Preface

Using computational techniques and methods, chemoinformatics aims to study and solve complex chemical problems. The collection of topics in this book aims to reflect the diversity of recent advances in chemoinformatics with a broad perspective which may be useful for scientists as well as for graduate students and engineers.

The main objective of this book is to provide innovative chapters on the growth of educational, scientific, and industrial research activities among chemists and chemical engineers and provides a medium for mutual communication between international academia and the industry. Reporting new methodologies and important applications in the fields of chemical informatics as well as includes the latest coverage of chemical databases, this book aims to present leading-edge research from around the world in the dynamic field of chemoinformatics.

Advanced Methods and Applications in Chemoinformatics: Research Methods and New Applications is made up of 17 chapters which will provide insight on this very topic as a whole.

Chapter 1 introduces quantitative structure activity relationship (QSAR) as a mathematical representation of biological activity in terms of structural descriptors. The chapter will present density functional theory based reactivity indices are applied as chemical descriptors in QSAR analysis for ecotoxicological studies on a group of aromatic compounds.

Chapter 2 indicates that the feasibility of replacing a given molecule by similar ones in the composition of a complex drug is studied. In taxonomy the detailed comparison of the sequences of biomolecules, proteins or nucleic acids, allows the reconstruction of a molecular phylogenetic tree.

Chapter 3 explains that nanomaterials are becoming an important component of the modern life and have been the subject of increasing number of investigations involving various areas of natural sciences and technology. However, theoretical modeling of physicochemical and biological activity of these species is still very scarce.

Chapter 4 reviews the active learning methodology, and a new one that aims at generating successively new samples in order to reach an improved final estimation of the entire search space investigated according to the knowledge accumulated iteratively through samples selection and corresponding obtained results, is presented. The methodology is shown to be of great interest for applications such as high throughput material science and especially heterogeneous catalysis where the chemists do not have previous knowledge allowing to direct and to guide the exploration.

Chapter 5 studies molecular similarity using a particular type of neural networks: the Kohonen networks (also called "SOM" Self- Organizing Maps), applying the nearest neighbor algorithm to the projection of the molecules (coordinates) in the constructed MAP.

Chapter 6 is a QSAR/QSPR study with a graph-theoretical centered on a vertex degree based on simple, general (or pseudograph), and complete graphs has shown the ability of the, connectivity, pseudoconnectivity and dual indices to achieve a quite good model of activities (*LogP*) in six different media and of four properties of two different and highly heterogeneous classes of compounds.

Chapter 7 explains that the logistic temporal solution of the generalized Michaelis-Menten kinetics is employed to provide a quantum basis for the tunnelling time and energy evaluations of Brownian enzymic reactions. The mono-substrate and mixed inhibition cases are treated and the associated quantum diagrams of the reaction mechanisms are depicted in terms of intermediate enzyme complexes.

Chapter 8 provides an overview of the most important feature selection methods, their advantages, disadvantages and applications in SAR and QSAR is given.

Chapter 9 presents the approximate analytical and numerical solution of cubic autocatalytic reaction-diffusion equations. There is a great deal of interest in chemical reactions which exhibit oscillatory solutions. These oscillations occur due to feedback in the system either chemical feedback such as autocatalysis or temperature feedback due to non-isothermal reaction.

Chapter 10 reviews the application of Quantitative Structure-Activity Relationships for the treatment of molecules involving thousands of atoms, such as proteins, nucleic acids (DNA, RNA), or polysaccharides. This is a new developing area of interest in Chemoinformatics, and it is expected to have a growing number of applications during the forthcoming years. Among the several points to be addressed during the modeling of macromolecules, the most important one appears to be the accurate representation of the chemical structure through numerical descriptors. It has to be noticed that descriptors based on optimized three-dimensional geometry are difficult to specify, and it is also a drawback the fact that the experimental geometry is not available.

Chapter 11 analyzes virtual screening advantages and the classification of virtual screening approaches. Also discussed is the current and potential importance of virtual screening for drug development in Latin America. Finally, the authors present a brief overview on virtual screening perspectives.

Chapter 12 generalizes the sol-gel made titanium dioxide nanostructure thin films deposited on special substrates such as glasses, mica, steels, textiles, fibers, and other organic/inorganic substrates were reviewed. Through this review, several distinctive properties such as optical, electrical, photocatalytic, morphological, and mechanical properties of TiO_2 nanostructured thin films were described.

Chapter 13 surveys the application of the electrostatic potential at nuclei (EPN) as a reactivity index in quantifying hydrogen bonding as well as different reactions of organic compounds. Numerous applications showed that the EPN index, an accurate quantum mechanical quantity, predicts with remarkable accuracy the energy shifts accompanying hydrogen bonding.

Chapter 14 explains the era of computers and the development of computer science, quantum chemists were among the first scientists to explore the potentialities of the new tool, and even to collaborate in its development. In this way, they also became participants in what many dubbed as the Second Instrumental Revolution in chemistry.

Chapter 15 discusses some of the most common techniques which are widely used in bioinformatics and chemoinformatics. Most of the drugs produce their effect by interacting with the target molecules via different interactions. However, these interactions are tough to be calculated without use of robotics techniques.

Chapter 16 presents the symbolic time course equations corresponding to a general model of a linear compartmental system, closed or open, with or without traps and with zero input. Special attention

is given to the open systems, for which an exhaustive kinetic analysis has been developed to obtain important properties.

Chapter 17 focuses on extended topochemical atom (ETA) indices, a relatively new class of topological descriptors. ETA indices contain important information regarding the nature of the atoms, bonds, atomic electronic environment and consider the contribution of different functional groups, molecular fragments, and branching to the response as evidenced by different reports showing their successful application in modeling different endpoints including toxicity, drug activity, and physicochemical properties.

With this collection, this book will provide innovative chapters on the growth of educational, scientific, and industrial research activities among chemists and chemical engineers and provides a medium for mutual communication between international academia and the industry.

Eduardo A. Castro
Research Institute of Theoretical and Applied Physical-Chemistry (INIFTA), Argentina

A. K. Haghi
University of Guilan, Iran