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Special Issue Reprint

## Computational Approaches

**Edited by: Anna Maria Almerico and Marco Tutone**

This Special Issue is a collection of research articles in which computational methods were utilized for the development of new drugs, or the repurposing of an old drug for the treatment of new diseases. Moreover, these approaches helped to predict the metabolic fate of a drug candidate and to highlight the potential toxicity of the drug candidate, reducing the number of compounds to be tested. Virtual screening and machine learning tools were revealed to be of great interest in the field of pharmaceutical sciences, pharmacology, chemical biology, and bioinformatics.

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