Computer-assisted lead finding and optimization : current tools for medicinal chemistry

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Abstrak

Computer-assisted techniques are well-integrated in modern drug discovery and used for the finding of new leads, the optimization of receptor or enzyme affinity, as well as of pharmacokinetic and physicochemical properties.
In this book an account is found of current strategies used in computer-assisted drug design. Important topics include progress in chemometrics, molecular modeling and three-dimensional QSAR approaches. Relatively new mathematical methods such as genetic algorithms or artificial neural networks and fuzzy logic have found their application in rational molecular design. As is amply illustrated, based on recent developments in these disciplines, important progress has been made in lead finding strategies. This is of great importance to the pharmaceutical industry.
Thus, all scientists investigating quantitative structure-activity relationships in their broadest sense, in medicinal, agricultural, or environmental chemistry will benefit from this book.