Science on the Web: from chaos to community

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The Internet has already had a major impact on the way scientists work – having spurred the development of intranet systems in most pharmaceutical companies – but the Web is in danger of becoming an unmanageable resource. With the advent of Web-based communities such as ChemWeb, a wealth of on-line information has become better organized and more available. Yet Web communities hold the promise of even more. Ultimately, they could help to level the playing field for drug discovery. Our challenge is to continue to build true Web communities in a way that supports the culture and tradition of scientific communication.

No matter what information it offers, the Web's very scope and chaotic nature can make it inefficient and time-consuming for researchers to use. For example, on-line patent data, once the province of indexing and abstracting services, is now available for free through some government Web sites. But as on-line patent data sources multiply and the sheer volume expands, it can actually take longer to navigate patent information. The Web may get bigger and faster, but it does not necessarily speed the work of drug discovery. And today, speed is what pharmaceutical R&D is all about.

Intelligent Web design

It is challenging to design Web resources for researchers who either may not know what things they want, or who want disparate things, or who interpret things in different ways. The answer is to think beyond providing ad hoc data and computational resources – to creating electronic environments, true Web communities. A good example is BioMedNet, an on-line club for biological and medical researchers. With over 175,000 members, BioMedNet has become an important fixture in on-line scientific debate, a center for scientific journalism and a major repository of journals and databases – all of which can be searched through the flexible, high-speed BiblioteK search engine.

Conceived by the founders of BioMedNet, ChemWeb, the Web's worldwide club for chemists, was launched in April 1997, as an on-line community that would support many of a chemist's daily activities. In keeping with the established culture of the Web, membership is free and there is no charge for participation in many ChemWeb events. ChemWeb generates income by providing information tools and services that typically one would find in a corporate research department – and some sophisticated options that are exclusive to ChemWeb. In less than a year we had seen ChemWeb's active on-line membership grow to more than 20,000 members.

Scientific Web communities like BioMedNet and ChemWeb are succeeding for several reasons.

- By consolidating resources, they ensure that users can do much of their on-line work in a single location, without jumping from one site to another.
- They keep up to date with the latest in on-line information resources and technology. For example, users can search much of the contents of ChemWeb by chemical structure and reaction, as well as retrieving text through BiblioteK – integrated search capabilities with a sophistication that is not available even in the best corporate research departments.
- These on-line communities connect people and ideas, using Web technology to provide virtual lectures, seminars and real-time publishing.

Databases and literature

It takes a critical mass of information sources to attract researchers consistently to one Internet site. In the case of ChemWeb, publishers including Current Drugs, Elsevier Science and Gordon & Breach together offer more than 40 journals through the site, and that number should exceed 200 by the end of this year. One of the new journals on ChemWeb, *Current Opinion in Drug Discovery and Development*, is the first substructure searchable journal available on the Internet. The Institute for Scientific Information's Reaction Citation Index, which becomes available in June of this year, will dramatically expand access to journal articles.

ChemWeb databases include the Investigational Drugs (IDdb), NCI-3D, IFI/Plenum CLAIMS/U.S. Patents, OHS Material

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Safety Data Sheets and soon, the Available Chemicals Directory and the Chapman & Hall combined chemical dictionaries. The Royal Society of Chemistry, Elsevier Science, Micropatent and Responsive Database Services have all announced plans to bring additional databases and/or journals to ChemWeb.

Building a community

A Web site can become the nucleus of a research community only when scientists themselves continuously shape its content. At the urging of many researchers, ChemWeb has addressed some of the Web's most nagging problems and promising frontiers. The ChemDex Resource Directory, originally developed at the University of Sheffield, is an Oracle-based resource that helps chemists find what they want among almost 4,000 chemistry Web sites – and with direct links to those sites. That number will soon grow to 7,000. In the coming months ChemDex will critically review selected chemistry Web sites in depth.

'Virtual lectures,' accompanied by on-line debates, on topics such as the chemical chaos of the Internet, the launch of Chemical Markup Language and on-line modeling tools have attracted hundreds of researchers from around the world. Because of their popularity, these on-line lectures will soon supplement text and graphics with a live audio feed.

ChemWeb's Shopping Mall provides more than just a place to buy things – it is one of the only ways for scientists to locate and evaluate valuable software, as well as books and services. The Job Exchange has become a major clearing house for careers in chemistry. The Conference Database is probably the most comprehensive calendar of world events in chemistry.

The Alchemist, the only major chemistry 'WebZine', provides some of the liveliest journalism available to anyone following news and developments in the research world. The Alchemist has covered several stories long before its print counterparts and provoked many on-line discussions. In the future, ChemWeb will help accelerate both the approval and publication of peer review articles.

In addition, chemists soon will be able to arrange electronic gatherings through the ChemWeb Meeting Room. Users will be able to control this electronic conferencing facility to provide the degree of privacy or inclusiveness they desire. ChemWeb is also planning computational services, offering a variety of calculation engines to support three-dimensional modeling and theoretical chemistry for example.

The Internet is only a few years old. With continuous pressure to accelerate drug discovery and cut costs in areas such as travel and facilities, researchers will continue to turn to the Web. What they find there and how often they return will have much to do with how well we design Web communities.

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