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Special Issue Reprint

In Silico Drug Design and Discovery

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This Reprint presents the Special Issue “In Silico Drug Design and Discovery: Big Data for Small-Molecule Design, 2nd Edition”, bringing together the editorial and eight peer-reviewed contributions that reflect current advances in computational strategies for small-molecule research. The collection covers structure-based modeling, molecular dynamics, virtual screening, chemoinformatics, drug target affinity prediction, reactive metabolite assessment, and generative artificial intelligence for molecular design. Across different therapeutic areas, the contributions show how data mining, bioinformatics, machine learning, and experimental validation can be combined to improve target analysis, lead identification, and hypothesis generation. By highlighting both methodological innovation and biologically relevant applications, this Reprint offers an updated overview of how big data-driven in silico approaches are reshaping modern drug discovery.

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