Special Issue

Recent Advances in Virtual Screening 2.0

Message from the Guest Editor

This Special Issue is the continuation of our previous special issue "Recent Advances in Virtual Screening". Finding new leads is an essential step in projects to develop and discover new drugs. There are two alternatives for achieving this goal: (a) experimentally testing compound libraries to find molecules that show any level of the desired bioactivity (a process known as high throughput screening and (b) a cheaper alternative that aims to computationally predict the bioactivity of interest in files containing molecular databases (known as virtual screening, VS). This Special Issue of IJMS will focus on recent advances in VS with particular emphasis on tools (either local or on-line) or databases that can be used for free for non-profit research or education. "Novel tools and VS must be either validated in silico or in vitro before first submission."

Guest Editor

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Deadline for manuscript submissions

closed (30 September 2021)



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Message from the Editor-in-Chief

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