

► The PDA: Making headway into a new frontier

Life sciences in the palm of your hand

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During his Nobel lecture at Stockholm University in Sweden, Alan Heeger pulled out a personal digital assistant (PDA) and proudly held it up so the crowd could marvel at its brilliant display screen (1). Heeger, one-third of the 2000 Nobel Prize in Chemistry team, helped to develop the world's first polymer-based plastic material to make this screen possible. Although chemists contributed indirectly to the PDA's development, handheld devices are gaining popularity with life sciences researchers as more integrated applications for the wireless technology emerge. And the biotechnology industry is just now making strides in incorporating the technology as it discovers the convenience of these handheld units.

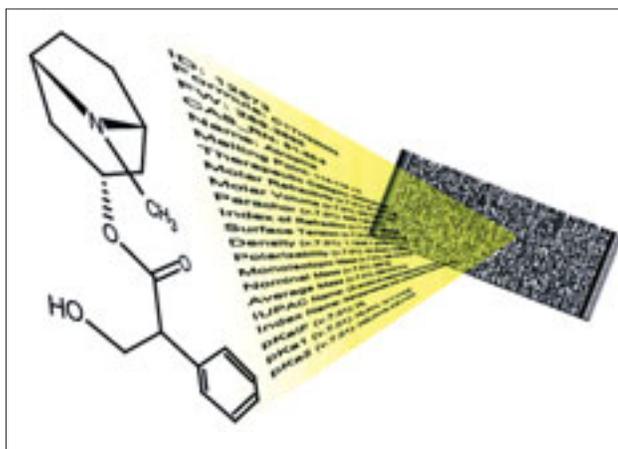
PDA integration

"Mobile computing in drug discovery is just beginning to be explored," says Robert S. DeWitte, director of medicinal chemistry solutions at software manufacturer Advanced Chemistry Development (ACD/Labs, www.acdlabs.com), but several scenarios jump out immediately.

Medicinal chemists today use desktop software to identify reasons why their molecules have poor ADME properties and to proactively design improvements to their compound series, DeWitte explains. "Now here's the mobile part: Pop the structures onto your PDA, head to the bench, and use the convenient handheld applications to do all the nitty-gritty calculations—molar equivalents and amounts to weigh—all in real time at the bench," he adds. "We see this as just one of the many potential mobile accelerators available to drug discovery research."

Although offering a lot of promise, handheld devices have not penetrated the

biotechnology area as widely as they have the health care field and segments of the pharmaceutical industry. However, the biotechnology industry has started to embrace the PDA and benefit from advances made in other sciences. Hence, the PDA's growing popularity is opening up an array of new opportunities as well as challenges for the biotech industry.



Communicating chemistry through bar codes: ACD/ChemCoder encodes chemical structures into 2D bar codes. (Image courtesy of ACD/Labs.)

Incorporating portable information devices is not a novel concept, but the challenge for life sciences software manufacturers is to identify and design mobile applications that are practical, reliable, and capable of continuous interaction. After all, handheld integration is supposed to increase efficiency, improve communication among researchers, and accelerate drug discovery.

However, mobile systems are typically slow and have limited interfaces. Although today's devices are smaller and more powerful than ever before, they are still somewhat limited in handling additional applications. Ted Hawkins, activity base product manager at biological data management provider ID Business Solutions (IDBS, www.idbs.com), points out that PDAs

are "useful for the simple scoring of observations, but the problem is there is not enough real estate for the biologists to use for real analysis. For biological data capture, a PDA cannot present the data in a usable format, as it lacks the space to see the data." And although adding software enhances functionality, memory and storage space is limited. Faced with these challenges, handheld scientific software companies are providing ways not only to make information mobile but also to enable users to customize their own systems.

Software applications

Programming innovations have brought technology from the desktop PC and the Internet to the PDA. Using wireless technology, users can input data directly into a pocket device's operating system and transfer the information to a remote desktop. Pharmaceutical companies—such as Aventis (www.ventis.com) and Ionix Pharmaceuticals (www.ionixpharma.com)—are finding that in addition to decreasing errors associated with data input and streamlining workflow, handhelds ensure the full use of back-end systems and data integrity.

Behavioral pharmacologists at Aventis Pharmaceuticals, an Aventis Pharma subsidiary in Bridgewater, NJ, have developed a handheld program using a custom-designed Excel-based template and featuring a user interface designed by IDBS. The unit allows scientists to capture behavioral assay data directly into IDBS's ActivityBase database, a software suite for managing and integrating cheminformatic data generated from high-throughput screening, secondary screening, ADME (absorption, distribution, metabolism, and excretion), DMPK (drug metabolism and pharmacokinetics), toxicology, in vivo, and other pharmacology assays. A data entry workbook can be created either manually or automatically using Excel or Visual

Basic for Applications, where experimental parameters can be entered as necessary. The recorded test data is uploaded from the PDA to a PC-based workbook via the handheld software and then imported into IDBS's ActivityBase.

Similarly, to capture, manage, and integrate biological, chemical, and inventory data at its Cambridge, U.K., site, Ionix is using the ActivityBase Inventory Management module to control its work process from registration of novel molecules to compound management, where researchers enter and manipulate data from screening and secondary assays. "Efficiency has been significantly enhanced by using the automation facilities of ActivityBase, which allow real-time screening data entry and analysis, providing a single repository of information for both chemists and biologists," Ionix says.

Researchers must also design improved compound analogues without sacrificing potency related to solubility, permeability, plasma protein binding, tissue partitioning, and blood-brain barrier penetration. And until recently, software had not addressed this concern. The ACD/ MedChem Advisor provides a means to develop potential new chemical structures by predicting physicochemical properties including logD, logP, pKa, and aqueous solubility. The PDA software enables medicinal chemists to easily share their drug design ideas and plans with colleagues.

In another example, Pocket Hyperchem, a software program developed by scientific molecular modeling company Hypercube (www.hyper.com), facilitates communication between the PDA and PC, allowing researchers to draw and download structures directly from the handheld device to the desktop. While there are several modeling programs, Hyperchem was the first chemistry software to run on Windows CE-based devices. And, as an added benefit, its use is not restricted to chemical modeling. Software enhancements allow for rendering protein structures—encompassing coils to helical cylinders—as well as recognizing secondary structures that allows information from the Brookhaven Protein Database to be captured and retained.

Hypercube also has tackled one, if not the most, notable deterrent to handheld integration, namely cooperative communication.

Typically, there are synchronization barriers between handheld units and desktop devices. However, the Pocket HyperChem and HyperChem workstation communicate intelligently, meaning there is no need to download information from the handheld to the desktop. Hence, scientists can move to using a handheld device and still have easy access to the main databases.

Such devices are used not only by industry but also by academia. At the University of North Carolina at Wilmington (www.uncw.edu), chemistry department chairman Charles R. Ward has implemented the device as a learning aid in lectures, as well as in the laboratory.

Additionally, as part of a research initiative funded by the NIH Small Business Technology Transfer Program (<http://grants1.nih.gov/grants/oe/htm>), Hypercube and the University of Florida are collabor-

ating to develop a modeling tool researchers can use to study proteins. Through Hypercube's research into wireless technology using chemistry models, its scientists, led by CEO and President Neil Ostlund, plan to expand model rendering to observe 3D protein structures. A group led by University of Florida (www.ufl.edu) evolutionary chemist Steve Benner is providing expertise in evolutionary protein changes that will be evaluated using Hypercube's modeling technology.

Encoding data

Combining novel software with enhanced inventory encoding provides a means of cataloging chemical structures and addressing inventory control and data management concerns. ACD/ChemCoder, with its PDA-based structure-viewing capability, encodes chemical structures and related information into a 2D bar code. A chemical structure is drawn, and a PDF417 bar code is created that contains associated text data such as laboratory information management system identification. When scanned, the encoded chemical structure can be displayed on an OS-based unit or the ACD/ChemPalm. It affords scientists the ability to scan bar-coded bottles and determine the substance by chemical structure and vice versa. The ACD/ChemCoder is available for the Palm OS and the Pocket PC.

For the PDA to be fully integrated into researchers' routines and maximize a company's resources, the handheld units will have to provide a clear benefit. "The key is to support biologists in their daily work," IDBS's Hawkins says, "while integrating seamlessly with chemistry and bringing these data together in a framework for decision-making at the enterprise level." And through software and user interface improvements, handhelds integrated with other laboratory systems are heading toward the mainstream rather than being just an interesting add-on. The reality of performing time-consuming calculations and downloads is becoming a relic of the past, replaced by software and hardware that are transferable as well as transportable.

Reference

- (1) Fairley, P. *Technol. Rev.*, Jan/Feb 2002, pp 48–52. ■

PDA software for life sciences applications

BioCoRE

www.ks.uiuc.edu/Research/biocore/announce/pdaSupport.shtml

Biology Study Guide 1.1

www.palmgear.com/index.cfm?fuseaction=software.showsoftware&prodid=15585

Biotechnology Glossary 1.2

www.pdacentral.com/epoc/preview/227366.html

Chembase 1.0

www.pdacentral.com/epoc/preview/79254.html

palmPCR

www.palmgear.com/index.cfm?fuseaction=software.showsoftware&prodid=15585

For a more extensive list, visit www.library.ualberta.ca/pdazone/science/index.cfm#chemistry and www.mysyware.com for Pocket PC, Windows CE, or Windows Mobile devices.