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Nota di contenuto	section 1. Introduction -- section 2. Enzymatic catalysis : multiscale QM/MM calculations -- section 3. Protein motions : flexibility analysis -- section 4. Approaches to intrinsically disordered proteins -- section 5. Large-scale dynamics -- section 6. Ensemble methods.
Sommario/riassunto	<P>This groundbreaking work addresses a crucial paradigm shift in structural molecular biology, illustrating how protein dynamics plays a central role in various functions, including enzymatic catalysis, protein-protein interactions, and the organization of complex assemblies. The book presents modern computational techniques for the characterization of proteins and their dynamic properties. The computational methods specifically address the dynamical aspects of protein functionalities, with special emphasis on the analysis of complex assemblies and intrinsically disordered proteins. </P>