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The Ideal Substituent Set Should Span Orthogonal Dimensions of Parameter Space; The Ideal Set Should Contain the Minimum Number of Substituents Necessary to Avoid Chance Correlations and Still Meet the Desired Goal; Target Compounds Should Be Chosen to Preserve Synthetic Resources But Should Not Be Chosen Just Because They Are Easy to Synthesize; The Derivatives Must Be Stable under the Conditions of Bioevaluation; Analysis Strategies; The Topliss Tree; Free-Wilson Analysis; A Strategy for Lead Optimization Using Multiple Linear Regression Analysis; Choose the Optimal Pattern for Substitution; Choose the Factors (Parameters) That Are Likely to Be Important

Sommario/riassunto

This book is an account of current developments in computational chemistry, a new multidisciplinary area of research. Experts in computational chemistry, the editors use and develop techniques for computer-assisted molecular design. The core of the text itself deals with techniques for computer-assisted molecular design. The book is suitable for both beginners and experts. In addition, protocols and software for molecular recognition and the relationship between structure and biological activity of drug molecules are discussed in detail.