Preface

Methodologies and Applications for Chemoinformatics and Chemical Engineering is aimed at providing comprehensive coverage on the latest developments of research in the ever-expanding area of theoretical and computational chemistry and their applications to broad scientific fields spanning physics, chemistry, biology, materials, and so on. A common misconception about Chemoinformatics is that it is difficult; it is not. It requires effort and dedication, focus and insight, like any other discipline, but its fascinating nature and findings can be explained easily.

Where does this come from then? The reasons are probably two: the first is counter-intuitiveness. The world at the quantistic level has strange, unusual rules, mainly due to its probabilistic nature and the fact that the world we appreciate with our senses focuses on a completely different scale.

The second reason is the tight bond between the language of chemistry and the language of computers. To properly convey the formal message and explore the facts, understanding of a proper computational framework is fundamental. However, to explain the specific meaning of the findings does not require complex mathematics: a clear explanation of the meaning of pages of convoluted equations is possible, just seldom found.

The aim is to provide both a rigorous view and a more practical, understandable view of methodologies and applications for chemoinformatics and chemical engineering in parallel. Although its aim is not divulgative, this book wants to satisfy readers with both direct and lateral interest in the discipline. It will show equations, but also concepts. The uninterested reader can skip the equations and pick only the final concrete message, hopefully with unaltered results. Although the lack of mathematical formalism will introduce more difficulty in understanding future concepts, it should not preclude people with lateral interest in the discipline to understand the fundamental points.

With the proliferation of sub-fields in the application of theoretical chemistry and the explosion of applications in various scientific fields, it is difficult these days for us to keep up with all the new research developments in these cross-disciplinary fields. This book will serve as a major single source of information on the latest research that can be broadly defined to be in the general area of theoretical and computational chemistry. This book includes original contributions on broad aspects: from both the development of fundamental theoretical methodology and computational algorithm, to extensive numerical applications, specific scientific problems ranging from gas-phase to condensed phase, and biological systems. It covers general research areas broadly defined as quantum chemistry, chemical dynamics, statistical mechanics, and chemical biology.
This volume is structured into different parts devoted to chemoinformatics, chemical engineering, and applications. Every section of the book has been expanded where relevant to take account of significant new discoveries and realizations of the importance of key concepts. Furthermore, most chapters provide instructions about algorithms and knowledge representation. Emphases are placed on the underlying fundamentals and on acquisition of a broad and comprehensive grasp of the field as a whole.

The coverage also ranges across the broad field of computational chemistry, an area that has recently seen rapid development at the forefront of scientific research and technology, such as QSTR (Quantitive-Structure-Toxicity-Relationship) and self-organizing neural networks to study molecular similarities.

Since we aim at building a bridge between different research communities that are approaching chemical systems from different perspectives, the chapters of this book are related to dynamic aspects of chemical engineering and chemoinformatics.

The book is devoted to the publication of chapters on the uses of computers in theoretical investigations of molecular structure, function, interaction, and design as well. The scope of the book also includes new aspects of molecular modeling and computational chemistry, including, for instance, the study of molecular shape and properties, molecular simulations, protein and polymer engineering, drug design, materials design, structure-activity, and structure-property relationships.

This volume brings new knowledge to the attention of our readers. As such, this volume not only reports results, but also draws conclusions and explores implications of the work presented. Routine applications of standard modeling approaches, providing only very limited new scientific insight, did not meet our criteria for publication of this volume. Reproducibility of reported calculations is an important issue. Wherever possible, the authors enhanced their chapters with supplementary data, for example, in “Retrained Classification of Tyrosinase Inhibitors” and “In Silico Potency Estimation by Using Atom-Type Linear Indices: A Powerful Tool for Speed up the Discovery of Leads”.

This volume reports new methodology and/or important applications in the fields of chemical informatics and molecular modeling. Specific topics include the representation and computer-based searching of chemical databases, molecular modeling, computer-aided molecular design of new materials, catalysts, development of new computational methods or efficient algorithms for chemical software, and biopharmaceutical chemistry, including analyses of biological activity and other issues related to drug discovery.

The reader will stay abreast of database search systems, use of graph theory in chemical problems, substructure search systems, pattern recognition and clustering, analysis of chemical and physical data, molecular modeling, graphics and natural language interfaces, bibliometric and citation analysis, and synthesis design and reactions databases (e.g., in “Bundlet Model for Single-Wall Carbon Nanotubes, Nanocones, and Nanohorns”).

Most chapters of this volume provide a balanced introduction to chemoinformatics and chemical engineering. Suitable for both experimentalists and theoretors, a wide range of samples and applications are included, drawn from all key areas. The book carefully leads the reader through the necessary equations providing information explanations and reasoning where necessary and firmly placing each equation in context.

A. K. Haghi
University of Guilan, Iran