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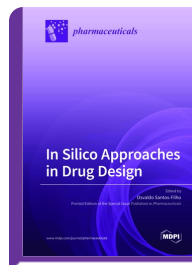
Special Issue Reprint

In Silico Approaches in Drug Design

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This reprint is a collection of 31 original papers and four reviews, published from 2021 to 2022, focused on the application of a wide range of computational tools in medicinal chemistry projects: from molecular docking to artificial intelligence approaches.

Applications of in silico tools are crucial in the early stages of drug design, such as planning more efficient and economic synthetic routes for chemical administration, screening of huge databases, as well as proposing hypotheses for probable mechanisms of action of drugs in macromolecular targets. Such endeavors are extremely complex and require the usage of modern and sophisticated approaches, such as artificial intelligence, data mining, computational molecular simulations through classical mechanics and quantum mechanics, molecular docking, chemoinformatics, applied mathematics, and biostatistics.



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