

Square Plugs and Round Holes - using Accord Enterprise in a Heterogeneous Software Environment

- Dr Chris Enkvist, Karo Bio, speaks at AccelrysWorld 2005

Karo Bio (www.karobio.com) is a leading drug discovery and development company focused on nuclear receptors, an important class of drug targets for the development of novel pharmaceuticals in major disease areas.

Dr Chris Enkvist, responsible for chemo and bioinformatics software and related application development at Kara Bio, spoke at the AccelrysWorld 2005 user event and conference on the role of Accord Enterprise Informatics (AEI) in chemical data integration.

AEI products integrate to offer an Oracle®-based enterprise-wide solution for chemical information management. These products draw on the power of the Accord Chemistry Engine and Oracle databases to store, search, and analyze chemical structures, related biological and chemical data, experimental results, and registration information.

Karo Bio AB has several databases and information sources e.g. chemical compound and information databases, inventory (chemical, solution, plates) databases, safety and information databases, and databases containing screening results from biological assays. Information from these sources should be accessible as flexibly as possible so that the data may smoothly integrate with 'any' application or software package the end user wishes.

"At Kara Bio we do not have massive amounts of data but do have many different data sources and research areas. Combine this with a small budget, both with regards to time and money, and flexible and dynamic requirements with respect to both applications and data content, and you have a complicated information problem," began Dr Enkvist.

"The first step in our solution was to migrate all our databases to the same database platform. We chose Oracle owing to its performance, security and scalability, along with its cross-referencing capabilities - vital with multiple databases," continued Dr Enkvist.

However, Oracle alone can not deal with chemical structures. "AEI was used as our chemistry database system because it not only enables Oracle to handle chemical structure data, but it also has a very easy-to-use API (application program interface) and it provides easy methods for building web based tools," continued Dr Enkvist. "In addi-

tion to these benefits, AEI has integrated methods for accessing any Oracle based database."

"The choice of using AEI as the fundamental building block of the federative layer was very simple - if the non-chemical/AEI data were ever to be made searchable from within the AEI framework, e.g. Accord for Excel Enterprise, the lookup tables and views had to be constructed no matter what," said Dr Enkvist. "By immediately focusing on making the non-AEI data available within the AEI framework several additional benefits could be reaped. The overall data model didn't have to be invented from scratch saving a lot of time, money, and headaches."

"New data sources could be added in incremental steps as the system was online throughout the implementation process, eliminating the need to wait for everything to be setup before the system could be used," added Dr Enkvist. "But perhaps the most important benefit of using AEI is that it provided tools that enabled most of the implementation work to be done in-house and easily customized to satisfy not only our needs today but also those of tomorrow."

"AEI enabled all the data to be merged in to one place and made completely searchable," explained Dr Enkvist. "When data can be accessed in the Accord Enterprise database it is very easy to access this data from 3rd party products or homebuilt applications."

"The usage of primarily web based solutions enables the users to access data from more or less any computer which can access the internal network thus significantly reducing the cost of software and IT resources," continued Dr Enkvist. "The familiarity of web interfaces reduces the learning threshold and simplifies the introduction of new tools and routines. After all, user acceptance is paramount! Furthermore, as the federative layer provides access to several different databases the information barriers between 'my data' and 'other people's data' can be eradicated as all data will be provided in the same interface/browser."

"When data can be accessed through web pages integration with 3rd party software is often trivial. Spotfire is one example where linking and viewing of web pages is a built-in functionality and hence easily integrated with the federative layer."

"However, the major benefit for the end user is that search and report interfaces can be easily customized, either by in-house IT or by the users themselves to fit their explicit needs and requirements," concluded Dr Enkvist.