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Titolo	Molecular orbital calculations for biological systems [[electronic resource] /] / edited by Anne-Marie Sapse
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Descrizione fisica	1 online resource (248 p.)
Collana	Topics in physical chemistry
Altri autori (Persone)	SapseAnne-Marie
Disciplina	541.280285 547.70448 547/.70448
Soggetti	Molecular orbitals Biomolecules Peptides Amino acids Antineoplastic agents
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Contents; Contributors; Introduction; 1 Ab Initio Calculations; 2 An Introduction to the Theoretical Basis of Semi-Empirical Quantum-Mechanical Methods for Biological Chemists; 3 The Molecular Electrostatic Potential: A Tool for Understanding and Predicting Molecular Interactions; 4 Applications of Density Functional Theory to Biological Systems; 5 On Comparing Experimental and Calculated Structural Parameters; 6 Ab Initio Studies of Anti-Cancer Drugs; 7 Ab Initio Calculations of Amino Acids and Peptides; Index; A; B; C; D; E; F; G; H; I; K; L; M; N; O; P; R; S; T; U; V; W; X; Z
Sommario/riassunto	This is a hands-on guide for the growing number of researchers in organic chemistry, biochemistry and molecular biology who would like to augment their experiments with theoretical calculations. Given the

current availability of sophisticated software, non-quantum chemistry practitioners can obtain accurate computational results and save significant amounts of laboratory time. This book teaches the use of quantum chemical computer programs while side-stepping the complex mathematical details.

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