Frontiers in Computational Chemistry

About the eBook

Frontiers in Computational Chemistry 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

- The Use of Dedicated Processors to Accelerate the Identification of Novel Antibacterial Peptides
- Computational Chemistry for Photosensitizer Design and Investigation of DNA Damage
- How to Judge Predictive Quality of Classification and Regression Based QSAR Models?
- Density Functional Studies of Bis-alkylating Nitrogen Mustards
- From Conventional Prodrugs to Prodrugs Designed by Molecular Orbital Methods
- Structural and Vibrational Investigation on a Benzoazin Derivative with Potential Antibacterial Activity
- First Principles Computational Biochemistry with deMon2k
- Recent Advances in Computational Simulations of Lipid Bilayer Based Molecular Systems
- Data Quality Assurance and Statistical Analysis of High Throughput Screenings for Drug Discovery

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