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Editorial Note

Development Editor Note: Biomolecular Modeling

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Now days, the structure of biomolecules modeling has been increased popularly with the use of integrative, information-driven computational methods. In the fields of computational structural biology there are some key areas of interest for information-driven, integrative modeling and discuss how they relate to ongoing challenges. Molecular modeling encloses all methods, theoretical and computational, used to model or mimic the behavior of molecules. The atomistic level description of the molecular systems is the common feature of molecular modeling methods. This may include treating specific modeling neutrons and protons with its quarks, anti-quarks and electrons with its photons, atoms as the smallest individual unit. The methods are used to study molecular systems ranging from small chemical systems to large bio molecules and material assemblies in the fields of computational chemistry, computational biology, drug design and materials science. To perform molecular modeling of any reasonably sized system inevitably computers are required, but the simplest calculations can be performed by hand.

One factor of molecular modeling is Molecular mechanics, it involves the use of classical mechanics to describe the physical basis behind the models. Atoms (nucleus and electrons collectively) as point charges with an associated mass is typically described by molecular models. The interactions between neighboring atoms are described by representing chemical bonds and Van der Waals forces. The coordinates are assigned in Cartesian space or in internal coordinates by atoms, and can also be assigned velocities in dynamical simulations. The velocities assigned by atoms are related to the temperature of the system and a macroscopic quantity. The collective mathematical expression is termed a potential function and is related to the sum of potential and kinetic energies are equal to the system internal energy (U), a thermodynamic quantity. The potential energy which is minimized by the methods are termed energy minimization methods (e.g., steepest descent and conjugate gradient), while molecular dynamics are the methods that model the behavior of the system with propagation of time.

Membrane protein modeling is another field which has recently attracted attention and has seen many developments. It is considered as one of the most difficult kinds of systems traditionally because of the nature of the lipid bilayer which requires that, either it is dissolved with detergents and reconstituted or that native or native-like membrane mimetics are used to study with experimental structural biology methods. With success for X-ray and NMR the former is easier and has been used but the questions are raised because of the effect of the detergent has on the 3D structure. The physiological conditions are much closer to use of native or native-like membrane mimetics, this means any structure that determined this way should be closer to its counterpart in the cellular environment, but many challenges are introduced in sample preparation and measurements. Therefore computational methods remain an attractive alternative for the study of membrane-bound or membrane-associated proteins and their complexes. As such blind challenges have been and will remain important catalysts for further development and advances the field would clearly benefit from truly integrative blind modeling challenges.