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Preface

The developments in information technology in the last decades of the 20th century have fundamentally changed the way in which scientific information is being communicated and used. Today's students probably hardly realize that less than 25 years ago computer searches for both primary literature references and factual scientific data were impossible, simply because the technology still had to be developed and the data files still had to be built. Similarly, in chemistry, molecular modeling was a hardly-existent computational chemistry niche, only practiced at those few institutes that could afford the very expensive specialized hardware. And where the Internet, the Web, and the CD now play a major role in science and education, these fields have been the almost exclusive domain of printed information for centuries and up to the last two decades of the past one.

A scientific discipline where the impact of these changes has been particularly significant is (bio)chemistry. Access to not only the primary literature but, possibly even more importantly, to the factual primary data about millions of chemical compounds, to reactions, structures, and spectra, and to the genomic data of various organisms including humans, can only be provided by digital storage and retrieval techniques. Computerized information storage and retrieval and computational chemistry and molecular modeling are now an essential part of chemical research and the scope of these activities reaches from organic synthesis and physical chemistry to molecular biology.

This book seeks to document some key developments in computerized chemical information handling in the last two decades of the past century and to bridge to recent cheminformatics research by covering selected topics in the fields of organic synthesis, drug design, crystallography, modeling and chemistry teaching. I have been fortunate to have found renowned experts in these fields, among which some of my former co-workers at the Dutch CAOS/CAMM Center, willing to contribute with chapters on the history, the research topics and the service facilities at their institutes and in their fields of expertise.

To put the developments into a historic perspective, I have chosen to include, as opening chapters, three review articles on the founding, the history, and the operation of three different representative European computer chemistry institutes; one in the Netherlands, one in the UK and one in Germany. These introductory chapters are personal accounts of history and development and clearly show the different approaches and aims in setting up these (academic) research and/or service facilities for computer-aided chemistry and cheminformatics.

In Chapter 1, I survey the development of the former CAOS/CAMM Center, a Dutch inter-university institute focusing on cheminformatics services with cheminformatics research as a spin-off activity. In Chapter 2, the Chemical Database Service in the UK, where cheminformatics services are the main activity, is reviewed and

described by Bob McMeeking and Dave Fletcher. Johnny Gasteiger and Tim Clark have contributed Chapter 3, in which they describe their computational chemistry and computer-assisted synthesis design research, eventually leading to the founding of the Computer Chemie Centrum in Erlangen, Germany.

A number of selected topics in the fields of organic synthesis, drug design, crystallography, modeling and chemistry teaching, fields where the impact of cheminformatics developments has been particularly significant, are treated in depth in the following chapters, thus bridging from history to current research and the state-of-the-art. Chapter 4 is devoted to organic synthetic analysis, and Martin Ott, involved for almost two decades in the development of the LHASA program and now at the CMBI at Nijmegen University, reviews methods for computerized treatment of synthetic analysis and describes the LHASA program.

The current use of cheminformatics methods and tools in drug design and lead optimization in pharmaceutical research is treated in Chapter 5 by Jan Kelder, Markus Wagener and Marco Timmers of the Organon Research laboratory in Oss, Netherlands.

Crystallographic and modeling topics are covered in Chapters 6 and 7. In Chapter 6 Sam Motherwell, a long-time (co-)developer of the Cambridge Crystallographic Database, outlines the data archiving function and reviews the research applications of this huge repository of crystallographic research data.

In Chapter 7 Paul Verwer, now at the Dept. of Solid State Chemistry, Nijmegen University, Netherlands, and Frank Leusen from the University of Bradford, UK, treat recent developments in (applications of) small molecule modeling and structure prediction.

Information technology and, in particular, developments in computer graphics have not only significantly influenced chemical research but also chemical education in the last two decades of the 20th century. When, in the mid-80s, it became possible and affordable to use the chemist's language, i.e. structural formulae, in communicating with computers, this technology – to manipulate molecules and molecular ensembles in 3D on a computer screen – penetrated into the PC world within only a few years. This spawned the development of new educational tools. CDs appeared as a supplement to textbooks. Stand-alone PC programs could handle structure data files, and Internet-accessible tutorials became available for individual or classroom teaching. Many individual and cooperative initiatives have resulted in tools, which go far beyond the possibilities of printed text. In particular, new possibilities have emerged to teach the 3-D nature and the flexibility of molecules in reactions.

In Chapter 8 Hens Borkent, now at the CMBI, Nijmegen University, Netherlands, addresses these developments and the question of how far newly-developed tools have been successful and lasting.

Jan H. Noordik
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