

Strengthening Cheminformatics at Incyte - Migrating from RS³ to Accord Enterprise Informatics -

a discussion with Dr Ken Abremski, Senior Director, Applied Technology

Abstract

In January 2005, Incyte Corporation, a company that develops small molecule drugs for conditions such as HIV, diabetes, oncology and inflammation, delivered faster compound registration to its chemists and improved customization capabilities to its Informatics developers by migrating its corporate registry system from Accelrys' RS³ to Accord Enterprise Informatics (AEI).

Why Incyte Chose to Migrate

As the repository for all of its chemistry data, structures and associated biological assay information, Incyte's corporate registry system is used by its chemists and biologists to both enter data and query for information. As a result, the system must offer end-users speed and ease of use, while also providing Incyte's Informatics developers with flexibility for customization and future development.

With these demands in mind, Incyte chose to migrate its system to AEI, an Oracle-based, enterprise-wide solution for chemical information management that builds on the strengths of their existing system through integration with Accord technology to provide a modern, richly featured solution.

AEI provides a powerful chemistry engine and an open and flexible backend that features a data catalog for flexibly linking to other Oracle databases, a list manager for storing and managing lists and queries, and standard PL/SQL development capabilities. These features of AEI enabled developers at Incyte to build a custom web-tool for structure input, searching, and viewing. With the tool, end-users simply input a structure and its associated information, hit search, and either select one of the hits already registered in the database or create a new structure.

As described below, using AEI as the basis for their corporate registry system offered Incyte two main advantages—significantly faster compound registration for chemists and improved customization capabilities for Informatics developers.



Solutions used

Accord Enterprise Informatics
Accelrys Migration Services

Industry sector

Biotechnology

Organization

Incyte Corporation

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Significantly Faster Compound Registration

The AEI-based system has significantly sped up structure and substructure searching. Dr. Abremski explains, "All of the chemists are very happy with the structure searching. They noticed the speed up right away. Structure searches that were taking up to 30 seconds in the old RS³ system are now taking 1 second or less." Dr. Abremski continues, "On top of this, I believe AEI can better handle different kinds of structures."

Flexible Customization

Because AEI provides the ability to access the Oracle database with standard PL/SQL programming, Incyte's developers were able to build a custom interface directly in the database, which was a big advantage over the previous system. Dr. Abremski explains, "From the developer side, we're trying to build clients that have built-in business rules and are user-friendly for our chemists and biologists. So, having PL/SQL development capabilities makes our job easier. From the user side, they really never noticed a difference because the interface was the same as it was in the past—except it was now significantly faster."

On top of this, with an AEI-based solution, Incyte's system is built on a chemistry engine that can continually evolve in terms of its capabilities, whereas the chemistry features in their old RS³-based system were more static in nature. As a result, when user needs change in the future, developers have an easier time adapting the system to meet new requirements.

The Migration and Maintenance Experience

As part of the migration process, an Accelrys cheminformatics expert consulted with Incyte's Informatics group in a series of pre-planning meetings in order to ensure the migration process went smoothly and downtime was minimized. "It was all planned very well," comments Dr. Abremski. "Accelrys was very responsive to our expectations around the migration. If any questions came up, they were answered pretty quickly."

In addition to installing AEI, Incyte's Informatics team also upgraded from Oracle 8i to Oracle 9i at the same time. The team did not attempt to run any systems in parallel, but instead told end-users that the system would be down temporarily. They planned for the migration to take five days, but everything went so smoothly that it ended up taking only two and a half days. The team was able to seamlessly bring the system back up after the migration and end-users could immediately log in. Dr. Abremski comments, "This went very smoothly compared to some other systems that we've had to get installed. In fact, it went so smoothly that it's difficult for me to remember the migration two years later."

After the migration, there were no issues or surprises that came up. "I think we were pretty well prepared," says Dr. Abremski. "The people at Accelrys were very knowledgeable and certainly our chemistry users were very happy with the speed up in the searching. The system has been a low maintenance, rock solid performer over the years we've had it."

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