



Structure-Property Correlations in Drug Research (Biotechnology Intelligence Unit)

Han van de Waterbeemd

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This book provides an overview of statistical chemometric methods used in the rapidly changing arena of drug discovery. It deals with physicochemical molecular descriptors, modern statistical methods to study structure-property and structure-activity relationships, including three-dimensional QSAR approaches and the concepts of molecular diversity. All scientists who investigate quantitative structure-activity relationships in medicinal, agricultural, or environmental chemistry will benefit from this book.

Key Features

- * Presented in a theoretical as well as practical manner
- * Provides an excellent introduction and recent overview of the field
- * Addresses a rapidly changing area in a timely manner
- * Includes concise updates of
- * The use of chemical descriptors
- * Modern statistical approaches
- * Comprehensive reviews of the literature in 3D-QSAR
- * Concepts and applications of molecular similarity and diversity

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