

## Reinvention of the Journal of Molecular Graphics and Modelling: News and Views

Chemical Design Automation News (CDAN) was launched by Polygen Corporation in April 1986 as a newsletter for the molecular modelling and computational chemistry community. Under the energetic editorship of Barbara F. Graham, CDAN was a substantial, informative newsletter carrying news and features of interest to this burgeoning discipline in both academia and industry. CDAN rapidly became established with up to six issues annually and grew in reputation and was often cited like a journal.

During the early 1990s, Polygen (by then absorbed by Molecular Simulations Inc.) felt that the time was right for the newsletter to become independent. After some negotiation, CDAN was picked up by the publisher of this Journal. Editorial control was taken by the Molecular Graphics and Modelling Society (MGMS). A few years ago, CDAN was merged into this journal to focus all the publishing activities of the MGMS in one publication. During this period, Cecilia H. Blaney capably served as editor.

As part of our ongoing efforts to shape a new journal tailored for the current needs of the members of MGMS and the Computers in Chemistry Division of the American Chemical Society, we are delighted to announce that Dr. Shauna Farr-Jones has been appointed editor of a new section of the journal called News and Views. This section will subsume the role of CDAN and feature commentary, book reviews, software reviews, announcements, meeting reports, and stories on a variety of topics pertinent to our readers. Abstracts from meetings will be published as requested by our affiliated professional societies.

Dr. Farr-Jones is a researcher with biochemistry, business, finance, and molecular modeling experience at the Department of Pharmaceutical Chemistry, University of California, San Francisco. Originally from Canada, she obtained a B.Sc. (Hons.) from Southampton University, a M. Phil. from the University of Surrey, and a Ph.D. in Biochemistry from Tufts University. Presently, she is an assistant researcher at UCSF, where she works on applying NMR and computational methods for protein structure determination. She has published papers with Fred Cohen, Thomas James, and Ken Dill.

Dr. Farr-Jones plans to use her experience in free-lance writing and market research to reshape the News and Views section. She is working on a number of changes which will serve and respond to the interests of the molecular modelling—computational chemistry community. We welcome Dr. Farr-Jones to the Journal.

In addition, we note the establishment of a new web presence to assist individuals who wish to contact the editors. The URL for the new web site is http://chem.iupui.edu/~boyd/jmgm.html. The site supplements the functions of existing web sites pertaining to the Journal, i.e., http://www.elsevier.nl/locate/jmgm/, http://chemweb.com/, and http://sciencedirect.com/.

Roderick E. Hubbard, D.Phil. Donald B. Boyd, Ph.D. Editors, *Journal of Molecular Graphics and Modelling*