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Special Topic

Molecular Modeling in Drug Design

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Over the past several years there has been a steadily evolving use of molecular modeling as a tool in drug design.[1] Most medicinal chemists in industry, institutes, or academia now have access to this technique and it is taking its place as an integral part of rational drug design.

Although medicinal chemists are increasingly interested in utilizing molecular modeling, the situation with regard to hardware and software for modeling work is rather confusing for the nonexpert. In addition, in view of the many publications now appearing in the medicinal chemistry literature involving molecular modeling, there is a clear need for a set of guidelines for publication of such studies. Since this is a very new field, there are no authoritative agreed upon standards for publications. The situation is somewhat akin to the early days of QSAR where a publication[2] by a group of experts on guidelines and standards proved to be extremely valuable in assuring that published work did meet appropriate criteria.

Recognizing this situation the Provisional Section Committee on Medicinal Chemistry of IUPAC,[3] under the chairmanship of Professor C. G. Wermuth, Strasbourg, France, decided to establish a Working Party with the objective of providing some clarification for the medicinal chemist of the uses, capabilities, and compatibility of available computer hardware and software for computer-assisted molecular modeling, and to provide a set of guidelines for publication of molecular modeling studies.

As a member of the Provisional Section Committee on Medicinal Chemistry, I was asked to form a small Working Party of international molecular modeling experts and serve as chairman and medicinal chemist. Drs. Jeffrey M. Blaney, Dupont, U.S.A.; N. Claude Cohen, Ciba-Geigy, Switzerland; Peter Gund, Merck Sharp & Dohme, U.S.A.; and David C. Barry, ICI, U.K., generously agreed to serve as members of the Working Party. Dr. J. G. Vinter, SK&F, U.K., also contributed to the early activities of this group.

The Working Party set out to produce three articles in fulfillment of its mission, these being (1) Guidelines for Publications in Molecular Modeling Related to Medicinal Chemistry, (2) Survey of Molecular Modeling Software, (3) Survey of Molecular Modeling Hardware. To bring these articles effectively before the medicinal chemical community, publication in the *Journal of Medicinal Chemistry* was sought. Dr. Philip S. Portoghese, Editor-In-Chief, has kindly facilitated arrangements under which they will be published as a series of three Special Topics.

The first of these, *Guidelines for Publications in Molecular Modeling Related to Medicinal Chemistry*, follows. It was written by Peter Gund with input from the other Working Party members and advice and comments from other experts in the field.

(1) Gund, P.; Halgren, T. A.; Smith, G. M. *Annu. Rep. Med. Chem.* **1987**, *22*, Chapter 27.
(2) Craig, P. N.; Hansch, C.; McFarland, J. W.; Martin, Y. C.; Purcell, W. P.; Zahradnik, R. *J. Med. Chem.* **1971**, *14*, 447.
(3) W. Bartmann, Hoechst AG, FRG; H.König, Knoll AG, FRG; M. Ohno, Japan; H. Timmerman, Vrije University, Netherlands; J. G. Topliss, Parke-Davis, U.S.A.; C. G. Wermuth, University Louis Pasteur, France; D. Witiak, Ohio State University, U.S.A.

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