



## Practical Global Optimization Computing Methods in Molecular Modelling

By Jiapu Zhang

LAP Lambert Academic Publishing Okt 2011, 2011. Taschenbuch. Book Condition: Neu. 220x150x12 mm. This item is printed on demand - Print on Demand Neuware - Due to the unstable, noncrystalline and insoluble nature of some proteins, the technologies such as X-ray crystallography, NMR (nuclear magnetic resonance) spectroscopy and dual polarization interferometry etc sometimes cannot produce the 3D structures of these proteins. In this condition, molecular modeling (MM) might have been the only strategy to get the 3D structures. The non-covalent interactions such as hydrogen bonding (HB), ionic interactions (SB), Van Der Waals forces (VDW), and hydrophobic packing (HP) are driving the proteins to be able to perform their biological functions. The author has found some SBs play a key role in prion diseases revealed from rabbit prion protein. Neurodegenerative diseases are amyloid fibril diseases. This book studies the HB, VDW, HP interactions for MM of amyloid fibrils in global optimization (GO). The GO MM-algorithms of this book should be very useful in materials science, drug design, IT, operations research, biostatistics and bioinformatics etc research fields. This book was written without advanced mathematical formulas thus it is easily readable for people in wide areas of sciences, engineering, IT, medicine, physiology, education, etc...



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