

Journal of Molecular Graphics and Modelling

www.elsevier.com/locate/JMGM

Journal of Molecular Graphics and Modelling 21 (2003) 321

Editorial Foreword

In July 2001, IUPAC held its first General Assembly in the southern hemisphere in Brisbane, Queensland. It was also the first time the General Assembly was held simultaneously with the IUPAC World Chemistry Congress. The combined meeting attracted approximately 1500 scientists from around the world. Two of the five themes in the scientific congress were organized by the Asian Federation for Medicinal Chemistry (AFMC), and the Federation of Asian Chemical Societies (FACS), and the Congress and Assembly were hosted by the Royal Australian Chemical Institute (RACI).

The theme of the biomedical section of the Congress was "Challenges for Drug Discovery and Development in the Twenty-first Century". There was also a substantial theme relating to "Chemistry by Computer" recognizing the fact that there are now three ways of conducting science—theory, experiment, and simulation or modeling. These two themes alone contained over 100 high quality papers delivered as oral presentations, with many more papers given as posters.

The five papers in this special issue, presented by authors from Australia, Japan, and Singapore, give a taste of the diversity of work presented at the Congress. The featured authors present work relating to modeling of interstellar chemistry (Birch Medalist John Bowie), the use of novel pharmacophore methods to discover HIV reverse transcriptase inhibitors (Renate Griffiths, and Paul Keller), novel methods of visualizing and navigating massive SAR data sets (Yoshimasa Takahashi), the use of soft computing methods to find eukaryotic promoter sites in gene sequences (Vlad Bajic and Vlad Brusic), and design of supramolecular structures from models of cyclic peptide scaffolds (Fairlie).

I thank the authors who contributed their interesting and high-quality work. This issue could not have been completed without the valuable and rigorous refereeing of the journal's editorial board members and other anonymous chemists, whom I want to heartily acknowledge. On the editorial side, thanks are due to Elsevier Science, which is publishing this special issue, and to Andy Holder, for his advice and encouragement.

The RACI and MGMS are jointly hosting an international molecular modeling and drug discovery conference in Lorne, Victoria, Australia between 5 and 10 February 2003 AIMECS01 congress in Brisbane, Australia (http://www.chem.csiro.au/raci/biomolecular). I invite readers to attend this major meeting and become more involved with molecular design in the Asia-Pacific region.

David A. Winkler CSIRO Molecular Science, Private Bag 10 Clayton South MDC3169, Australia Tel.: +61-3-9545-2477; fax: +61-3-9545-2446 E-mail address: dave.winkler@csiro.au (D.A. Winkler)