

[SCIENCE/Chemistry / Physical & Theoretical]

量子生化学 (全2巻) Quantum Biochemistry

Chérif F. Matta (ed.): Mount St. Vincent University, Halifax, Canada



本書について

全2巻からなる本書は、生化学計算の理論的基礎、生体分子、反応、遷移状態の解明、配座可動性の決定、薬剤設計などの主題をカバーする。DNA、RNA、酵素、ビタミン、複素環化合物など重要な化合物クラスが幅広く取り上げられる。収録論文にはAda Yonath (2009年)とJerome Karle (1985年)という二人のノーベル化学賞受賞者による寄稿も含む。

TABLE OF CONTENTS

I. THEORETICAL METHODS TAILORED FOR LARGE BIOMOLECULES

Quantum Crystallography and the Kernel Energy Method
New DFT Functionals Capturing Dispersion Forces in Biomolecules
Linear Scaling and Divide-and-Conquer Methods
Transition State Theory of Biochemical Reaction
The Fast-Marching Method for Predicting the Products of Enzyme-like Chemical Catalysis
Solvent Effects in Biochemistry
Biochemical Applications of the Quantum Theory of Atoms in Molecules
Quantum Chemical Topology and the Automatic Location of Active Centers in Biomolecules

II. BIOMOLECULES

Accurate Estimates of Stacking Energies in DNA and RNA
Chemical Modifications and Drug Interactions with DNA
Ionization of DNA and RNA bases
Proton Tunnelling in Nucleic Acids and Mutation
Amino Acids and Polypeptides
Energy-rich Compounds
Pteridines

Porphyrins
Carotenoids and Vitamin A
Quinones and Antioxidants
Carcinogenic Polycyclic Aromatic Hydrocarbons

III. BIOCHEMICAL REACTIONS AND TRANSITION STATES

Transition State of the Peptide Bond Formation in the Ribosome
Quantum Modeling of the Catalytic Mechanism of Aldose Reductase Based on Proton Mobility Revealed by Neutron and Subatomic Resolution X-Ray Crystallography
Time Resolved X-ray Diffraction Study of the Electron Density in Enzymatic Reactions
Seleno-Enzymes

IV. CONFORMATIONAL FLEXIBILITY OF BIOMOLECULES

The Conformations of Histamine

V. QUANTUM BIOCHEMISTRY IN DRUG DESIGN

The Design of Drugs for Epilepsy, Alzheimer, and Parkinson's Disease
Computational Chemistry in the Development of Potential Antidementia Inhibitors of Butyrylcholinesterase
Advances in Molecular Similarity Measures and their Uses in Drug Design

出版/予定: 2010年1月
ISBN13: 978-3-527-32322-7

ページ数(約): 976 (全2巻)
予価: US\$335.00 (2009年12月現在/変動あり)

◆ご注文は洋書店にお願いします

◆資料ご請求、ご質問は—— **ワイリー・ジャパン**

〒112-0002 東京都文京区小石川1-28-1

フロンティア小石川ビル4F

TEL 03-3830-1232 FAX 03-5689-7276

E-mail: marketing@wiley.co.jp

日本語ホームページ: www.wiley.co.jp

取扱書店