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Altri autori (Persone)	MannholdRaimund KubinyiHugo FolkersGerd
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Soggetti	Biomolecules Chemical reactions -- Computer simulation Chemicals -- Pharmacokinetics -- Forecasting Chemicals -- Physiological effect -- Forecasting Drug development Pharmaceutical chemistry Structure-activity relationships (Biochemistry) -- Computer simulation Pharmaceutical chemistry - Physiological effect - Forecasting Chemicals - Computer simulation Chemical reactions - Computer simulation Structure-activity relationships (Biochemistry) Computational Biology Models, Molecular Quantitative Structure-Activity Relationship Computer Simulation Drug Design Pharmaceutical Preparations Software Structure-Activity Relationship Biology Drug Discovery Computing Methodologies Chemicals and Drugs Models, Theoretical Biological Science Disciplines

	Chemistry, Pharmaceutical Biochemical Phenomena Information Science Pharmacological Phenomena Investigative Techniques Natural Science Disciplines Analytical, Diagnostic and Therapeutic Techniques and Equipment Pharmacology Physiological Phenomena Chemistry Chemical Phenomena Phenomena and Processes Disciplines and Occupations Pharmacy, Therapeutics, & Pharmacology History of Medicine Health & Biological Sciences Medicine
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Nota di contenuto	Molecular Interaction Fields; A Personal Foreword; Contents; Preface; List of Contributors; I Introduction; 1 The Basic Principles of GRID; 1.1 Introduction; 1.2 Philosophy and Objectives; 1.3 Priorities; 1.4 The GRID Method; 1.4.1 GRID Probes Are Anisometric; 1.4.2 The Target "Responds" to the Probe; 1.4.3 The Target is Immersed in Water; 1.5 The GRID Force Field; 1.5.1 The Lennard-Jones Term; 1.5.2 The Electrostatic Term; 1.5.3 The Hydrogen Bond Term; 1.5.4 The Other Terms; 1.6 Nomenclature; 1.6.1 "ATOM" Records; 1.6.2 "HETATM" Records; 1.7 Calibrating the GRID Force Field 1.7.1 Checking the Calibration1.7.2 Checking Datafile GRUB; 1.8 The Output from GRID; 1.8.1 GRID Maps from Macromolecules; 1.8.2 GRID Maps from a Small Molecule; 1.9 Conclusions; 2 Calculation and Application of Molecular Interaction Fields; 2.1 Introduction; 2.2 Calculation of MIFs; 2.2.1 The Target; 2.2.2 The Probe; 2.2.3 The Interaction Function; 2.2.3.1 Van der Waals Interactions; 2.2.3.2 Electrostatic Interactions; 2.2.3.3 Hydrogen Bonds; 2.2.3.4 Entropy; 2.3 Selected Applications of MIFs; 2.3.1 Mapping a Ligand Binding Site in a Protein; 2.3.2 Deriving 3D-QSARs 2.3.3 Similarity Analysis of a Set of Related Molecules2.4 Concluding Remarks and Outlook; II Pharmacodynamics; 3 Protein Selectivity Studies Using GRID-MIFs; 3.1 Introduction; 3.2 GRID Calculations and Chemometric Analysis; 3.2.1 Source and Selection of Target Structures; 3.2.2 Selection and Superimposition of Binding Sites; 3.2.3 Calculation of the Molecular Interaction Field; 3.2.4 Matrix Generation and Pretreatments; 3.2.4.1 Region Cut-outs; 3.2.5 GRID/PCA; 3.2.5.1 Score Plots; 3.2.5.2 Two-Dimensional Loading Plots; 3.2.5.3 Loading Contour Maps; 3.2.5.4 Problems of GRID/PCA 3.2.6 GRID/CPCA3.2.6.1 Block Unscaled Weights; 3.2.6.2 CPCA; 3.2.6.3

Identification of Important Variable Blocks for Selectivity; 3.2.6.4 Contour Plots; 3.3 Applications; 3.3.1 DNA Minor Groove Binding - Compare AAA and GGG Double Helix; 3.3.2 Dihydrofolate Reductase; 3.3.3 Cyclooxygenase; 3.3.4 Penicillin Acylase; 3.3.5 Serine Proteases; 3.3.5.1 S1 Pocket; 3.3.5.2 P Pocket; 3.3.5.3 D Pocket; 3.3.6 CYP450; 3.3.7 Target Family Landscapes of Protein Kinases; 3.3.8 Matrix Metalloproteinases (MMPs); 3.3.9 Nitric Oxide Synthases; 3.3.10 PPARs; 3.3.11 Bile Acid Transportation System
3.3.12 Ephrin Ligands and Eph Kinases3.4 Discussion and Conclusion; 4 FLAP: 4-Point Pharmacophore Fingerprints from GRID; 4.1 Introduction; 4.1.1 Pharmacophores and Pharmacophore Fingerprints; 4.1.2 FLAP; 4.2 FLAP Theory; 4.3 Docking; 4.3.1 GLUE: A New Docking Program Based on Pharmacophores; 4.3.2 Case Study; 4.4 Structure Based Virtual Screening (SBVS); 4.5 Ligand Based Virtual Screening (LBVS); 4.6 Protein Similarity; 4.7 TOPP (Triplets of Pharmacophoric Points); 4.8 Conclusions; 5 The Complexity of Molecular Interaction: Molecular Shape Fingerprints by the PathFinder Approach
5.1 Introduction

Sommario/riassunto

This unique reference source, edited by the world's most respected expert on molecular interaction field software, covers all relevant principles of the GRID force field and its applications in medicinal chemistry. Entire chapters on 3D-QSAR, pharmacophore searches, docking studies, metabolism predictions and protein selectivity studies, among others, offer a concise overview of this emerging field. As an added bonus, this handbook includes a CD-ROM with the latest commercial versions of the GRID program and related software.