

# Preface

Chemoinformatics is a key technology for today's synthetic/medicinal chemist. People with extensive knowledge of chemistry and computer skills are immensely required by the industry. Database producers, chemical software developers, and chemical publishers offer attractive opportunities to the chemoinformaticians. The present book is intended to be a useful practical guide on chemoinformatics for the students at graduate, postgraduate, and Ph.D. levels. There are a couple of books on the theory of chemoinformatics and plenty of scattered information is available on the web but a well structured *Do it yourself* book is urgently required. The idea is that the reader of any background should be enthused to follow the book and start using the computer or a computer enthusiast can start learning the basics of computational chemistry. With this objective in mind, numerous step by step practice tutorials, source code snippets, and *Do it yourself* exercise have been given for quick grasp of the subject. The book intends to put the students in the driver's seat to test drive the software, code snippets, and practice tutorials. Rules of thumb have been provided at the end of every chapter for specific practical guidance. The language has been intentionally kept simple, technical jargon wherever used has been thoroughly explained. Adequate bibliography has been provided for readers seeking advanced knowledge on any of the given topics. The chapters in the book are linked to each other and at the same time are independent of each other.

The book begins with an elementary chapter on how to read and write molecules into a computer and basic file format conversions. The second chapter teaches how to compute properties of molecules and store them in a database. The third chapter delves into the use of computed property data to build models employing machine learning methods. The fourth and fifth chapters deal with protein active site prediction and docking studies, both of which are essential for any successful drug design experiment. The sixth and seventh chapter focus on use of reaction and NMR chemical shift based fingerprints respectively, and their use of virtual screening—an important component in chemoinformatics. The eighth chapter deals with text mining and its role in chemoinformatics methods to discover a lead molecule. The ninth and tenth are technology focused chapters that demonstrate ways to handle big data using today's state of art workflows, portals deployed in distributed, cloud

computing platforms, and Android-based app development. To sum up, the purpose behind bringing out this book is to demystify and master chemoinformatics through a practical approach and make students aware of the latest developments in this field. After comprehending the entire book the reader will be able to appreciate the power of chemoinformatics tools and apply them for practical use.

Practical Chemoinformatics

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