1. Record Nr. UNINA9910704344603321

Titolo	NASA : earned value management implementation across major spaceflight projects is uneven : report to congressional requesters
Pubbl/distr/stampa	[Washington, D.C.] : , : United States Government Accountability Office, , 2012
Descrizione fisica	1 online resource (iii, 104 pages) : illustrations
Soggetti	Space flight - Management Aeronautics and state - United States
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Title from title screen (viewed Jan. 28, 2013). "November 2012." "GAO-13-22."
Nota di bibliografia	Includes bibliographical references.

2. Record Nr. UNINA9911019309903321

Titolo	Quantum Biochemistry / / edited by Cherif F. Matta
Pubbl/distr/stampa	Weinheim, : Wiley-VCH Verlag GmbH & Co., 2010
ISBN	9786612462917 9781282462915 1282462911 9783527629213 3527629211 9783527629220 352762922X
Descrizione fisica	1 online resource (980 p.)
Altri autori (Persone)	MattaCherif F
Disciplina	572
Soggetti	Quantum biochemistry Biochemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Quantum Biochemistry; Acknowledgment; Congratulations to Professor Ada Yonath for Winning the 2009 Nobel Prize in Chemistry; Introductory Reflections on Quantum Biochemistry: From Context to Contents; Contents; List of Contributors; Part One Novel Theoretical, Computational, and Experimental Methods and Techniques; 1 Quantum Kernels and Quantum Crystallography: Applications in Biochemistry; 1.1 Introduction; 1.2 Origins of Quantum Crystallography (QCr); 1.2.1 General Problem of N-Representability; 1.2.2 Single Determinant N-Representability; 1.2.3 Example Applications of Clinton.s Equations 1.2.3.1 Beryllium1.2.3.2 Maleic Anhydride; 1.3 Beginnings of Quantum Kernels; 1.3.1 Computational Difficulty of Large Molecules; 1.3.2 Quantum Kernel Formalism; 1.3.3 Kernel Matrices: Example and Results; 1.3.4 Applications of the Idea of Kernels; 1.3.4.1 Hydrated Hexapeptide Molecule; 1.3.4.2 Hydrated Leu1-Zervamicin; 1.4 Kernel Density Matrices Led to Kernel Energies; 1.4.1 KEM Applied to Peptides; 1.4.2 Quantum Models within KEM; 1.4.2.1 Calculations and Results Using Different Basis Functions for the ADPGV7b Molecule

1.4.2.2 Calculations and Results Using Different Quantum Methods for the Zaib4 Molecule1.4.2.3 Comments Regarding KEM; 1.4.3 KEM Applied to Insulin; 1.4.3.1 KEM Calculation Results; 1.4.3.2 Comments Regarding the Insulin Calculations; 1.4.4 KEM Applied to DNA; 1.4.4.1 KEM Calculation Results; 1.4.4.2 Comments Regarding the DNA Calculations; 1.4.5 KEM Applied to tRNA; 1.4.6 KEM Applied to Rational Design of Drugs; 1.4.6.1 Importance of the Interaction Energy for Rational Drug Design
1.4.6.2 Sample Calculation: Antibiotic Drug in Complex (1O9M) with a Model Aminoacyl Site of the 30s Ribosomal Subunit1.4.6.3 Comments Regarding the Drug-Target Interaction Calculations; 1.4.7 KEM Applied to Collagen; 1.4.7.1 Interaction Energies; 1.4.7.2 Collagen 1A89; 1.4.7.3 Comments Regarding the Collagen Calculations; 1.4.8 KEM Fourth-Order Calculation of Accuracy; 1.4.8.1 Molecular Energy as a Sum over Kernel Energies; 1.4.8.2 Application to Leu1-zervamicin of the Fourth-Order Approximation of KEM; 1.4.9 KEM Applied to Vesicular Stomatitis Virus Nucleoprotein, 33 000 Atom Molecule 1.4.9.1 Vesicular Stomatitis Virus Nucleoprotein (2QVJ) Molecule1.4.9.2 Hydrogen Bond Calculations; 1.4.9.3 Comments regarding the 2QVJ Calculations; 1.5 Summary and Conclusions; References; 2 Getting the Most out of ONIOM: Guidelines and Pitfalls; 2.1 Introduction; 2.2 QM/MM; 2.3 ONIOM; 2.4 Guidelines for the Application of ONIOM; 2.4.1 Summary; 2.5 The Cancellation Problem; 2.6 Use of Point Charges; 2.7 Conclusions; References; 3 Modeling Enzymatic Reactions in Metalloenzymes and Photobiology by Quantum Mechanics (QM) and Quantum Mechanics/Molecular Mechanics (QM/MM) Calculations
3.1 Introduction

Sommario/riassunto

Divided into five major parts, the two volumes of this ready reference cover the tailoring of theoretical methods for biochemical computations, as well as the many kinds of biomolecules, reaction and transition state elucidation, conformational flexibility determination, and drug design. Throughout, the chapters gradually build up from introductory level to comprehensive reviews of the latest research, and include all important compound classes, such as DNA, RNA, enzymes, vitamins, and heterocyclic compounds.The result is in-depth and vital knowledge for both readers already working in the