Bioorganic & Medicinal Chemistry 20 (2012) 5316

Contents lists available at SciVerse ScienceDirect

Bioorganic & Medicinal Chemistry

journal homepage: www.elsevier.com/locate/bmc

Preface

Chemoinformatics: Recent advances at the interfaces between computer and chemical information sciences, chemistry, and drug discovery

Nearly 25 years ago, the term 'chemoinformatics' first appeared in the scientific literature. However, scientific roots of this field can be traced back at least to the 1960s (if not beyond). Similar to the situation in bioinformatics, research activities that we would presently consider to fall into core areas of chemoinformatics (such as compound classification or database searching) existed long before this term was coined. However, even nowadays one is hard pressed to clearly define or delineate the chemoinformatics field. This is not unexpected for an interdisciplinary research field that continues to evolve at interfaces between computer and chemical information sciences, chemistry, and pharmaceutical research. Scientifically, the chemoinformatics field is highly diverse. Yet, there are least a few characteristics. First and foremost, many of the early chemoinformatics research and development activities have originated in pharmaceutical environments and a primary focus on drug discovery has remained a characteristic of the field to this date, despite its heterogeneity. The analysis and prediction of biological activities of small molecules continue to represent the most popular tasks in chemoinformatics, which are methodologically approached in rather different ways. Furthermore, a strong emphasis on method development represents another general characteristic. In fact, a plethora of chemoinformatics methods of very different design and computational complexity is currently reported, many of which might hardly ever be utilized in practical applications. However, over the years a number of chemoinformatics approaches have matured to the point that they are directly impacting experimental programs, for example, in targeted library design or practical virtual screening. All in all, the field continues to be in flux and this makes it particularly interesting to be a part of it.

When putting together a Special Issue on chemoinformatics, a few choices need to be made. For example, one might consider assembling a collection of articles around pre-selected topics or methodological concepts and hence attempt to provide a general overview of this field. Alternatively, one might structure an issue around selected authors and thus emphasize individual contributions. In organizing this Special Issue, the latter strategy was chosen. After all, research fields are shaped by individuals (especially if these fields are interdisciplinary in nature) who—as authors—should probably have the last word.

This Symposium-in-Print brings together leading investigators from Europe, the United States, and Japan, both from industry and academia. State-of-the-art contributions include review-type and original research articles. Together, the papers cover a wide range of topics within the chemoinformatics spectrum and do reflect the diversity of this field, as one would wish for. For example, different contributions focus on compound filter functions, clustering approaches, or machine learning methods such as variants of self-organizing maps. Furthermore, database mining and design approaches are presented as well as computational chemistry methods with relevance for drug design. Moreover, emerging themes such as activity landscape modeling are discussed and new concepts are introduced such as 'chemotography'. Because these contributions cover many aspects of the chemoinformatics spectrum, further supported by reviews, they do—at last—also provide a good (yet incomplete) overview of the field, although a clear priority was initially assigned to individual preferences of selected authors.

It is anticipated that this Symposium-in-Print will make an interesting read for experts, or aspiring experts, in chemoinformatics and/or computer-aided drug design (the boundaries are fluid here). In addition, it is hoped that this collection of articles might also be appealing to practicing chemists who wish to have a first glimpse, or deeper look, into this interdisciplinary area of research with high relevance for drug discovery.

I am very grateful to all authors who have agreed to contribute to this Special Issue.

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0968-0896/$ - see front matter
http://dx.doi.org/10.1016/j.bmc.2012.08.051