Available online at www.sciencedirect.com
SCIENCE DIRECT®
Journal of Molecular Graphics and Modelling 22 (2004) 465
Journal of Molecular Graphics and Modelling
www.elsevier.com/locate/JMGM

Foreword

In February 2003, the international conference on 'Bioactive Discovery in the New Millennium' was held in the seaside town of Lorne, Victoria, Australia. The meeting focused on cutting edge methods of discovering and developing new bioactive agents. It was a Gordon conference style residential meeting to maximize the interactions between the delegates. This proved very successful, especially for the student participants.

The conference was a joint meeting of

- the Biomolecular Chemistry Division of the Royal Australian Chemical Institute (RACI)
- the European Chapter of the Molecular Graphics and Modelling Society (MGMS)
- the Australian Molecular Modelling Workshop (MM2003)
- the Medicinal Chemistry project of the Federation of Asian Chemical Societies (FACS)

It aimed to facilitate dialog on multidisciplinary approaches to the design and development, not only of pharmaceuticals but also veterinary drugs, agrochemicals and other bioactive agents. Given the involvement of several specialist modelling societies, and the overlap with the Lorne structural biology conference, there was a focus on the use of computational methods and molecular modelling to design new bioactive agents using protein structure information. The conference attracted 175 participants from 19 countries, and 11 trade exhibitors. Approximately 100 papers were presented, roughly half oral and half posters.

Conference topics included: natural bioactive compounds; de novo design; molecular docking methods; novel organic and biomimetic synthesis, chemistry driven lead generation and optimization; quantitative structure–activity relationships (QSAR); soft computing methods and complex systems; measurement and modelling of ADME properties; informatics; quantum chemical methods and applications; high throughput structural biology, NMR studies of ligand–receptor interactions, molecular mechanics and dynamics; pharmacology; and toxicology.

The conference had a very strong line up of 20 plenary speakers including Nobel Laureate Prof. Peter Doherty. A "Startups and Spinoffs" workshop was also held, which explored the path between scientific discovery, invention and ultimately, a spinoff company. The aim was to allow researchers who had made the jump from pure research to a startup or spinoff company to explain how this was achieved, and to discuss the advantages and pitfalls of commercializing research outputs in various ways.

The seven papers in this special issue, presented by authors from Australia, USA, Germany, and the UK provide a taste of the diversity of work presented at the conference. The featured authors present work relating to selection of compounds for HTS using neural networks (Martyn Ford), the use of novel pattern recognition methods and worldwide grid computing to discover agents to counter bioterrorism (Graham Richards), accounting for solvent in ligand docking calculations (Glen Kellogg), pitfalls in the use of structure-based modelling of DM-PK (Bob Clark), robust methods for building models for predictive ADMET (Dave Winkler), quantitative structure-metabolism methods for predicting secondary metabolism (Paul Smith), and QSAR and QSPR based on surface properties (Tim Clark).

Acknowledgements

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.

David A. Winkler
CSIRO Molecular Science Private Bag 10
Clayton South MDC 3169, Australia
Tel.: +61-3-9545-2477; fax: +61-3-9545-2446
E-mail address: dave.winkler@csiro.au
(D.A. Winkler)
Available online 17 April 2004

1093-3263/$ – see front matter
doi:10.1016/j.jmgm.2004.03.005