Preface

In 2004, vol. 275 of the *Methods in Molecular Biology*™ series was published. This book, entitled *Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery*, presented an array of different chemoinformatics methodologies. Now, 6 years later, a second volume focusing on chemoinformatics is introduced with the title *Chemoinformatics and Computational Chemical Biology*. Besides new focal points, there is a link between these volumes because eight of the lead authors who contributed in 2004 also contribute to the new book.

Over the past years, the chemoinformatics field has further evolved and new application areas have opened up, one of which is highlighted in the new book. Other developing application areas for chemoinformatics approaches could have also been emphasized, but chemical biology, the study of biological functions and systems using small molecules, seemed particularly appropriate, given that this field is at least distantly related to pharmaceutical research, which has been one of the origins of chemoinformatics (and also a major focal point of the 2004 volume). Topics of interest in chemical biology that can be addressed with the aid of chemoinformatics methodologies include, among others, system-directed approaches using small molecules, the design of target-focused compound libraries, the study of molecular selectivity, or the systematic analysis of target–ligand interactions, all of which are discussed in the book.

Currently, both long-established computational approaches and new methodologies are considered part of the chemoinformatics spectrum, and the book also aims to reflect this situation. Thus, in addition to topics relevant for chemical biology, which are mostly discussed in the last third of the book, mainstays of chemoinformatics are covered including similarity methods, machine learning, probabilistic approaches, and fragment-based methods. Other contributions concentrate on structure–activity relationships and underlying activity landscapes, pharmacophore concepts, de novo ligand design, and chemical reaction modeling. Many contributions discuss issues related to virtual compound screening. Two chapters even go beyond the current chemoinformatics spectrum by describing knowledge-based modeling of G protein-coupled receptor structures and computational design of siRNA libraries. The book begins with a detailed introduction into the chemoinformatics field and its development and ends with a discussion of statistical standards for the evaluation of virtual screening calculations, a topic of general relevance.

This book has brought together a group of leading investigators, both from academia and industry, who have helped to shape the chemoinformatics field. Eighteen chapters were solicited from different investigators to cover various methodological aspects of chemoinformatics. As the book evolved, four contributions from our group were added to complement and further expand selected research areas. More than half of the 22 chapters have review-type character; the others describe an individual method or a class of methods. The sequence of chapters follows a logical flow, to the extent possible, and chapters having thematic connections are presented back-to-back.

It is hoped that this compendium of articles will be of interest to experts, but also newcomers to this exciting field. I am very grateful to our authors whose contributions have made this book possible.

Bonn, Germany, January 18, 2010 ***Jürgen Bajorath***

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