Record Nr. UNINA9910144116703321 Lipophilicity in drug action and toxicology [[electronic resource] /] / **Titolo** edited by Vladimir Pliska, Bernard Testa, and Han van de Waterbeemd Pubbl/distr/stampa Weinheim: New York,: VCH, c1996 **ISBN** 1-281-84266-4 9786611842666 3-527-61499-0 3-527-61498-2 Descrizione fisica 1 online resource (466 p.) Collana Methods and principles in medicinal chemistry;; v. 4 Altri autori (Persone) PliskaVladimir **TestaBernard** WaterbeemdHan van de Disciplina 615.7 615/.19 Soggetti Drug lipophilicity Toxicology Electronic books. 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 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 Method2.3.3 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

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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.