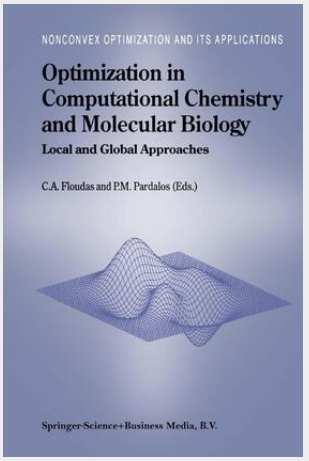
Pardalos / Floudas

Optimization in Computational Chemistry and Molecular Biology

Local and Global Approaches



Optimization in Computational Chemistry and Molecular Biology: Local and Global Approaches covers recent developments in optimization techniques for addressing several computational chemistry and biology problems. A tantalizing problem that cuts across the fields of computational chemistry, biology, medicine, engineering and applied mathematics is how proteins fold. Global and local optimization provide a systematic framework of conformational searches for the prediction of three-dimensional protein structures that represent the global minimum free energy, as well as low-energy biomolecular conformations. Each contribution in the book is essentially expository in nature, but of scholarly treatment. The topics covered include advances in local and global optimization approaches for molecular dynamics and modeling, distance geometry, protein folding, molecular structure refinement, protein and drug design, and molecular and peptide docking. Audience: The book is addressed not only to researchers in mathematical programming, but to all scientists in various disciplines who use optimization methods in solving problems in computational chemistry and biology.

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