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Putting MDL® Isentris® into practice

Three easy steps you can take now to gain *"data on demand, power for decisions"*

The question is: How do you implement a new approach like Isentris in the real world on top of an established order—without interrupting operations?

Integrating information and workflows with MDL® Isentris® provides unparalleled opportunities to improve productivity. MDL Isentris saves time, cuts costs and improves decision making. The question is: How do you implement a new approach like Isentris in the real world on top of an established order—without interrupting operations? The best place to start is with Elsevier MDL's experienced Consulting organization, a group that offers significant experience with implementation and migration projects at companies of all sizes, all around the world.

Here are three simple steps you can take today.

1. Start with a plan (and a Starter Kit!)

"Every migration begins with a plan, a detailed roadmap of how to achieve the desired goal," says John McCarthy, Vice President, Consulting Services. "In this plan we pinpoint the specific places where we can add value. We identify the key stakeholders, define the business objectives and understand the customer's workflows."

Isentris is tremendously flexible. Sometimes this benefit can present a challenge—many options and decisions lie before you. To help guide you through this process and limit the number of decisions, Elsevier MDL Consulting has developed Isentris Starter Kits that can get you up and running quickly (see page 12).

The goal is to begin with a standard Isentris implementation that meets a specific workflow need. Consulting delivers a fixed installation, configuration and setup with onsite training, lets you work with the system and then follows up with additional site support to address any workflow functionality or integration issues that may arise in the early stages of deployment. "Later, we can return to assess incremental improvements such as adding data sources, customized forms, fields or calculators and providing additional administrator or developer training," says McCarthy.

2. Prove value in the lab

With plan in hand, Elsevier MDL Consulting can develop a proof of concept that demonstrates the value of the solution in the lab. "The goal of this critical step is to show scientists that the Isentris solution works, that it saves them time and helps them make better decisions," says McCarthy. "At the same time, we need to show management that the solution improves efficiency, simplifies operations and enhances productivity."

Recently, a large U.S. pharmaceutical company asked Elsevier MDL consultants

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to replace the ISIS interface used by chemists and biologists in one particular therapeutic area with an Isentris interface. They wanted to see if they could still do everything they did with ISIS—but do it better with Isentris.

Within one week, the Consulting group had replaced selected Hviews with an Integrating Data Source (IDS)[1], replicated ISIS forms in Isentris, added the ability to see live IC50 curves, delivered new interactive Structure Activity Relationship (SAR) tables, integrated it all with Spotfire technology and enabled scientists to use the results of a search to generate PowerPoint reports for project team meetings (refer to Figures 1-3). The IDS provided a rich, flexible foundation for connecting data from relational and other data sources into a network model and presented the information in the hierarchical format that scientists prefer. Instead of having to use many static Hviews, the customer could employ the IDS to create flexible, dynamic views that were easy to browse and search and preserved hierarchical relationships.

"When we presented the prototype, company management was impressed," said McCarthy. "They told us they weren't supposed to reveal their excitement in meetings with a vendor, but we deserved a pat on the back for what we had accomplished in such a short period of time. We had successfully demonstrated that Isentris is more than just a replacement for ISIS, it far surpasses it."

3. Deploy in stages

Once Consulting has demonstrated the value of the Isentris solution, they can move on to deploy the software throughout the organization.

With regard to deployment, it is important to remember that MDL Isentris leverages your investment in existing MDL products and does not require rebuilding your informatics infrastructure. ***You can run Isentris concurrently with ISIS. As the two systems share key design and data representation features, you can take a step-by-step approach to migrating chemical structure repositories and workflow applications to Isentris***.

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[1] The MDL ISIS Hview (heterogeneous view) presents data in tree-structured views that are useful for searching content. However, the need to maintain hundreds of isolated Hviews in a system built on proprietary coding increases the complexity and cost of data storage. The MDL Isentris Integrating Data Source (U.S. patent pending) dynamically represents multiple derived hierarchies providing real-time updated views of data as well as powerful data pivoting and other list management capabilities that offer significant advantages over Hview technology.

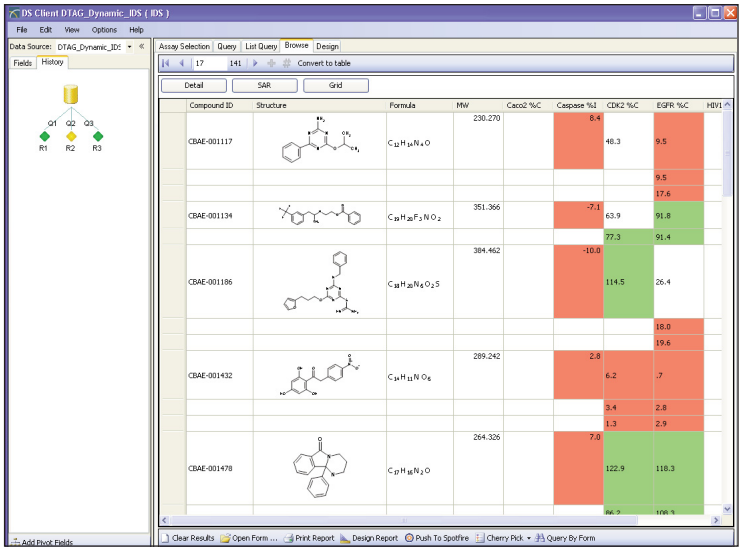

Figure 1: Interactive SAR tables with conditional formatting provide a quick overview of a compound's activity.

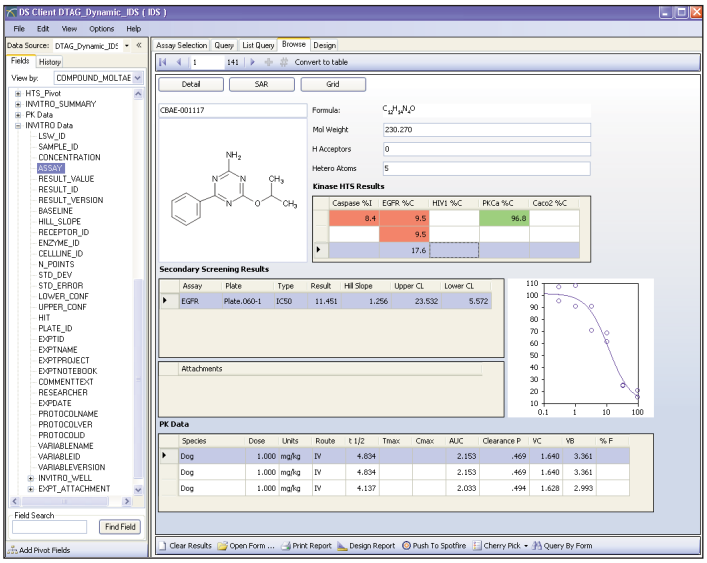

Figure 2: Isentris forms enable the scientist to see the level of detail required to understand the activity profile of a lead candidate.

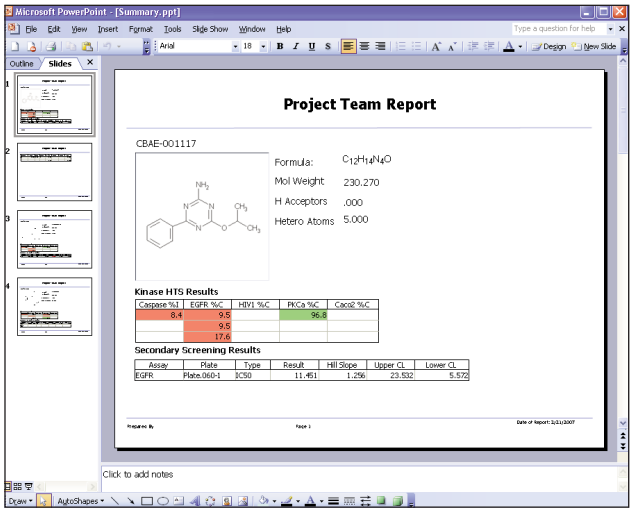

Figure 3: Isentris offers powerful, built-in reporting capabilities. A scientist can send the data from an Isentris form to a set of PowerPoint slides with the click of a button, saving hours of cutting and pasting in preparation for project review meetings.

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Organizations with hundreds of Hviews and applications can continue to use those systems alongside the new architecture. "You can deploy Isentris at your own pace, in a flexible manner, without interrupting your business," says McCarthy. "Whether you chose to install the new system as part of an effort to consolidate and decommission legacy applications or as a way to support new constituents in your research community, the choice is yours and your existing applications can continue to run."

Flexible deployment options further ease the transition to Isentris by offering a variety of migration approaches.

Project-based approach. Scientists at one company needed to shorten the time it was taking to collate the assay results necessary to understand the activity profiles of their lead compounds. At this company, it made sense to take a project-based approach to the Isentris migration. Consulting began the transition by implementing a new SAR interface and then proceeded to the deployment of a new Isentris-based registration system that supported the registration of biomolecules, a new strategic initiative for this organization. The customer is now assessing a new inventory and logistics solution.

Application-based approach. Depending on a company's needs and priorities, they might opt to follow an application-based transition, possibly swapping out ISIS for Excel with Isentris for Excel, and then retiring the ISIS Finders for accessing commercial databases in favor of the new Isentris client while leaving other in-house applications running. This approach enables a company to realize the benefits of Isentris immediately while also transitioning in-house-developed applications to the new environment in an orderly fashion.

Community-based approach. Other organizations have taken a community-based approach in which they first deploy Isentris to specific groups of researchers or specific research locations. For example, a team of pharmacologists who had not previously used ISIS is now using Isentris for Excel to reduce the time spent creating spreadsheets used to compare compound properties. As a result, they now have time for the more productive activities involved in understanding and analyzing the results of their research.

More and more companies are migrating to Isentris using whichever of these flexible approaches is most appropriate to their business needs. More than half of Elsevier MDL's top 30 customers, have now licensed MDL Isentris.

How can you determine if Isentris will benefit your organization?

First, let Consulting come to your site and show you how Isentris addresses your specific challenges. Contact your Elsevier MDL Account Manager and ask for a demonstration of Isentris.

"Second, you can take Isentris for a test drive. Ask your Elsevier MDL Account Manager to set up a conference room pilot of MDL Isentris so that you can spend some time assessing its capabilities," says McCarthy. "For example, see how the new Reaction Planner can help your medicinal chemists develop synthesis plans."

"Third, challenge Elsevier MDL Consulting to demonstrate the innovative, new capabilities that make Isentris so much better than ISIS," suggests McCarthy. "Ask us to do something specific like converting one of your ISIS Remote Access Files to an Isentris interface. Then let us demonstrate the many additional benefits Isentris brings to your researchers."■

The MDL® Isentris® Starter Kits:

Immediate access to an out-of-the-box Isentris solution

The MDL Isentris Starter Kits are defined consulting packages designed to help you quickly plan, implement and deploy out-of-the-box Isentris functionality including the installation, configuration of appropriate software[1], training and follow-up.

Contact your Elsevier MDL Account Manager for specifics and pricing.

Data access kits

MDL databases

Access to MDL databases covering chemical sourcing, synthetic methodology and bioactivity. This implementation enables scientists to access critical data, plan synthetic routes and simplify compound sourcing.

In-house database

This package includes access to MDL databases and an organization's in-house, proprietary database, enabling researchers to search, collate, analyze and share data from multiple data sources in support of critical decisions.

Discovery foundation kits

Chemistry

A chemical substance registration system. This implementation includes the ability to normalize and register chemical substances in an in-house database and access related biological information and MDL databases.

Biology

A biological assay data capture system. This package includes two protocols for capturing assay data and configuring the system to enable scientists to access biological and chemical data, as well as MDL databases.

Advanced discovery kits

Discovery I

An integrated suite of Isentris applications for managing chemistry workflows. This implementation enables scientists to plan synthetic routes, procure compounds and register substances through a notebook user interface.

Discovery II

An integrated suite of Isentris applications for managing biology and chemistry workflows. In addition to the Discovery I chemistry workflows, this implementation includes two protocols for capturing assay data, providing scientists with access to chemical and biological data.

[1] Software and database license and maintenance fees not included. Travel expenses billed separately.