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presents contemporary research on molecular modeling techniques used in drug discovery and the drug development process: computer aided molecular design, drug discovery and development, lead generation, lead optimization, database management, computer and molecular graphics and the development of new computational methods.

Contents

- ▶ Computational Strategies to Incorporate GPCR Complexity in Drug Design
- ▶ Knowledge-Based Drug Repurposing: A Rational Approach Towards the Identification of Novel Medical Applications of Known Drugs
- ▶ Tuning the Solvation Term in the MM-PBSA/GBSA Binding Affinity Predictions
- ▶ Recent Advances in the Discovery and Development of Protein- Protein Interaction Modulators by Virtual Screening
- ▶ Computational Design of Biological Systems: From Systems to Synthetic Biology
- ▶ Considering the Medium when Studying Biologically Active Molecules: Motivation, Options and Challenges
- ▶ A Novel Coarse-Grained Description of Protein Structure and Folding by UNRES Force Field and Discrete Nonlinear Schrödinger Equation
- ▶ Computational Chemistry Strategies Tackling Function and Inhibition of Pharmaceutically Relevant Targets

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