Golden Anniversary of the ACS Division of Chemical Information (1948−1998)

In the listing of "Historical Milestones of the ACS Division of Chemical Information (CINF)",[1] compiled for the 50th anniversary of the Division, there are three entries related to this *Journal*:

1961 ACS *Journal of Chemical Documentation* (*J. Chem. Doc.*) started (Herman Skolnik, editor)

1975 *Journal*'s name changed to *Journal of Chemical Information and Computer Sciences* (*J. Chem. Inf. Comput. Sci.*)

1985 *Journal of Chemical Information and Computer Sciences* celebrated its 25th anniversary with a Silver Anniversary issue

How the *Journal* came into being has been described in some detail previously.[2,3] When the Division was formed in 1948, it did not take long for it to become a forum for exchange of news and views on all aspects of chemical information through technical meetings and papers. But, relatively few of these technical papers could find a medium for publication. It took quite a few years of discussions, evaluations, and consultations, but finally in 1961, the ACS Board of Directors approved the publication of the *Journal of Chemical Documentation* upon the recommendation of the Divisional Publications Committee and appointed Herman Skolnik as its Editor.

The impetus for the introduction of the *Journal* came from the Division, and until 1971 a relatively high percentage of papers came from the Divisional programs. Eventually the *Journal* became a primary medium for papers written for publication, rather than presented at a meeting. Also, the international participation soon reached 50% and more.

Although the *Journal* has never been formally pronounced as the official organ of the Division and the Division has never attempted to influence the Editor's publication policies, very close ties have always existed between the Division and the *Journal*'s Editors [Herman Skolnik (1961−1982), Tom Isenhour (1982−1989), and Bill Milne (from 1989)]. Prominent and active members of the Division have served on the *Journal*'s Advisory Board. The Division directly has contributed by encouraging speakers at the Divisional symposia to submit the papers for publication in the *Journal*.

In a way, the Division has continued to regard the *Journal* as its own, even when its scope expanded to include computer science, as reflected in the title changed to the *Journal of Chemical Information and Computer Sciences* in 1975, and more recently to include chemical computation and molecular modeling, as reflected in specially created sections under those titles.

Therefore, it seems fitting that the *Journal* should celebrate in a small way the 50th anniversary of the Division by a section dedicated to the Division. The theme is not uniform. On purpose, we wished to provide some history in a couple of selected areas, to cover a few "hot" topics such as modern methods of communication among the chemists, structure searching and elucidation, and virtual compound libraries, and to focus on the ever important subject of information instruction, especially in the current changing access environment.

Edgar Meyer and Norma Funkhouser provide a history of networking, going back to the first online bibliographic search capability demonstrated by the Systems Development Corporation (SDC) in 1960 and the first networked retrieval of structural information from a biological database in 1971.

Gary Wiggins reviews the major uses of the Internet and presents a look at future developments. He discusses the electronic journals in some details, indicates the efforts to standardize codes and identifiers, and predicts that electronic journals will become the major source of primary information for chemists worldwide.

Wendy Warr, having referred to such Internet resources as electronic journals and discussion lists, describes and compares "virtual communities", or clubs, for chemists, such as ChemCenter from the ACS, chemsoc from the RSC, and ChemWeb.com from ChemWeb Inc.

Henry Rzepa *et al.* review the global use of an Internet standard based on chemical primary Multipurpose Internet Mail Extensions (chemical MIME) which is essential for

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the exchange among chemists of chemical information through e-mail and WWW-based communications.

Peter Willett *et al.* provide an overview of chemical similarity searching, starting with a historical review of fragment-based similarity searching and followed by a more detailed discussion of similarity and distance coefficients, of structural representations, and of applications of similarity searching. Areas where further work is required are highlighted.

Morton Munk traces the development of computer-based tools for structure elucidation and indicates that three major components of structure elucidation, spectrum interpretation, structure generation, and spectrum prediction, are amenable to computer modeling. The availability of spectroscopic databases of increasing diversity and quality will contribute to the development of further more powerful computer-based tools.

Richard Cramer *et al.* describe virtual compound libraries, that is, representations of all the molecules that might be obtained by the combinatorial chemistry resources. To be useful in molecule selection, a virtual library must be searchable in timely and relevant ways. That is a new approach to decision making in molecular discovery research.

Arleen Somerville reports on a survey of information instruction activities, identifies current trends, especially with respect to rapidly changing chemical resources, and points out the need for increased involvement by faculty and librarians and the need for funding of access to electronic information resources.

Both the Division and the *Journal* are looking forward to a continued successful cooperation in the years ahead.

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(1) Metanomski, W. V. *Chem. Inf. Bull.* **1998**, *50*(2), 7−8, 10−12.
(2) Skolnik, H. The Journal of Chemical Information and Computer Scientists: A 25 Year Perspective. *J. Chem. Inf. Comput. Sci.* **1985**, *25*, 137−140.
(3) Metanomski, W. V. *50 Years of Chemical Information in the American Chemical Society, 1943−1993*; ACS Division of Chemical Information: 1993; pp 27−29.

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