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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 Data7.3. 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
