

1. Record Nr.	UNISA996218390403316
Autore	Kubinyi Hugo
Titolo	QSAR : Hansch analysis and related approaches [[electronic resource] /] / by Hugo Kubinyi
Pubbl/distr/stampa	Weinheim ; ; New York, : VCH, c1993
ISBN	1-281-75888-4 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
Note generali	Description based upon print version of record.
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 Equations; 5.3. Partial Least Squares (PLS) Analysis and Other Multivariate Statistical Methods; 6. Design of Test Series in QSAR; 7.

Applications of Hansch Analysis; 7.1. Enzyme Inhibition  
7.2. Other in vitro Data 7.3. Pharmacokinetic Data; 7.4. Other Biological  
Data; 7.5. Activity-Activity Relationships; 8. Applications of Free Wilson  
Analysis and Related Models; 9. 3D QSAR Approaches; 9.1.  
Stereochemistry and Drug Action; 9.2. Active Site Interaction Models;  
9.3. Comparative Molecular Field Analysis (CoMFA); 9.4. Molecular  
Similarity QSAR Analyses; 10. Summary and Conclusions; References;  
Index

---

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

---