



Beilstein-Institut
zur Förderung der Chemischen Wissenschaften

International Workshop

**Molecular Informatics:
Confronting Complexity**

May 13th -16th, 2002

**Hotel Schloss Korb,
Missian-Eppan,
nr. Bozen, Italy**

Scientific Program

Overview

This workshop will address the new challenges that now face scientists in the post-genome era. In particular, the integration of two, until recently, disparate sciences - cheminformatics and bioinformatics. It is now essential to bridge the gap between chemists, dealing with the intricacies of drug discovery, and biologists, working with complex cell physiological systems, in order to make any real and significant advances in the areas of molecular structure-function relationships and drug-target specificity.

The flood of information being generated as a result of research into genomics and proteomics is often completely overwhelming. Consequently, successes tend to focus away from some of the significant issues relating to a better understanding of molecular systems which are still far from clear. The effective use of information derived from genomics and proteomics is of central importance and the ability to identify the most important data, to assess its accuracy and to be aware of any assumptions and limitations of hypotheses and predictive models is absolutely essential. Whereas the development of predictive models based on analogy has been very successful in chemistry and cheminformatics, the complex nature of biomolecular systems limits similar transference within bioinformatics. Without a critical analysis, in-silico discovery will be unable to be effectively integrated in the field of molecular informatics.

The following themes will be covered: 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 the use of high-throughput methods (biochips) for acquiring gene expression and protein binding information.

Scientific Program

Tuesday 14th

9.00	Opening Remarks and Greetings <i>Session Chair: Hugo Kubinyi</i>	Martin G. Hicks
9.15	Studies on yeast membrane transporters – how can computational biology help?	Carsten Kettner
10.00	Understanding the nature and consequences of protein folding and misfolding	Chris Dobson
10:45	Coffee	
11.15	Evolutionary perspectives on protein folding, structure and thermodynamics	Richard Goldstein
12.00	Prediction of protein structure and function on a genomic scale	Jeffrey Skolnick
12.45	Lunch <i>Session Chair: Holger Wallmeier</i>	
14.30	Pattern recognition in drug design	Graham Richards
15.15	Generating synthetically accessible ligands by de novo design	A. Peter Johnson
16.00	Tea	
16.30	Physicochemical properties and the discovery of orally active drugs: technical and people issues	Christopher Lipinski
17.15	Molecular feature mining for predictive toxicology	Luc De Raedt
18.00	Close	
19.00	Dinner	

Wednesday 15th

Session Chair: Günther Metz

9.00	Metabolic analysis as a tool in drug design	Athel Cornish-Bowden
9.45	Representing and analysing information on networks of cellular function	Shoshana Wodak
10.30	Coffee	
11.00	DNA-microarrays; technology and application	Jörg Hoheisel
11.45	Halolex: a lighthouse in the flood of information	Friedhelm Pfeiffer
12.30	Lunch	
14.30	Excursion	
20.00	Banquet	

Thursday 16th

Session Chair: John Bradshaw

9.00	Computer-aided design and screening of combinatorial drug libraries	William Jorgensen
9.45	New approaches to in-silico screening	Hans-Joachim Böhm
10.30	Coffee	
11.00	Hits, leads, and artefacts from molecular docking & other screens	Brian Shoichet
11.45	High throughput x-ray crystallography for drug discovery	Harren Jhoti
12.30	Lunch	

Session Chair: Christoph Steinbeck

14.30	Computer-assisted decision making in pharmaceutical research	Gerald Maggiora
15.15	Knowledge based lead finding by matching chemical and biological space	Karl-Heinz Baringhaus
16.00	Tea	
16.30	Providing cheminformatics solutions to medicinal chemists to support drug discovery decisions	Kevin Holme
17.15	Does quantum chemistry have a place in cheminformatics?	Timothy Clark
18.00	Summary	Gisbert Schneider
19.00	Dinner	