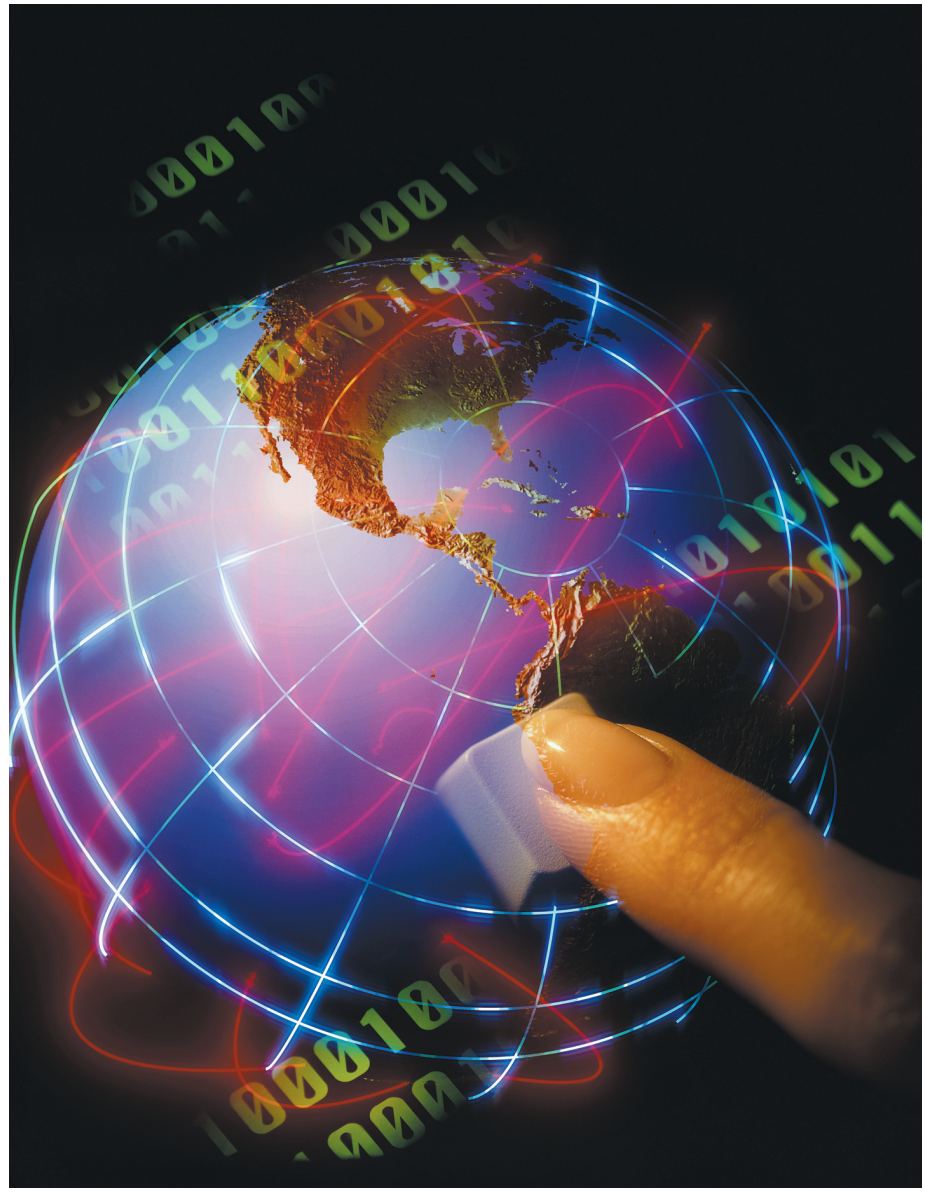
Does the Web Work for Analytical Chemists?

David Bradley

We have kept readers up to date with the latest developments on the Internet through the regular WebWorks column. But in a brief moment of doubt, Contributing Editor David Bradley wonders whether the Internet revolution, which has brought these masses of new tools to the desktop, is keeping the analyst away from the benchtop. Turns out his doubts were unfounded: Analytical scientists are mining the Internet for all kinds of information.



The list of online resources is burgeoning, with many at little or no cost. There are databases; tools for spectroscopy and related tasks (for example, see Advanced Chemistry Development at http://www.acdlabs.com/); virtual private networks (*1*); and brokerage sites for analytical services, such as LabSeek (http://www.labseek.com/) (*2*). There are e-commerce sites, such as ChemConnect (http://chemconnect.com/) (*3*); listservs; chat rooms; discussion groups; and virtual communities, such as ChemCenter (http://www.acs.org/), ChemWeb (http://analytical.chemWeb.com/), and ChemicalAnalysis.com (http://www.chemicalanalysis.com/) (*4*). Finally, who could forget the blight of the impatient—e-mail?

Norm Dovichi, an analytical chemist working on novel capillary electrophoresis techniques at the Uni-

versity of Alberta (Canada), is convinced of the "net" benefits. "Like all tools," he explains, "the Web has its appropriate uses." He finds it an outstanding complement to classroom instruction. "I routinely put my lecture notes on the Web when I teach large first- and second-year classes," he says (see http://hobbes.chem.ualberta.ca/). Last semester, he taught his senior-level bioanalytical chemistry students how to use the Web to find protein and DNA structure information. That part of the class was very popular with students because they learned how to use databases to solve real-world problems.

Other scientists, however, warn that distance learning is sometimes oversold. "Online materials are a useful supplement," says Kermit Murray of Emory University. "But they don't suffice as a stand-alone educational tool." There is an obvious need to balance time online with more traditional approaches to teaching.

Many **researchers** shop online, but **few** are ready to **purchase** instruments **sight** unseen.

It is beyond doubt that the Web is changing the way most analytical scientists use the library. In particular, databases such as MEDLINE (which can be accessed through many portals, including Internet Grateful Med at http://igm.nlm.nih.gov) have proved to be invaluable tools for quickly researching almost any topic. Its vast repository includes *Analytical Chemistry* and the *Journal of Chromatography*; however, the *Journal of the American Chemical Society* and several other primary analytical journals are not yet indexed, unfortunately. Collaborative initiatives to publish papers directly on the Web, such as BioMed Central in the United States and E-Biosci in Europe, are also underway, although many chemistry publishers are reluctant to be brought into the fold.

"The Web is a fantastic tool for accessing information," enthuses Dermot Diamond, director of the Biomedical and Environmental Sensor Technology (BEST) Centre at Dublin City University (Ireland). He says he uses it for regularly scanning electronic versions of journals. "I can easily download graphs and figures, take quotes from papers, and introduce them into lectures," he explains. Although he admits to still receiving paper journals, he says the speed of access to e-journals is a major benefit. Richard Crooks of Texas A&M University agrees. "I certainly check out instruments and things like that [online], but mostly, I use [the Web] to search the scientific literature, retrieve research papers, and take advantage of various library services."

The sentiment is echoed by Murray. For him, the availability of searchable information online is the most powerful aspect of the Web, but he also points to the increased speed of publication. With ACS's "ASAP" articles and the Royal Society of Chemistry's "Advance Articles", for example, scientists can see papers before print publication—in some cases, many weeks in advance. Similarly, the processing of papers is faster with online submission and review. (As testament to the growing popularity of this option, the journals *Science* and *Nature* had, at the time of writing, just announced that they would join the ranks of publishers accepting and reviewing papers via the Web.) Finally, Murray adds, the hyperlinking of references makes the experience of reading papers even easier.

When it comes to e-commerce, however, the Net seems to be enabling some academics to unravel themselves from red tape, while others are being bound more tightly. According to Dovichi, many academic chemists are unable to buy equipment directly via the Web. The typical university, he points out, usually obliges scientists to present several bids for equipment and to channel all requests for instrumentation through the institute's purchasing office.

"I suppose that 'buying equipment online' would mean filling out a form with your credit card number and pushing a button to complete the sale," adds Murray, "but I don't think that will happen with big purchases like instruments for a while." In part, that is because some face-to-face negotiation is required for items that cost more than a few hundred dollars, he notes. Nevertheless, the Web can help with finding equipment specifications and user opinions (*5*). Microelectrode chemist Zbigniew Stojek of the University of Warsaw (Poland) agrees. "We never order materials, instrumentation, or services without searching the Internet first," Stojek says. However, he concedes that electronic purchases of instrumentation and materials are still rare.

Diamond, who has recently been equipping the year-old BEST Centre, has a different perspective (and, perhaps, different bureaucratic constraints). "Obtaining specifications and prices for equipment using the Web is very important for us," he says, "[because] it enables us to purchase directly rather than go through layers of agents."

Reinhard Niessner's group at the Technical University of Munich (Germany) has perhaps found a happy medium. "We [buy] small stuff, such as chemicals, but nothing beyond $5000," he explains. "Above this price, personal contact is very important to ensure you get the right stuff for your application and the right price." Alain Berthod of the University of Lyon (France) agrees. "I would not buy an expensive scientific piece

of equipment without really seeing it, having it for a demo for a while, and so on," he says. "I may be old-fashioned, but I like [to get] a paper catalogue and then look up the latest price and model on the Internet."

Dovichi points to a spin-off benefit of e-commerce. He says that the swathes of information about all kinds of instrumentation on manufacturers' Web sites can be useful in preparing course notes. "Online catalogs," he explains, "are very convenient when preparing classroom lectures on instrumentation, both to obtain specifications and to gather photographs." Such information is freely available and presumably the "marketing" effect would provide enough of an incentive for any manufacturer to keep the site up to date.

Although seemingly the simplest of Internet functions, e-mail still remains perhaps the single most powerful tool available, because it provides quick, inexpensive, direct contact between individuals wherever and "whenever" they are in the world. There is, admittedly, not always the immediacy of a phone call, but e-mail has a critical added bonus in giving people slightly more time to think about replies, without the frustrating delays of "snail mail". E-mail also gives us the option of attaching additional information, such as a spectral chart or even a GC output, very readily—things that are simply impossible by fax or phone.

"E-mail is now a tool I could not live without," enthuses Berthod. "I [communicate] with my American and Canadian [colleagues], with the scientific journals I collaborate with, and with personal contacts by e-mail. [It's] free, fast, and exquisitely polite—you read it and answer it when you want!" Stojek points out that "scientific cooperation across borders and oceans is certainly much easier now." However, he has many colleagues who see the Internet as a time-wasting activity, and he himself recognizes the increasing number of commercial e-mails as a real problem.

Diamond, too, lists many Internet applications that he says analytical and other scientists use on a daily basis: everything from databases and journals to networking with colleagues and collaborators to publicizing his group's work (http://www.dcu.ie/research/best.html). "The trend will continue, and for analytical chemists, a major benefit will be remote accessing of information," he says. "We can keep in touch with what is happening from anywhere in the world." Ten years ago, the applications were simply impossible.

During 2000, Crooks says his team is going to hook up their X-ray photoelectron spectrometer to the Web (http://www.chem.tamu.edu/rgroup/crooks) so that users at remote sites can control it themselves. Because the machine was purchased with National Science Foundation funding, his group is trying to make it as accessible as possible to other researchers. In addition, they will be able to sell time on the machine to defer costs, he explains. "Remote control of expensive scientific instruments is going to be very big in the next year or two," he enthuses. Indeed, *Analytical Chemistry* reported on other Web-based "collaboratories" (*6*), including one from Phil Williams's group at the University of Nottingham (U.K.) in 1997 (*7*). This team developed the first interactive system based on the Web for analyzing and improving surface images from scanning probe microscopy.

Other applications, such as MS, are also set to make it big on the Internet. Murray says he has been promoting this resource for MS for about five years (see his FAQ page at http://userwww.service.emory.edu/~kmurray/mass-spec-resources.html). His popular index page of resources was bought by the publisher Wiley, which turned it into the MS Web portal *Base Peak* (http://base-peak.wiley.com/). Like others, he believes online instrumentation might have a role to play as educational tools. It should even be possible to create a virtual mass spectrometer for this purpose, he says. Indeed, various training and educational packages simulate spectrometers, and this software could very easily be ported from desktop computers to the Web.

Online **instrument** catalogs are **good** resources for preparing **lectures.**

Veteran Net users—that's anyone online since 1995!—can see where things might be heading. "There is a learning curve," says Murray. "It's probably true that expectations are greater now than they were several years ago, but there is much as yet unfulfilled promise for those online." Expectations and applications are growing. The Internet can only increase with them, and that might mean spending more time online and off-bench.

Time to log off, I think . . . for now.

References

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