

Drug Discovery in the Clouds

Alice McCarthy

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The concept of drug discovery often brings images of wet chemistry experimentation, large-scale automation, and biological assays—processes usually carried out in laboratory environments. But within the past few years, some companies are going virtual with their drug discovery efforts, taking advantage of the leaps in computing power and technology available through the cloud.

To meet the need of pharmaceutical and biotech companies, and a much larger cast of supporting and collaborating partners, a few commercial companies are now providing cloud-based drug discovery software services. The goal is to increase the power of collaboration while maintaining the highest levels of security, at the same time lowering the

discovery, you want to collaborate with whoever has the best in the world complementary capabilities. In a cloud-based world, there are essentially no barriers,” says Barry Bunin, CDD CEO and founder. “Users can work with whoever has the best complementary skills, technology, or services and control the intellectual property as needed, removing much of the technological and communication friction of traditional collaborations.” With cloud-based services, anyone with an internet connection and the proper security codes can fully participate in the drug discovery effort.

CDD’s product is not just a data facilitator or storage solution. It also includes proprietary software developed internally to expedite and simplify drug discovery

make the data meaningful,” he adds. These tools make it easy to work with biological information such as IC50, the Hill slope, and Z prime statistics, and on the chemistry side provide a similar ability to view molecules in 3D.

SCYNEXIS

SCYNEXIS has successfully collaborated with most of the world’s large pharmaceutical companies through its cloud-based discovery information software system called Hit Explorer Operating System (HEOS). Originally formed as a drug discovery service organization, SCYNEXIS saw the need in its own business model for a software tool to expedite communication with its clients. “We needed to find a way to best communicate and exchange proprietary information with our customers,” says Terry Marquardt, Executive Director, Market Development at SCYNEXIS. Toward that end, SCYNEXIS started developing HEOS in 2001.

The company hired former Rhone-Poulenc IT Director Fredric Bost to lead the HEOS development effort. “SCYNEXIS developed HEOS as a cloud-based application to address the growing new paradigm in drug discovery that increasingly involves collaboration between different companies and organizations,” explains Bost. “It enables geographically-dispersed scientists – not only from different departments, but also different companies with different processes and cultures – to collaborate together and exchange data and still function as a team.”

HEOS started as a tool to help all collaborating partners exchange data without fouling each other’s central databases. But about four years ago, SCYNEXIS began receiving requests from non-CRO clients for licensing access to its HEOS software package. At that time, the company expanded its business model to include the HEOS software as a stand-alone service. “Since it has been available as a cloud-based service, it offers extreme flexibility to everyone,” says Marquardt. Projects are easily

***“In a cloud-based world there are essentially no barriers.”—
Barry Bunin, CEO, Collaborative Drug Discovery***

need for sometimes voluminous internal computer power and IT overhead.

To date, two companies are proving that the sky is no longer the limit for drug discovery. Collaborative Drug Discovery (CDD) of Burlingame, California, and SCYNEXIS, based in Research Triangle Park, North Carolina, have emerged as the leaders of these services offering private, secure, cloud-based drug discovery software platforms. Both highlight the collaborative nature of their products and the reduced costs provided by the barrier-free virtual world of cloud computing—and both are finding users interested in pursuing drug discovery in a hosted colocation service in the cloud.

Collaborative Drug Discovery

Collaborative Drug Discovery’s (CDD) software has literally been in the cloud since the company was founded over 7 years ago and is probably the earliest entry into the field. As its name implies, collaboration is the focal point of the software. “From a collaborations perspective, to be maximally efficient for drug

projects. CDD has developed tools that recognize chemistry structures (which represent potential composition patents) and bioactivity data (representing utility patents) —the core of chemical registration and structure-activity relationships (SAR).

“We have put a lot of work into the design and ease-of-use of the software, so it is easy to use,” says Bunin, who conceived of the CDD business model while an “entrepreneur in residence” at Eli Lilly working on identifying innovative business models for drug discovery. He had previously founded another company, Libraria (now Eidogen-Sertanty), where he built the first gene family-wide SAR and combinatorial reaction databases. While at Lilly, Bunin found the support and seed funding to demonstrate the efficiency of cloud-based management and distributed drug discovery and conceived of the CDD prototype. “We have developed a very useful software platform that adds a lot of value. It is not just putting data in the cloud. It is a whole series of tools that

divided up with seamless information exchange based on user security settings. He adds, "This makes it very easy for our customers to organize several different projects without having to upload all the information repeatedly. The whole process is just so simple."

Like CDD, SCYNEXIS' services go beyond simple data storage and sharing. They, too, have developed a proprietary system to help scientists work with chemistry and biology information, and they have embedded popular drug discovery pharma tools into HEOS—well-known tools like Accelrys's Pipeline Pilot and TIBCO's Spotfire—that are easily recognized industry standards. Users can run Pipeline Pilot protocols on top of data captured in the cloud and run Spotfire lead optimization on the data from a web window. To maximize HEOS' availability, SCYNEXIS formed a marketing agreement with Accelrys to market the service.

When SCYNEXIS first started offering its HEOS software, most of the projects involved big numbers from data-heavy efforts including combinatorial chemistry, large chemical libraries, and high-throughput screening (HTS) campaigns, but the company finds that over the past couple of years, clients are reaching for HEOS more for lead optimization and preclinical work. "Now we can easily capture and manage even more biological and chemical data, all information that is relevant for a drug discovery effort," adds Bost.

Diverse User Base

Both CDD and SCYNEXIS find that customers come in two general varieties—the large company or collaboration interested in expediting drug discovery among many parties and the relatively smaller academic laboratory or biotech company who rely on cloud-based

services to handle all their drug discovery data and informatics. But within collaboration, the size and mission of the participants can vary widely from a remote field office in a disease-endemic region to a professor's research laboratory half a world away to the global headquarters of a major pharmaceutical company.

Projects range from a simple database that is used once to companies who have signed on for years to have all their data in the cloud. Scaling collaborations becomes easier to facilitate because one does not have to create multiple databases that need to be uploaded multiple times. Data can be tagged, much like in Flickr for photographs, and consequently be available for multiple projects. "Having the service in the cloud means that it is much easier to scale multiple collaborations with finite headcounts, since you only upload your molecules and libraries once," says Bunin.

Neglected Diseases

Because of their success working with a varied customer base, SCYNEXIS and CDD have both successfully participated in drug discovery efforts involving neglected diseases—multiparticipant projects that necessitated the use of a cloud-based product. "We found that working in the cloud helped our clients with researchers over quite a wide global distribution, including regions of the world where neglected diseases are rampant," says Bost, who recently cowrote a paper about the solutions offered by cloud-based informatics services in neglected disease collaborations (Bost et al., 2010).

A cloud-based architecture allows researchers in remote areas with sometimes limited technological resources to be full participants in the research project. "All they have to have is access to the Internet and the proper security codes,"

adds Bost. This avoids the requirement for software downloads every few weeks to all participating computers, and it ensures that users in various working environments—companies, academia, and public health—all participate fully in the projects. The software acts as the glue for bringing together all the various types of researchers and organizations.

SCYNEXIS is going another step beyond a computer connection to make its services available on mobile devices. One can download the HEOS iPhone application to stay on top of ongoing projects.

Secure Environments

Data security and privacy are central to the success of these cloud-based tools. "One can easily make your microscope or telescope as small or as large as you want to in terms of permissions to maintain security and maximally mine the data," says CDD's Bunin. CDD cites its 100% security record over its history and 26,000 customer logins as a testament to its security and increasing customer base. Similarly, SCYNEXIS claims a faultless HEOS security history. "We've worked with most of the top ten pharma companies that included use of HEOS as part of the project," says Marquardt. "We've completed many projects with these companies using real, confidential data and information and have never had a security or data breach in the cloud environment."

REFERENCE

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Alice McCarthy (alice@alicemccarthy.com) is a science writer based in Gloucester, MA.