## THE VEIL OF COMMERCIALISM

Occasionally, there arises an issue so fundamental that it cannot be ignored. The issues in this case are the artificial impediments to publication of experimental data which preclude the examination by the scientific community of the basis on which significant conclusions are drawn. In particular, the letter from Dr. Frederic M. Richards, which is co-signed by over 200 scientists and printed in this issue, addresses the delay between determination and announcement of crystal structures and the availability of coordinates. As proteins which are potential therapeutic targets have been solved, the commercial pressure on investigators to withhold the information and distribute it selectively in return for research support has become the rule rather than the exception. While this is an understandable response in times of limited funding and an exploding array of new biotechnology ventures, it strikes at a fundamental tenet of science. Science progresses by verification of observations and testing of the resulting conclusions by other investigators. Withholding crucial data circumvents this essential aspect and reduces a scientific contribution to the equivalent of a rumour. The editors of the *Journal of Computer-Aided Molecular Design* believe it essential for the scientific community to address its own ethical questions in a responsible manner and support both the essence and the intent of the letter from Dr. Richards and colleagues. We intend to abide by these guidelines and encourage other journals to take a similar stance.

We also believe this issue extends far beyond the crystallographic community. The computational chemistry community has a number of similar problems which need to be addressed in a responsible manner. One of the motivations in starting this journal was to promote the publication of machine-readable data which would allow scrutiny by other investigators of the models which arise, often from months of work and hundreds of cpu hours. In a similar vein, the development of commercial modeling packages has stimulated the field, but proprietary concerns have limited publication of force field parameters and algorithms. These limitations present impediments, sometimes insurmountable, to the critical evaluation of results arising from such systems. We believe it is time for the computational community to address this issue, and call for editors to question the validity of publication of results which are compromised in this fashion.

We also note with some pride the announcement in this issue of the availability of machine-readable supplements to five papers published in volume one of the journal. This service to the community on a cost-reimbursement basis by Dr. James B. Dunbar of the Center for Molecular Design at Washington University to provide copies of the data on either IBM or Macintosh disks deserves both our thanks and support. The editors are considering requiring submission of coordinate data in machine-readable form for future papers in this journal to assist in both evaluation of the papers by the referees and the scientific community. We would appreciate comments from our readers as to the desirability of this course of action and to potential impact upon submission of manuscripts.

In summary, the scientific community has a fundamental responsibility to insure that the results reported in papers in scientific journals can be put to the test of reproducibility. In our opinion, results which cannot be verified by others violate the criteria of a scientific hypothesis and do not

deserve space in a scientific journal. With increasing volume, the forces of advertising and marketing are making their inroads into the scientific community. We need to be vigilant regarding our standards to insure that the veil of commercialism does not descend over our area to compromise the scientific process and impede progress.

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