Oracle *at* Work

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— Douglas McArthur, scientific programmer for MDL Information Systems, Inc.

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Manual labeling of test tubes and bottles worked fine when pharmaceutical and biotechnology companies were testing just 100 chemical compounds per week. But when research labs began using robots to help them test up to 10,000 compounds a day, a new drug discovery and chemical testing process called High Throughput Screening (HTS) was introduced.

Though the methodology has been in the making for almost five years, most pharmaceutical and biotech companies are just now implementing HTS. MDL Information Systems, a leading developer of chemical information systems, is the first to build a complete cross-platform client/server solution for managing HTS. And they did it with Oracle Power Objects (OPO).

MDL, a longtime Oracle partner, built MDL SCREEN, its application for HTS automation, in OPO, and now sells it as part of a package that works with Oracle SQL*Net and the Oracle7 database. In fact, OPO's native access to Oracle7 servers, drag-and-drop binding, and database-aware controls were among the reasons why MDL chose OPO as the tool with which to build MDL SCREEN. "OPO's tight integration with an Oracle database was extremely attractive to us," says MDL SCREEN chief engineer Douglas McArthur. "It saved us literally thousands of lines of code."

Tailored Solutions To Complex Problems

For the few companies who tried to move to HTS before MDL SCREEN became available, their scientists were experimenting with everything from Microsoft Excel spreadsheets to what McArthur likes to call "home-brew" databases to manage their lab data. But there were problems inherent in attempting to manipulate large amounts of complex data with these tools.

"The problem with homegrown databases is that they don't have the flexibility needed for large amounts of data," McArthur says. "Oracle7 can handle the interactions between many tables and relationships, and can grow as the data grows."

Though the development team at MDL knew that using an Oracle database to store information garnered on chemical compounds would be their best bet, choosing a tool to build the new overall solution was much more difficult.

Business Profile

Founded in 1978, MDL Information Systems, Inc. is a leading worldwide provider of solutions for research and development in the pharmaceutical, chemical, agrochemical, and biotechnology industries. These solutions include scientific information management systems, databases, and services to aid individuals, research teams, and corporations in the discovery and development of new products. Company headquarters are in San Leandro, California, and the company has offices throughout the U.S., Europe, and Japan.

Solution Snapshot

Primary use:
Tracking and managing large volumes of data during HTS, a new drug discovery and chemical testing process

Hardware:
DEC Alpha, Silicon Graphics, and IBM RS/6000 servers; Macintosh and PC clients

Oracle products:
Oracle Power Objects,™ SQL*Net,® Oracle7™

Benefits

- Serves as a comprehensive automated testing solution for drug discovery organizations

- Protects highly sensitive test results

- Provides an easy-to-navigate interface, with visual objects that represent familiar scientific validation and process-directed activities

- Stores and makes readily available large and growing amounts of test data

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Why Oracle Power Objects

At first, MDL considered using a combination of two different tools to build MDL SCREEN separately on each platform. But building the product once, rather than twice, seemed like the smartest move.

"We had to deliver on both the Mac and the PC," McArthur says. "Oracle Power Objects allowed us to do that with limited customization work." Oracle Power Objects is Oracle's powerful, yet low-cost and easy-to-use tool for Visual Basic programmers. And it's fast—whether upsizing a table, downsizing a database, or even migrating a database from one database server to another, it can all be done with drag-and-drop ease.

McArthur and one other programmer were able to build MDL SCREEN, a complex 150-form application with reporting options and hundreds of stored procedure calls, in just four months.

"We made the right choice," says MDL SCREEN Product Manager Lee Amon. "We have finished development in an astoundingly short period of time, and we have a product that works well, looks good, and is cross-platform."

The Right Choice

MDL client Neurocrine Biosciences, Inc., would be the first to agree that MDL's choice was a good one. Neurocrine's Dimitri Gregoriadis, senior research scientist in neuroscience, explains why.

"At Neurocrine, our neuroscience and immunology disciplines give us the ability to identify specific and selective chemical compounds from a library of tens of thousands that help treat a variety of neurological and neuropsychiatric diseases. Each target requires a different and specific set of procedures (called an 'assay') that can differentiate and identify unique chemical compounds that will interact with that specific target. We use high-throughput screening of multiple chemical libraries as a way in which to identify such 'starting' molecules and then chemically modify them into specific and selective drugs."

Keeping track of thousands of compounds and their effects in a wide variety of assays can prove to be quite daunting, however. "In the past," Gregoriadis explains, "we used spreadsheets to keep track of not only the compound's physical properties, but also its effects on all of the assays related to the targets we were investigating. Each target and its associated assays were usually kept in one spreadsheet. These spreadsheets all resided on multiple desktop computers. An obvious major shortcoming of a system like this was the tedious job of obtaining all of the information related to a specific compound across the therapeutic areas in the company. In addition, in order to generate a "compound profile," multiple spreadsheets had to be accessed and queried for the information. What we clearly needed was a more integrated system; one that can track data across all of the programs within a company."

MDL SCREEN provides Neurocrine with a desktop solution that can accurately and quickly respond to inquiries about the effects of the compounds they research. "What we need to be able to do," Gregoriadis says, "is sample the database and quickly and accurately get a product profile of specific compounds. This is exactly what MDL SCREEN is designed to do." In a world that is desperately awaiting cures for far too many debilitating afflictions and diseases, MDL SCREEN may be just what the doctor ordered.

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