecular dynamics (MD) simulation help to cast in-depth dynamic insights toward protein targets, guiding rational structure-based drug design. Moreover, marching progresses in mathematics and computer science such as artificial intelligence and deep learning all profoundly promote the field of computation-aided drug discovery. This current Special Issue aims to supply a forum for disseminating state-of-the-art advances in computational strategies applied to drug discovery. Both methodological breakthroughs and their cutting-edge applications on therapeutic agent development are of interest. We look forward to your contribution to this Special Issue.

Guest Editor

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