Biomolecular simulations : methods and protocols

Abstrak

Over the past 40 years the field of molecular simulations has evolved from picosecond studies of isolated macromolecules in vacuum to studies of complex, chemically heterogeneous biological systems consisting of millions of atoms, with the simulation time scales spanning up to milliseconds. In Biomolecular Simulations: Methods and Protocols, expert researchers illustrate many of the methods commonly used in molecular modelling of biological systems, including methods for electronic structure calculations, classical molecular dynamics simulations and coarse-grained techniques. A selection of advanced techniques and recent methodological developments, which rarely find coverage in traditional textbooks, is also introduced. Written in the highly successful Methods in Molecular Biology series format, chapters include general introductions to well-established computational methodologies, applications to real-world biological systems, as well as practical tips and general protocols on carrying out biomolecular simulations. Special emphasis is placed on simulations of proteins, lipids, nucleic acids, and carbohydrates. Authoritative and practical, Biomolecular Simulations: Methods and Protocols seeks to aid scientists in further simulation studies of biological systems.