



## A Virtual Screening & Molecular Docking Study of Thiadiazoles:

By Utkarsh Raj

LAP Lambert Academic Publishing Feb 2012, 2012. Taschenbuch. Book Condition: Neu. 221x147x13 mm. This item is printed on demand - Print on Demand Neuware - In structure-based drug design, the three-dimensional structure of a drug target interacting with small molecules is used to guide drug discovery. 'Structure-based drug design represents the idea that you can see exactly how your molecule interacts with its target protein. This structural information can be obtained with X-ray crystallography or nuclear magnetic resonance spectroscopy (NMR). Originally, structure-based drug design was equated with de novo design or building a molecule from the ground up. Structure-based drug design relies on knowledge of the three dimensional structure of the biological target obtained through methods such as x-ray crystallography or NMR spectroscopy. If an experimental structure of a target is not available, it may be possible to create a homology model of the target based on the experimental structure of a related protein. As experimental methods such as X-ray crystallography and NMR develop, the amount of information concerning 3D structures of biomolecular targets has increased dramatically. Current methods for structure-based drug design can be divided roughly into two categories : Ligand-based drug design & receptor-based drug design. 56 pp....



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