



# Molecular Structures and Structural Dynamics of Prion Proteins and Prions [ Mechanism Underlying the Resistance to Prion Diseases /

Zhang, Jiapu

Springer

Life sciences Molecular biology Chemistry, Physical and theoretical  
 Bioinformatics Proteins Biophysics Biological physics Life Sciences  
 Protein Structure Molecular Medicine Computational Biology  
 Bioinformatics Theoretical and Computational Chemistry Biophysics and  
 Biological Physics

Monografia

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  $\alpha$ 2sprotein structural conformational $\alpha$ 3s diseases. PrPC is predominant in  $\alpha$ -helices but PrPSc are rich in  $\beta$ -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

**Título:** Molecular Structures and Structural Dynamics of Prion Proteins and Prions [Recurso electrónico] Mechanism Underlying the Resistance to Prion Diseases by Jiapu Zhang

**Editorial:** New York [etc.] Springer

**Descripción física:** XIX, 355 p. 179 il., 176 il. in color

**Mención de serie:** Focus on Structural Biology 1571-4853 9

**Contenido:** 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

**Detalles del sistema:** Modo de acceso: World Wide Web

**Fuente de adquisición directa:** Springer (e-Books)

**ISBN:** 9789401773188 978-94-017-7318-8 9789401773171

**Punto acceso adicional serie-Título:** Focus on Structural Biology 1571-4853 9

---

## Baratz Innovación Documental

- Gran Vía, 59 28013 Madrid
- (+34) 91 456 03 60
- [informa@baratz.es](mailto:informa@baratz.es)