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ROLE OF MOLECULAR MODELLING IN DRUG DESIGN

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ABSTRACT: - Molecular modeling includes all theoretical methods and computational techniques used to model or mimic the behavior of molecules. The techniques are used in the fields of computational chemistry, drug design, computational biology and materials science for studying molecular systems ranging from small chemical systems to large biological molecules and material assemblies. One can perform simplest calculation manually. But the computers are required to perform molecular modeling of any complex or reasonably sized system. Atomic level description of molecular system is the common feature of molecular modeling techniques. This may include treating atoms as the smallest individual unit (the Molecular mechanics approach), or explicitly modeling electrons of each atom (Parsons et al., 2005).

INTRODUCTION:

Molecular models commonly represent atoms (nucleus and electrons collectively) as point charges with a relevant mass. Spring-like interactions (representing chemical bonds) and van der Waals forces will describe interactions between neighboring atoms Vander Waals forces are usually described by Lennard-Jones potential. The electrostatic interactions has been computed using Coulomb's law. Atoms are assigned coordinates in Cartesian space or in internal coordinates, and can also be assigned velocities in dynamical simulations. The atomic velocities are related to the temperature of the system, a macroscopic quantity. The collective mathematical expression is known as a potential function and is related to the system internal energy (U), a thermodynamic quantity equal to the sum of potential and kinetic energies. Methods which minimize the potential energy are known as energy minimization techniques (e.g., steepest descent and conjugate gradient), while methods that model the behavior of the system with propagation of time are known as molecular dynamics (Leach, 2001).

COMPUTATIONAL CHEMISTRY:

Computational chemistry is a branch of chemistry that uses computer simulation to assist in solving chemical problems, to study the fundamental properties of atoms, molecules and chemical reactions using quantum mechanics and thermodynamics. Computational chemist helps manufacturers design more productive and efficient processes, characterizes new compounds and materials, and helps other researchers extract useful knowledge from more number of data. Computational chemists may use simulations to identify sites on protein molecules that are most likely to bind a new drug molecule or create models of synthesis reactions to demonstrate the effects of kinetics and thermodynamics on the amount and kinds of products. They can also explore the basic physical processes underlying phenomena such as superconductivity, energy storage, corrosion, or phase changes. The pharmaceutical industry, a major employer of computational chemists, has historically focused on the discovery and design of new small molecular therapeutics (Smith, 1997).

DRUG DESIGN:

Drug design is the inventive process of finding new medications based on the knowledge of a biological target. The drug is most commonly an organic small molecule that activates or inhibits the function of a biomolecule such as a protein, which inturn results in a therapeutic benefit to the patient. Drug design involves the design of molecules that are complementary in shape and charge to the biomolecular target with which they interact and therefore will bind to it. Drug design frequently but not necessarily relies on computer modeling techniques.

Pharmacophore approaches have become the major tool in drug discovery the past century's and particularly facing the demand for reducing the current expensive cost is associated with drug discovery. This type of modeling is often referred to as computer-aided drug design. The computer-aided molecular model is valuable tool for rational drug design. The Drug design that relies on the knowledge of the 3D structure of the bimolecular target is known as structure-based drug design. In addition to small molecules, biopharmaceuticals and especially therapeutic antibodies are an increasingly important class of drugs and computational methods for improving the affinity, selectivity, and stability of this protein-based therapeutics have also been developed (Yang, 2000).

MATERIAL SCIENCE:

The interdisciplinary field of materials science mainly involved in discovery and design of new materials, with a special importance on solids. The intellectual origins of materials science stem from the Enlightenment, when researchers began to use analytical thinking from chemistry, physics, and engineering to understand ancient, phenomenological observations in metallurgy and mineralogy. Material science still includes elements of physics, chemistry, and engineering. As such, the field was long thought of as a sub-field of these related fields. Materials science is recognized as a specific and distinct field. The scientific problems faced by humans are due to the limitations of the materials that are available and as a result, breakthroughs in materials science are likely to have a significant impact on the future of technology. Material scientists attention on understanding how the history of a material (its processing), influences its structure, and thus the material's properties and performance. The understanding of processing-structure-properties, relationships is called the material paradigm. (Eddy et al., 2008).

COMPUTATIONAL BIOLOGY:

Computational biology involves the development and application of data-analytical and theoretical methods, mathematical modeling and computational simulation techniques to the study of biological, behavioral, and social systems. Computational biology is different from biological computation, which is a subfield of computer science and computer engineering using bioengineering and biology to build computers, but is similar to bioinformatics, which is an interdisciplinary science using computers to store and process biological data (Kitano et al., 2002).

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