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.

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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