IMPEDIMENTS TO THE SCIENTIFIC METHOD

The publication of 'Guidelines for Publications in Molecular Modeling Related to Medicinal Chemistry' by Peter Gund, David C. Barry, Jeffrey M. Blaney and N. Claude Cohen in the *Journal of Medicinal Chemistry* [31 (1988) 2230-2234] is a noteworthy event. The Editors concur with most, if not all, of the recommendations and plan to implement several of them as part of this Journal's policy. As a whole, we find the underlying philosophy sound, that is, the scientific process depends on exchange of information and the ability to judge the merits of a piece of work by its reproducibility. This premise was one of the underlying motivations for the inception of the *Journal of Computer-Aided Molecular Design*. Included with this issue is a questionnaire to help determine how the Journal can best provide machine-readable information to help expedite the scientific process. As a matter of course, the Editors now strongly recommend that data in machine-readable form be provided with manuscripts to assist not only those researchers wishing to reproduce the reported experiments, but also reviewers in their considerations. In addition, papers dependent on software or algorithms will be considered only if the editors believe that adequate access by the scientific community to the software or algorithms is available.

One recommendation (Section I.g.) in the article by Gund et al. reflects a potential conflict between patent law and the scientific process and is quoted below:

> 'As previously recommended by the IUPAC with respect to QSAR studies, authors should REFRAIN FROM PUBLISHING PREDICTED ACTIVITIES OF SPECIFIC UNKNOWN STRUCTURES, since that may compromise the patentability of such structures if they are active, so there is reduced incentive to synthesize these materials.'

We believe this to be a misguided recommendation and encourage such publications as a means to truly verify the predictability of methodology. While it is true that commercial interests may be less likely to synthesize a compound with published predicted activity, we find that unlikely in our current milieu of competitiveness and search for new lead structures. We believe groups of scientists concentrating on methodological approaches exist which lack the resources to synthesize and test their predictions. Certainly, throwing down the gauntlet in public should generate a response. Even if that response is limited to the academic community because of commercial restriction, the scientific process can still continue. The alternative would be to restrict our field only to groups capable of synthesis and biological evaluation.

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