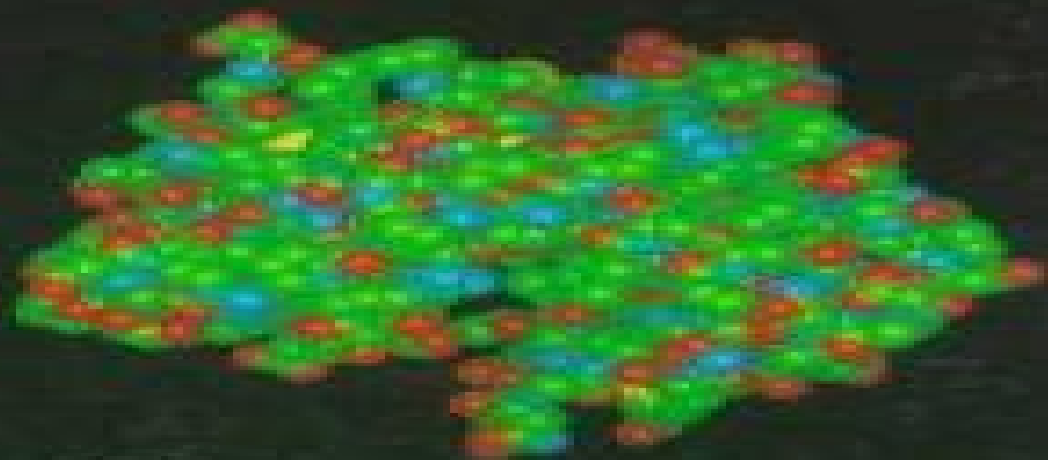
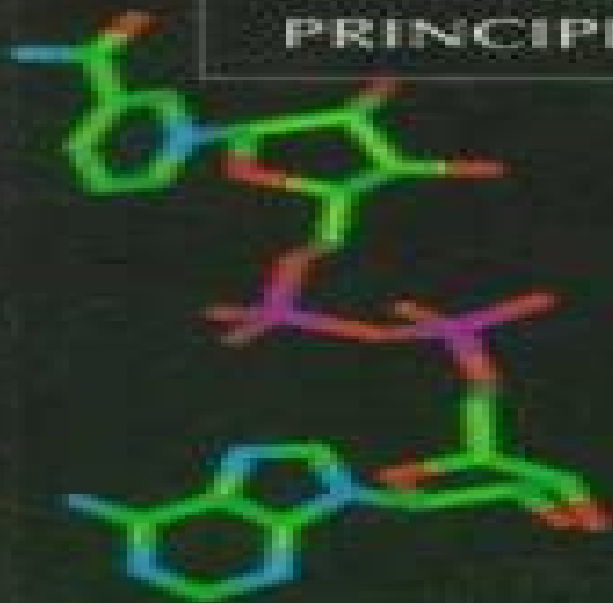


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MOLECULAR MODELLING PRINCIPLES AND APPLICATIONS



Molecular Modelling Principles And Applications

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been developed in the field of CDFT These methodologies have been used to explore mutual relationships between the descriptors of CDFT namely electronegativity hardness etc The mutual relationship between the electronegativity and the hardness depend on the electronic configuration of the neutral atomic species The volume attempts to cover almost all such methodology Conceptual Density Function Theory and Its Application in the Chemical Domain will be an appropriate guide for research students as well as the supervisors in PhD programs It will also be valuable resource for inorganic chemists physical chemists and quantum chemists The reviews research articles short communications etc covered by this book will be appreciated by theoreticians as well as experimentalists

Computational Tools for Chemical Biology Sonsoles Martín-Santamaría, 2017-10-25 The rapid development of efficient computational tools has allowed researchers to tackle biological problems and to predict analyse and monitor at an atomic level molecular recognition processes This book offers a fresh perspective on how computational tools can aid the chemical biology research community and drive new research Chapters from internationally renowned leaders in the field introduce concepts and discuss the impact of technological advances in computer hardware and software in explaining and predicting phenomena involving biomolecules from small molecules to macromolecular systems Important topics from the understanding of biomolecules to the modification of their functions are addressed as well as examples of the application of tools in drug discovery glycobiology protein design and molecular recognition Not only are the cutting the edge methods addressed but also their limitations and possible future development For anyone wishing to learn how computational chemistry and molecular modelling can provide information not easily accessible through other experimental methods this book will be a valuable resource It will be of interest to postgraduates and researchers in the biological and chemical sciences medicinal and pharmaceutical chemistry and theoretical chemistry

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Volume 3 Hans-Georg Elias, 2005 Providing a broad survey of the entire field Macromolecules integrates representations of chemistry physics and technology as well as including precise descriptions of basic phenomena and balanced treatments of facts and theory *QSAR and Molecular Modeling Studies in Heterocyclic Drugs II* S.P. Gupta, 2006-06-22

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Anne Christianson,1997 *Journal of the Physical Society of Japan* Nihon Butsuri Gakkai,2011 *Computer Aided Design of Selective Cytochrome P450 Inhibitors* Andreas Verras,2005 I have generated a virtual library of imidazole based compounds and used an altered form of the DOCK algorithm CovDOCK to screen these compounds against heme containing proteins I was able to generate high affinity ligands for P450cam An L244A mutant of P450cam was generated and used to test our ability to generate selective ligands Using our methods I was able to generate ligands which only inhibit the mutant enzyme The library was expanded with more substituted imidazoles and screened against a viable drug target Mycobacterium tuberculosis CYP51 After one round of compound development I was able to find micromolar inhibitors I also demonstrated that the methods and library are easily applicable to new protein systems To explore differences of the imidazole compounds in binding and inhibition I carried out stopped flow kinetics experiments and further UV spectroscopic studies I find that mono and disubstituted imidazoles bind distinctly to wild type P450cam The natural substrate also affects both classes of ligands uniquely To explore the mitigated affinity for imidazole of the L244A mutant I have done crystallography studies I report the structures of the substrate free mutant and imidazole co crystallized wild type and mutant proteins I present a possible explanation for the mitigated imidazole affinity based on structural factors observed when juxtaposing the wild type and mutant structures *Calculating Precise and Accurate Free Energies in Biomolecular Systems* Michael R. Shirts,2004

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