1. Record Nr. UNINA9910830089003321 Autore Kubinyi Hugo Titolo QSAR: Hansch analysis and related approaches [[electronic resource] /] / by Hugo Kubinyi Weinheim: New York,: VCH, c1993 Pubbl/distr/stampa 1-281-75888-4 **ISBN** 9786611758882 3-527-61682-9 3-527-61683-7 Descrizione fisica 1 online resource (254 p.) Collana Methods and principles in medicinal chemistry;; v. 1 Disciplina 572.072 615 615.1901 Soggetti QSAR (Biochemistry) Pharmaceutical chemistry Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Description based upon print version of record. Note generali Nota di bibliografia Includes bibliographical references (p. [183]-210) and index. Nota di contenuto QSAR: Hansch Analysis and Related Approaches; Content; 1. Introduction; 1.1. History and Development of QSAR; 1.2. Drug-Receptor Interactions; 2. Biological Data. The Additivity of Group Contributions; 3. Parameters; 3.1. Lipophilicity Parameters; 3.2. The Measurement of Partition Coefficients and Related Lipophilicity Parameters; 3.3. Lipophilicity Contributions and the Calculation of Partition Coefficients; 3.4. Polarizability Parameters; 3.5. Electronic Parameters: 3.6. Steric Parameters: 3.7. Other Parameters: 3.8. Indicator Variables; 4. Quantitative Models 4.1. The Extrathermodynamic Approach (Hansch Analysis)4.2. The Additivity Model (Free Wilson Analysis); 4.3. The Relationships between Hansch and Free Wilson Analysis (The Mixed Approach); 4.4. Nonlinear Relationships; 4.5. Dissociation and Ionization of Acids and Bases; 4.6. Other QSAR Approaches; 5. Statistical Methods; 5.1. Regression Analysis: 5.2. The Significance and Validity of QSAR Regression

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Sommario/riassunto

Finding the new remedy for a certain disease: an inspired goal. QSAR, an invaluable tool in drug design, aids scientists to attain this aim. This book is a long-awaited comprehensive text to QSAR and related approaches. It provides a practice-oriented introduction to the theory, methods and analyses for QSAR relationships, including modelling-based and 3D approaches. Hugo Kubinyi is a leading expert in QSAR. Readers will benefit from the author's 20 years of practical experience, from his careful calculations and recalculations of thousands of QSAR equations. Among the topics cov