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## PREFACE

Managing and effectively utilizing large collections of highly diverse chemical data – especially when chemical structures are involved – is a major challenge for the chemical and pharmaceutical industries and universities, as well as for the producers of large publicly available databases. Automated techniques, such as, combinatorial chemistry coupled with high throughput screening result in the routine generation of enormous amounts of data. Methods of information handling such as knowledge discovery and data mining, machine learning, statistical analysis, and visualization, whose origins lie outside chemistry, are becoming more and more applicable in the area of chemical sciences. The aim of this workshop was to bring together experts from chemical and non-chemical fields to discuss new and better methods for handling and analyzing large amounts of data of a chemical nature.

The remote location of Schloss Korb – set on a hillside overlooking Bozen/Bolzano – provided the ideal venue for the participants to spend time discussing issues of interest and to make contact with scientists from different disciplines. The format of these workshops, with ample time for discussion between the lectures and afterwards at lunch and dinner, provided the participants with something rarely found at larger meetings – time to think and time to talk.

Over three days we heard a series of invited talks, which covered the following areas:

- Knowledge Discovery and Data Mining
- Information Extraction and Text Mining
- Data Compression and Clustering of Large Data Sets
- Chemical Structure Representations
- Structure Browsing and Similarity Indexes
- Virtual Screening and Library Design
- Property Prediction
- Visualization of Data and Physicochemical Properties

The scientific program was compiled by Martin Hicks (Beilstein-Institut), Gerald Maggiora (Pharmacia) and Peter Willett (University of Sheffield).

The Beilstein-Institut organizes and sponsors scientific meetings, workshops and seminars, with the aim of catalyzing advances in chemical science by facilitating the interdisciplinary exchange and communication of ideas amongst the participants. We were very pleased that speakers from both inside and outside the mainstream chemical community accepted invitations to speak. The resonance that we had both during and after this workshop clearly reflected the attractiveness of the scientific program and the format of the workshop.

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, as well as to the speakers and participants for their contributions in making this workshop a success.

Werner Brich

Martin G. Hicks