



Drug Design: Structure- and Ligand-Based Approaches

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Structure-based (SBDD) and ligand-based (LBDD) drug design are extremely important and active areas of research in both the academic and commercial realms. This book provides a complete snapshot of the field of computer-aided drug design and associated experimental approaches. Topics covered include X-ray crystallography, NMR, fragment-based drug design, free energy methods, docking and scoring, linear-scaling quantum calculations, QSAR, pharmacophore methods, computational ADME-Tox, and drug discovery case studies. A variety of authors from academic and commercial institutions all over the world have contributed to this book, which is illustrated with more than 200 images. This is the only book to cover the subject of structure and ligand-based drug design, and it provides the most up-to-date information on a wide range of topics for the practicing computational chemist, medicinal chemist, or structural biologist.

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