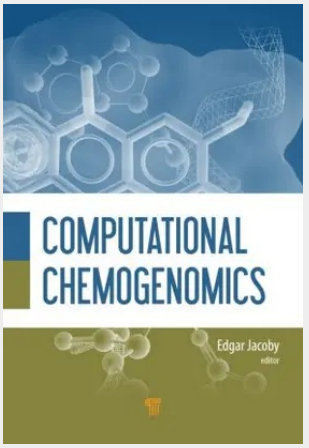
Jacoby

Computational Chemogenomics

This book focuses on applications of compound library design and virtual screening to expand the bioactive chemical space, to target hopping of chemotypes to identify synergies within related drug discovery projects or to repurpose known drugs, to propose mechanism of action of compounds, or to identify off-target effects by cross-reactivity analysis. Both ligand-based and structure-based in silico approaches, as reviewed in this book, play important roles for all these applications. Computational chemogenomics is expected to increase the quality and productivity of drug discovery and lead to the discovery of new medicines.



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