

PREFACE

The Beilstein Institute organizes and sponsors scientific meetings, workshops and seminars, with the aim of catalysing advances in chemical science by facilitating the interdisciplinary exchange and communication of ideas amongst the participants.

This workshop – *Molecular Informatics: Confronting Complexity* - addressed some of the new challenges that face scientists in the post-genome era, in particular, the integration of two, until recently, disparate sciences – chemistry and biology. The underlying theme of the workshop was to gain insight into the behaviour of biological and molecular systems through the application of molecular informatics.

The flood of data being generated as a result of research into genomics and proteomics is often overwhelming. Well publicised successes tend to draw the focus away from some of the significant issues relating to a better understanding of molecular systems which are still far from clear. Whereas the development of predictive models based on analogy has been very successful in chemistry and cheminformatics, the non-linear nature of biomolecular systems, often with multiple pathways, restricts similar transference within bioinformatics. However, without a critical analysis, taking into account the assumptions and limitations of hypotheses and predictive models, advances in molecular informatics will not assume significance. Before this can be effectively carried out, more effort needs to be made in bridging the gap between chemists, dealing with the structure and properties of molecules, and biologists, working with complex molecular and cell physiological systems.

Participants, as well as, speakers were confronted with the following complex challenges from cheminformatics and bioinformatics: knowledge discovery and data mining, rational drug design, prediction of small molecule bioavailability (ADME Tox) properties, protein structure and function determination, new methods of drug-target modeling, cellular metabolism and metabolic pathways, and the use of high-throughput methods (biochips, x-ray crystallography) for acquiring gene expression and protein structure, as well as, binding information.

This meeting did not set out to solve all problems, but to initiate a dialog between scientists of different disciplines. Over the three days of the workshop, the participants not only heard excellent talks, took part in lively discussions, but in the time between the official sessions of the scientific program, exchanged ideas and thoughts and generally made a valuable and personal contribution to bridging the gap!

We would like to thank particularly the authors who provided us with written versions of the papers that they presented. Special thanks go to all those involved with the preparation and organization of the workshop, to the chairmen who piloted us successfully through the sessions, and to the speakers and participants for their contribution in making this workshop a success.

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