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	Autore	NISSMAN, David B.
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Nota di contenuto	Lipophilicity in Drug Action and Toxicology; Preface; A Personal Foreword; List of Contributors; Contents; 1 Lipophilicity : The Empirical Tool and the Fundamental Objective . An Introduction; 1.1 Setting the Scene; 1.2 Biological Aspects; 1.3 The Molecule in the Background; 1.4 Some Pragmatic Aspects; 1.4.1 Definitions and Symbols; 1.4.2 Experimental Techniques; 1.4.3 Computational Procedures; 1.5 Objectives of the Book; References; 2 Lipophilicity: A History; 2.1 Introduction; 2.2 Measurement of Lipophilicity; 2.3 Calculation of Lipophilicity; 2.3.1 Substitution Method 2.3.2 Fragment Additivity Method 2.3.3 Fragmentation into Atoms; 2.3.4 Molecular Orbital Calculations; 2.3.5 Calculations Based on Surface Area; 2.4 The Nature of Lipophilicity; 2.4.1 Relation to Other Molecular Properties; 2.4.2 Thermodynamics of Partitioning; 2.4.2.1 Phase Transfer; 2.4.2.2 The Aqueous Phase and the "Hydrophobic Bond"; 2.5 Lipophilicity and Biological Activity; References; 3 Thermodynamics of van der Waals and Hydrophobic Interactions; 3.1 Introduction; 3.2 Outline of Thermodynamics and Auxiliary Disciplines; 3.3 Intermolecular Interactions of the van der Waals Type 3.3.1 The Physical Nature of van der Waals Interactions 3.3.2 Classification of van der Waals Clusters; 3.3.3 Calculation of the Interaction Energy; 3.3.3.1 Nonempirical ab initio Variational Method; 3.3.3.2 Density Functional Theory; 3.3.3.3 Semiempirical Methods; 3.3.3.4 Empirical Procedures; 3.3.4 How to Obtain a Consistent Set of Various Calculated Properties for van der Waals Clusters; 3.3.4.1 Potential Energy Surface (P . E . S.); 3.3.4.2 Stabilization Energy; 3.3.4.3 Empirical Potential; 3.3.4.4 Vibration Frequencies; 3.3.4.5 Computer Experiments 3.4 Processes Involving Hydrophobic Effects 3.5 Specific Illustrations; 3.5.1 Ab initio Evaluation of a Consistent Set of Various Properties of the Benzene ... Arn Cluster; 3.5.1.1 Potential Energy Surface; 3.5.1.2 More Accurate Calculations for the Global Minimum; 3.5.1.3 Preparation of the Empirical Potential; 3.5.1.4 Vibrational Frequencies; 3.5.1.5 Molecular Dynamics Simulations; 3.5.2 Monte Carlo Free Energy Perturbation Calculation : Solvation Free Energy of Methanol and Ethane; References; Appendices; 4 Intramolecular Interactions Encoded in Lipophilicity : Their Nature and Significance 4.1. Introduction : The Concept of Molecular Structure 4.1.1 The Elementary and Geometric Levels of Description; 4.1.2 The Stereoelectronic Levels of Description; 4.1.3 Social Molecules; 4.2 Intermolecular Forces Encoded in Lipophilicity; 4.2.1 Recognition Forces in Molecular Pharmacology and Biology; 4.2.2 Factorization of Molecular Lipophilicity; 4.2.3 Polar Interactions Encoded in Lipophilicity; 4.2.4 Nonpolar Interactions Encoded in Lipophilicity; 4.2.5 Recognition Forces Encoded in Lipophilicity; 4.3 Intramolecular Interactions Affecting Lipophilicity; 4.3.1 Electronic Conjugations 4.3.1.1 In Aromatic Systems
Sommario/riassunto	In keeping with the outstanding importance of lipophilicity in biosciences, this volume examines all its facets in more than twenty contributions from leading experts. It offers a thorough and highly topical survey of this rapidly developing field of research. Color plates demonstrating structural aspects, a vast number of references, and the

straightforward presentation of the material make this volume a
invaluable tool for all researchers involved in drug design or in the
investigation of drug action.
