
IUPAC Forum

On the Reality of Virtual Libraries

by Paul Erhardt

During one of the activities of the Chemistry and Human Health Division, namely a medicinal chemistry subsection meeting directed toward harmonizing nomenclature in the area of combinatorial chemistry, we became aware of a movement to obtain patent protection of virtual libraries. Such patents have been sought most often on the basis that a library has been pre-selected to be "drug like" in its make up. Along these same lines, it appears that Chemical Abstracts Service CA Registry numbers are now being sought for the compound members within virtual libraries. Concerned about these developments for the reasons mentioned below, we welcome the views of the readership to clarify what position might actually be best to advocate as we all continue to proceed into the rapidly evolving future of drug discovery.

Since its formalization as a discipline nearly 100 years ago, medicinal chemists have contemplated what structural features a new therapeutic agent ought to contain in order to exhibit the most desirable pharmacological profile. Simply drawing such conceptions on paper, however, has never been regarded as an adequate basis for a patent even when the conceived family of structures is new and novel. This is because the patenting process has traditionally also emphasized a reduction to practice (e.g., actual synthesis of a number of representatives so as to encompass the breadth or "scope" of the proposed family of structures) along with a demonstration of potential utility by at least a real, if not the preferred, embodiment of the concept (e.g., positive

responses from the synthesized members upon their study in a biological model indicative of the anticipated response being sought in humans).

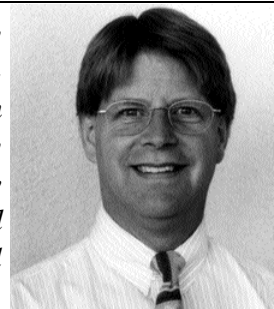
Today, it is possible with the aid of computers, to draw huge numbers of "virtual compounds" that can be thought of as drug like in their overall character based upon our notions of what types of parameters are generally required for such behavior. While this might constitute conception relative to a particular molecular scaffold to be deployed for a given therapeutic indication, it does not constitute either a reduction to practice or an actual demonstration of utility. In some ways, this situation is reminiscent of issues raised within the *Journal of Medicinal Chemistry* several years ago. In the midst of the so-called "heyday of rational drug design," this audience stepped forward to express its reluctance to engage in the wholesale publication of proposed new drug molecules that had not actually been synthesized. This is because it was recognized that this type of public disclosure could bar the patenting of such structures at a later point and could thus serve to discourage, rather than to encourage, the true pursuit of compounds deemed to be of therapeutic value. Finally, it might also be suggested that for similar reasons, prudence ought to be exercised relative to the potential assignment of CA Registry numbers to virtual compounds whether or not patents are being pursued.

Paul Erhardt is a professor at the University of Toledo, Ohio, USA, and is the director of the University Center for Drug Design & Development. He is also the current vice president of the IUPAC Chemistry and Human Health Division.

IUPAC News

The Analytical Chemistry Division

It seems extremely arrogant and naïve to assume that 10 individuals can possibly keep up with and do their part to drive forward a field as large and diverse as analytical chemistry. Yet that is the task of the IUPAC Analytical Chemistry Division Committee. To accomplish it, these 10 analytical minds work as a team, apply their own quality control (QC)/quality assurance (QA) procedures, and adopt new managerial strategies and organizational initiatives. In this article, we have asked the new Division president, David Moore, to explain what the Analytical Chemistry Division (ACD) does and how its members are selected.



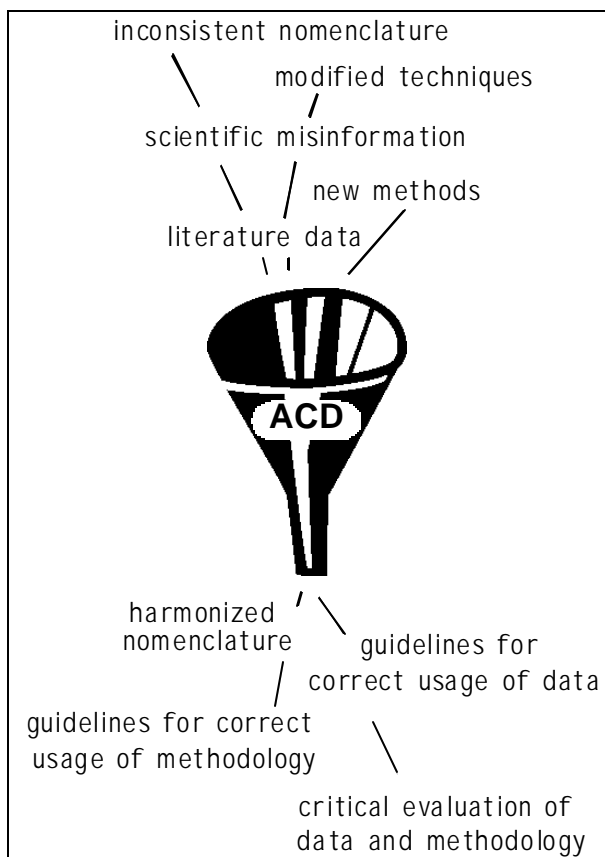
David Moore

Analytical Chemistry—A Discipline At the Heart of IUPAC

by David Moore

Analytical chemistry is a scientific discipline that develops and applies methods, instruments, and strategies to obtain information on the composition and nature of matter in space and time, as well as on the value of these measurements (i.e., their uncertainty, validation, and/or traceability to fundamental standards).

For more than 50 years, the role of the IUPAC ACD has been to catalyze interactions between the scientific community and users of analytical methodology and data and between the scientific community and beneficiaries of analytical results, such as international organizations (IAEA, OECD, WHO), accreditation bodies (ISO), standards bodies (BIPM, NIST), chemical societies, and society as a whole. The process involves taking input, such as literature data, information about sources, inconsistent nomenclature, newly developed or modified methods and techniques, and scientific misinformation, and then performing harmonization of nomenclature, critical evaluation of data and methodology, formulation of guidelines for correct usage of data and methodology, and promotion of analytical chemistry to society in general.



Where Role and Structure Define an Organization

In response to the recent IUPAC reorganization, the ACD also reorganized—through a phased process over

the past four years—into a smaller structure with well-defined roles for committee members. These roles cover the various fields within analytical chemistry: methods (general aspects, separations, spectrochemical, electrochemical, nuclear chemical) and applications (particularly to environmental and human health problems). To enable analytical chemists to choose the methods best suited for specific applications, the roles of the ACD encompass:

- the critical and comparative evaluation of established and emerging analytical methods (including the harmonization of associated terminology, proficiency testing, and other inter-laboratory comparisons);
- the recommendations for sample collection, preparation, storage, and handling;
- the compilation of data used in analytical chemistry and their critical evaluation; and
- the definition of recommended methods and proper application of QC and QA procedures.

To optimally perform its required duties under a smaller structure, the division committee established several new managerial and organizational initiatives. Roles and responsibilities were established for each category of division committee membership. Each titular member (TM) of the division committee is encouraged to organize an advisory group in order to help them develop and/or select projects in response to pressing needs in a given area. An advisory group should therefore have a global view and experience in a specific area, in order to aid in identifying and soliciting new projects. Associate members of the committee are to provide focused representation in a particular area of analytical chemistry or to establish a tight link to other IUPAC committees, such as the Committee on Chemistry Education, the Interdivisional Committee on Terminology, Nomenclature and Symbols, or the Committee on Printed and Electronic Publications. National representatives are nominated by IUPAC National Adhering Organizations that are not otherwise represented on the committee (up to six are appointed). Each national representative is linked to a TM according to their expertise, with the goal of ensuring they participate and are tutored in project proposal reviews and ACD planning activities.

A shortcoming and criticism of IUPAC has been its lack of internal and external communication as well as relevance to the community. We have addressed the internal communication issue by establishing a regular e-mail newsletter (“Teamwork”) to keep members apprised of their responsibilities, upcoming events, new project proposals, and deadlines. As discussed below, initiatives to improve relevance have begun with a fresh review and selection process for new projects. External communication has been improved by better dissemina-

tion of project results. Moreover, we are establishing a directory of expertise database to allow us to locate experts according to a set of keywords related to their own field of expertise. Each person that has served the IUPAC ACD on a commission or project task group in the past decade or more will be recorded. New task group and division committee members, as well as experts involved in project review, will be added.

Electing *the* 10 ACD Committee Members

The smaller size of the division membership has also increased the difficulty in maintaining continuity over many years. We have addressed this problem by establishing a revolving election, whereby half of the committee is elected each biennium to facilitate four-year terms.

New ACD committee members are elected through a process defined in the IUPAC Bylaws. Nominees are selected by a Nominating Committee composed of five members: two from the ACD and three other well-known external analytical chemists, one of whom is appointed to be the chair. It is necessary for the Nominating Committee members to be very active to ensure a supply of fresh blood to the division committee, to ensure geographical diversity, and complete representation of the different branches of analytical chemistry. After the slate of nominees is complete, the IUPAC Secretariat handles the election itself via e-mail ballot. The electorate consists of the division committee titular members, associate members, and national representatives; project and task group leaders of current projects and projects scheduled to be completed during the current biennium; and nominating committee members not otherwise eligible.

Selecting the Most Relevant Projects

The ACD has a limited project budget, and yet, there are pressing needs within the international analytical chemistry community. The ACD therefore established a selection process for funding project proposals, based on a set of priorities.

After ensuring that a project proposal is complete, the Division president assigns one or two TMs to check the financial feasibility and practicality of the project. If needed, the proposed task force leader (or Task Group Chairman [TGC]) is asked to modify and resubmit the proposal. The Division president then recommends at least two external reviewers (either as suggested in the project proposal form or others as deemed appropriate) and transmits their names to the Secretariat, which handles the correspondence. Upon receipt of the reviewers comments, the Division president either accepts the reviews or asks the TGC to modify and resubmit the proposal.

A complete and annotated model project proposal is available on the ACD Web site. To be approved, projects should demonstrate clear evidence of advance plan-

ning and should describe the process that will be used to complete the project. Appendix A of the model proposal provides an example of such advance planning.

Following the initial review, and twice a year, the division committee carries out the selection and funding of projects, giving priority to pressing needs in given areas. The ACD committee is, however, concerned that all the different subject areas in analytical chemistry are covered in as equitable a fashion as possible. April 30 and October 31 are the deadlines for submitting completely reviewed proposals and initiating the selection process. The projects that are considered good, but cannot be funded, are then carried forward for the next selection, if so desired by the TGC.

The ACD has adopted the following general guidelines for project priority:

- IUPAC objectives met
- Task group membership complete with appropriate expertise and diversity
- Funding amount appropriate and justified
- High scientific value to user groups per cost
- Subject area coverage balance
- Cost sharing with other funding agencies so that funds are leveraged
- High visibility and usability of product
- Dissemination plan complete and appropriate

Monitoring Projects

Individual TGCs are responsible for the implementation of their projects and the management of their project budgets. Practically, a TM of the division committee is assigned to track a given project, as soon as funding is approved. Each TGC is asked to send a progress report to the Division vice president semi-annually (at the end of June and December), stating the completion of milestones, indicating whether any difficulties have been encountered, and stating whether the project is likely still to meet its completion date. All these reports are collated and forwarded to all ACD members so that they can add comments when needed. The expenditures are handled and tracked by the Secretariat.

Completing a Project

The final product of a project—usually a manuscript—is sent to the Division secretary (a copy also goes to the Division president), who then sends it to two or three ACD members for internal review, and also to three external reviewers named by the TM monitoring the project. The Division secretary then collects the reviews and returns them to the TGC for incorporation into a revised camera-ready manuscript. If the project involves nomenclature or terminology, an additional review process through the ICTNS is then initiated to further ensure consistency with previous publications, as well as worldwide consultation.

Does it Just End There?

No, the next stage is the dissemination plan, one of the most important parts of any IUPAC project. This is how terminology recommendations, for instance, are made known to practitioners or to the intended audience. Therefore, the implementation of the dissemination plan will be monitored. Again, an assigned TM will liaise with the TGC. As each step in the dissemination plan is executed, the TGC is asked to notify the assigned TM. This tracking system is to supplement the semi-annual progress reports and to help the ACD to improve on external communication.

What Does the Future Hold?

A major undertaking that looms just over the horizon is the revision of the Orange Book (Compendium of Analytical Nomenclature), which is being posted on the IUPAC Web site. Each chapter is slated to be systematically updated over the next few years according to the latest recommendations in each field. In the future, each project that recommends terminology will also provide for a mechanism to update the relevant entries in the Orange Book.

Project proposals are always welcome. In addition, ideas for projects and/or pressing needs within the analytical chemistry community can be communicated to anyone on the division committee so that a task force can be organized.

Dr. David Moore is a technical staff member at the Los Alamos National Laboratory, New Mexico, USA, and is the current president of ACD. He has been involved in the Analytical Division since 1988, and a member of the division committee since 1998.



www.iupac.org/divisions/V

2002 Winners of the IUPAC Prize for Young Chemists

On 14 May 2002, IUPAC today announced the winners of the IUPAC Prize for Young Chemists, an award for the best Ph.D. thesis in the chemical sciences, as described in a 1 000-word essay. The winners are:

- Jeroen J. L. M. Cornelissen, University of Nijmegen, The Netherlands (currently at IBM Almaden research Center, San Jose, CA);
- Jinsang Kim, Massachusetts Institute of Technology, Boston, MA, USA (currently at the California Institute of Technology, Pasadena, CA);
- Stefan Lorkowski, University of Münster, Germany;

- Simi Pushpan, Indian Institute of Technology, Kanpur, India.

The four winners will each receive a cash prize of USD 1 000 and a free trip to the IUPAC Congress, 10-15 August 2003, Ottawa, Canada. Each prize winner will also be invited to present a poster at the IUPAC Congress describing his/her award winning work.

Applications for the 2003 Prize are now being solicited, as described on the IUPAC Web site.

The essays describing the winners' theses also can be found on the Web site and cover a wide range of subject matter:

- Dr. Cornelissen, "Polymers and Block Copolymers of Isocyanopeptides—Towards Higher Structural Order in Macromolecular Systems;"
- Dr. Kim, "Supramolecular Assemblies of Conjugated Sensory Polymers and the Optimization of Transport Properties;"
- Dr. Lorkowski, "Differential Gene Expression in Human Macrophages During Foam Cell Formation;"
- Dr. Pushpan, "Core Modified N-confused and Expanded Porphyrinoids: Syntheses, Characterization and Photodynamic Activity."

There were 40 applicants from 20 countries. The Prize Selection Committee was comprised of Members of the IUPAC Bureau with a wide range of expertise in chemistry. The Committee was chaired by Dr. Alan Hayes, IUPAC Past President.

In view of the quality of many applications, the Committee decided also to give four Honorable Mention awards to:

- Christopher J. Kuehl, University of Utah, USA (currently at Los Alamos National Laboratory, NM);
- Gábor Lente, University of Debrecen, Hungary;
- Shinsuke Sando, Kyoto University, Japan (currently at Stanford University, CA, USA);
- Izabela Tworowska, Polish Academy of Sciences, Lodz, Poland (currently at Rice University, Texas, USA).

The Honorable Mention Award winners will receive a cash prize of USD 100 and a copy of the Compendium of Chemical Terminology, the IUPAC "Gold Book."

The awards to the four winners of the IUPAC 2002 and those of 2003 will be made during the Opening Ceremony of the IUPAC Congress in Ottawa, Canada.



www.iupac.org/news/prize/2002_winners.html