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Titolo	Molecular Structures and Structural Dynamics of Prion Proteins and Prions : Mechanism Underlying the Resistance to Prion Diseases / / by Jiapu Zhang
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ISBN	94-017-7318-1
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Descrizione fisica	1 online resource (366 p.)
Collana	Focus on Structural Biology, , 1571-4853 ; ; 9
Disciplina	616.83
Soggetti	Proteins Molecular biology Bioinformatics Chemistry, Physical and theoretical Biophysics Biological physics Protein Structure Molecular Medicine Computational Biology/Bioinformatics Theoretical and Computational Chemistry Biological and Medical Physics, Biophysics
Lingua di pubblicazione	Inglese
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Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Basic Knowledge -- The Homology Structure and Dynamics -- The NMR Structure and Dynamics of the Wild-type and Mutants -- Compared with the NMR Structure and Dynamics of Humans and Mice -- Compared with the NMR Structure and Dynamics of Dogs and Horses -- Compared with a Homology Structure and Dynamics of Buffaloes -- Compared with NMR Structure and Dynamics of Elks -- Compared with the X-ray Structure and Dynamics of Rabbits -- Surface Electrostatic Charge Distributions -- The Hydrophobic Region PrP(109–136) -- The Hybrid Method of Steepest Descent - Conjugate Gradient with Simulated Annealing -- Hybrid Method of Discrete Gradient with Simulated Annealing or Genetic Algorithm -- A Novel Canonical Dual

Global Optimization Computational Approach -- The Hybrid Method of Evolutionary Computations with Simulated Annealing -- Simulated Annealing Refined Replica Exchange Global Search Algorithm -- LBFGS Quasi-Newtonian Methods for MM Prion AGAAAAGA Amyloid Fibrils -- Particle Swarm Global Optimization Search Algorithm -- A Summary of the Research Works on AGAAAAGA.

Sommario/riassunto

This monograph is the first easy-to-read-and-understand book on prion proteins' molecular dynamics (MD) simulations and on prions' molecular modelling (MM) constructions. It enables researchers to see what is crucial to the conformational change from normal cellular prion protein (PrPC) to diseased infectious prions (PrPSc), using MD and MM techniques. As we all know, prion diseases, caused by the body's own proteins, are invariably fatal and highly infectious neurodegenerative diseases effecting humans and almost all animals for a major public health concern. Prion contains no nucleic acids and it is a misshapen or conformation-changed protein that acts like an infectious agent; thus prion diseases are called “protein structural conformational” diseases. PrPC is predominant in -helices but PrPSc are rich in -sheets in the form as amyloid fibrils; so very amenable to be studied by MD techniques. Through MD, studies on the protein structures and the structural conversion are very important for revealing secrets of prion diseases and for structure-based drug design or discovery. Rabbits, dogs, horses and buffaloes are reported to be the few low susceptibility species to prion diseases; this book's MD studies on these species are clearly helpful to understand the mechanism underlying the resistance to prion diseases. PrP(1-120) usually has no clear molecular structures; this book also studies this unstructured region through MD and especially MM techniques from the global optimization point of view. This book is ideal for practitioners in computing of biophysics, biochemistry, biomedicine, bioinformatics, cheminformatics, materials science and engineering, applied mathematics and theoretical physics, information technology, operations research, biostatistics, etc. As an accessible introduction to these fields, this book is also ideal as a teaching material for students.