



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

*Han van de Waterbeemd*

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**Structure-Property Correlations in Drug Research (Biotechnology Intelligence Unit)** Han van de Waterbeemd

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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