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## Recent Advances in Drug Design

Guest Editor:

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Deadline for manuscript  
submissions:

**closed (30 September 2021)**

### **Message from the Guest Editor**

Dear Colleagues,

This Special Issue will focus on recent improvements on water mapping algorithms for SBDD and machine learning algorithms (neural networks, support vector machine, etc/) from researchers involved in computer science, which will suggest molecular descriptors of binding phenomena and tools from graph theory for mapping the binding area, aiming at filtering the best candidate molecules during a virtual screening procedure. Additionally, manuscripts that mainly describe computational studies should be accompanied by experimental validation.



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# Special Issue



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## Editor-in-Chief

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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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