Predicted Compounds—Alleged Biological Activity

The IUPAC Commission on Medicinal Chemistry conducted a study of some of the consequences arising in the past decade from applying computer-assisted techniques to the quantitative analysis of relationships between structure and biological activity.

The IUPAC Commission recently published a report entitled " 'Predicted' Compounds with 'Alleged' Biological Activities from Analyses of Structure–Activity Relationships. Implications for Medicinal Chemists"[1]. The report examines the effects on patentability resulting from the publication of such "predicted" compounds that have not been synthesized and concludes with the following two recommendations:

1. Medicinal chemists who publish predictions of allegedly active compounds should be urged to consider it their responsibility to synthesize and test such compounds or to arrange to have this work done. "Predictions" *per se* are of little practical value unless the underlying hypotheses are tested experimentally.
2. Journal editors and editorial boards should consider the adoption of policies which discourage the publication of manuscripts containing "predictions" if they are not accompanied by the synthesis and testing of the predicted compounds.

Copies of the complete report are available from the IUPAC Secretariat, Bank Court Chambers, 2/3 Pound Way, Cowley Center, Oxford, OX4 3YF, United Kingdom, or from the undersigned.

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Received December 22, 1975.

[1] "IUPAC Information Bulletin," No. 49, Mar. 1975, pp. 12–20.

Bioavailability Information

For the past year, I have served as the Academy of Pharmaceutical Sciences' representative to the APhA Bioavailability Project Steering Committee. As I am sure you are aware, this Committee has been overseeing the writing of bioavailability monographs on selected drug products. The nine drugs to be studied in the third phase of the Project include: acetaminophen, chlordiazepoxide, conjugated estrogens, ferrous sulfate, meprobamate, papaverine (sustained release), penicillin V potassium, sulfisoxazole, and thyroid.

The discussion and analysis of information supplied by manufacturers and/or distributors of drug products are major factors of each monograph. However, one problem the Committee has encountered is correctly identifying the appropriate individual within a company to contact for information.

Since industrial pharmaceutical scientists reading this Journal are the primary individuals within their companies concerned with the bioavailability issue, I am asking each to determine if any their products is being evaluated. In addition, I would appreciate it if they would communicate with Dr. Richard P. Penna, Staff Project Director at APhA headquarters, the name of the appropriate individual within the firm who should be directly contacted to provide bioavailability information.

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Received December 22, 1975.