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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