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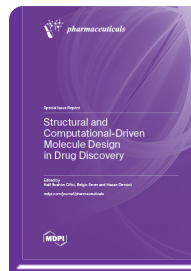
*Special Issue Reprint*

## **Structural and Computational-Driven Molecule Design in Drug Discovery**

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This Special Issue aimed to provide deep mechanistic insights into strategies in structural dynamics studies and computational methods. The areas of research included but were not limited to the following: structural dynamics studies, computer-aided drug designs, molecular dynamic simulations, molecular docking, virtual screening, QSAR, and in silico ADMET analyses.



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