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Autore	Fernández Stigliano Ariel
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Soggetti	Proteins Cell membranes Molecular biology Pharmaceutical technology Biophysics Biological physics Protein-Ligand Interactions Membrane Biology Molecular Medicine Pharmaceutical Sciences/Technology Biological and Medical Physics, Biophysics
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Nota di contenuto	The Aqueous Interface of a Soluble Protein or the Birth of Epistuctural Biology -- Electrostatic Exploration of Biomolecular Interfaces: The Chemical Function of Interfacial Water -- Semiempirical Solution to the Protein Folding Problem Through a Combination of Structural and Epistuctural Approaches -- Packing Defects and Protein Hydration: Dynamics of the Aqueous Interface -- Proteins in the Order-Disorder Twilight: Unstable Interfaces Promote Protein Aggregation -- Evolution of Protein Structure Degradation and Lessons for the Drug Designer -- Chemical Functionality of the Aqueous Interface in Soluble Proteins -- The Biomolecular Interface as a Selectivity Filter for Drug-Based Targeted Therapy -- Wrapping-Based Re-Engineering of an Anticancer Drug to Make it Safer -- Biomolecular Interfaces Provide Universal

Markers for Drug Specificity and Personalized Medicine -- Controlling Induced Folding Through Wrapping Drug Design -- Wrapping Drug Combinations for Therapeutic Editing of Side Effects: Systems Biology Meets Wrapping Technology -- Multi-Target Control of Drug Impact: A Therapeutic Imperative in Cancer Systems Biology -- Engineering Therapeutic Alignments between Immune Response and Molecularly Targeted Cancer Treatment -- High-Level Quantum Chemistry Empowers the Wrapping Technology for Drug Design -- Epilogue -- Appendix 1. Code for Dehydron Identification -- Appendix 2. Solutions of Problems.

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Sommario/riassunto

The book focuses on the aqueous interface of biomolecules, a vital yet overlooked area of biophysical research. Most biological phenomena cannot be fully understood at the molecular level without considering interfacial behavior. The author presents conceptual advances in molecular biophysics that herald the advent of a new discipline, epistructural biology, centered on the interactions of water and biomolecular structures across the interface. The author introduces powerful theoretical and computational resources in order to address fundamental topics such as protein folding, the physico-chemical basis of enzyme catalysis and protein associations. On the basis of this information, a multi-disciplinary approach is used to engineer therapeutic drugs and to allow substantive advances in targeted molecular medicine. This book will be of interest to scientists, students and practitioners in the fields of chemistry, biophysics and biomedical engineering.

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