

Chapter 5

Physicochemical Parameters of QSAR

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Introduction

The enormous effort to comprehend the impact of organic substances on living beings is one of the fastest growing professions of that portion of the global human consciousness still preoccupied with serious problems. This essentially entails comprehending how organic substances interact with macromolecules, like as membranes and organelles. Organic compounds interact with biological systems to generate their effects. Chemist concern for a deeper understanding of how ligands relate to macromolecules is bound to grow significantly in the global fight against death as industrialized nations step up their efforts to eradicate toxic chemicals from the environment and control disorders. Quantitative structure-activity relationships, or QSAR, are a key paradigm for comprehending these linkages [1, 2]. One such method that enables the multidisciplinary investigation of information on substances including the areas of chemistry, physics, biology, and toxicity is quantitative structure activity relationship (QSAR) modeling. It offers a framework for creating mathematical relationships between the behavioural expressions of (structurally) comparable molecules and their chemical characteristics. An effective mathematical method serves as the foundation for the whole technique [3-6]. Modern drug design heavily relies on quantitative structure-activity relationships (QSARs), which are an extremely fast and less expensive substitute for medium in vitro

A TEXTBOOK OF COMPUTER AIDED DRUG DESIGN



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ABOUT THE BOOK

The “*A Textbook of Computer Aided Drug Design*” is intended for Bachelor and Masters Pharmacy students and is based on the syllabus of Pharmacy Council of India (PCI). The authors did their utmost to deliver the book in a more visually appealing manner.

This book provides up-to-date information on bioinformatics tools for the discovery and development of new drug molecules. It discusses a range of computational applications, including three-dimensional modelling of protein structures, protein-ligand docking, and molecular dynamics simulation of protein-ligand complexes for identifying desirable drug candidates. Moreover, it presents structure and ligand-based drug design tools to optimize known drugs and guide the design of new molecules. The book also describes methods for identifying small-molecule binding pockets in proteins, and summarizes the databases used to explore the essential properties of drugs, drug-like small molecules and their targets. In addition, the book highlights various tools to predict the absorption, distribution, metabolism, excretion (ADME) and toxicity (T) of potential drug candidate.