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Pharmacophore Hypothesis and Molecular Comparisons -- 18. Quantitative Structure–Activity Relationships -- 19. From in vitro to in vivo: Optimization of ADME-Tox Properties -- 20. Protein Modeling and Structure-Based Drug Design -- 21. A Case Study: Structure-Based Inhibtor Design for tRNA-Guanine Transglycosylase -- Part V. Drugs and drug action: Successes of structure-based design -- 22. How drugs act: Concepts for therapy -- 23. Inhibitors of hydrolases With an acyl-enzyme intermediate -- 24. Asparticprotease inhibitors -- 25. Inhibitors of hydrolysing metalloenzymes -- 26. Inhibitors of transferases -- 27. Inhibitors of oxidoreductases -- 28. Agonists and antagonists of nuclear receptors -- 29. Agonists and antagonists of membrane-bound -- 30. Ligands for channels, pores and transporters -- 31. Ligands for surface receptors -- 32. Biologicals: Peptides, proteins, nucleotides and macrolides as drugs.

Sommario/riassunto

Unique work on structure-based drug design, covering multiple aspects of drug discovery and development. Fully colored, many images, computer animations of 3D structures (these only in electronic form). Makes the spatial aspects of interacting molecules clear to the reader, covers multiple applications and methods in drug design. Structures by mode of action, no therapeutic areas. Of high relevance for academia and industrial research. Focus on gene technology in drug design, omics-technologies computational methods experimental techniques of structure determination multiple examples on mode of action of current drugs, ADME-tox properties in drug development, QSAR methods, combinatorial chemistry, biologicals, ribosome, targeting protein-protein interfaces.