

MDL[®] ISENTRIS[®] 2.0:

Data on demand. Power for decisions.

In recent years, the volume and complexity of data handled by pharma, biotech and chemical research organizations have continued their upward trend, while research directors have aspired to bridge diverse elements of the research process. A 2006 study by Health Industry Insights™ identified data integration as pharma's top IT priority going into 2007¹.

To meet this integration challenge, Elsevier MDL has invested significant resources to develop a new-generation information system that extends well beyond the capabilities of MDL[®] ISIS.

The result is MDL[®] ISENTRIS[®], a system that provides a scientist-centered research environment that blends information access and workflow applications for enhanced decision-making. The ISENTRIS 2.0 release will be available in December 2006.

What is ISENTRIS?

For scientists, ISENTRIS manages day-to-day research—activities such as capturing data, accessing information from diverse sources, analyzing results and sharing ideas. A self-service environment, ISENTRIS gives scientists the control to quickly create their own views of data, for example, SAR tables, and act on them.

More than an application, though, ISENTRIS is a system that integrates data from multiple sources into workflows and supports rapid application development based on industry-standard technology. Organizations can tailor data, in-house applications, MDL applications and specialized software from other vendors into researchers' workflows.

"MDL ISENTRIS is really the informatics foundation for the lab of tomorrow," says Dr. Trevor Heritage, senior vice president and chief scientific officer, Elsevier MDL. "It addresses the integration challenge

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Meeting real needs

ISENTRIS is improving data management today at research organizations around the world, helping researchers get to the data they need, when they need it and in the format they want.

Recordati moved to ISENTRIS because difficulties accessing data and searching for information were slowing scientists, according to Carlo Riva, head of chemical synthesis in the Pharmaceutical R&D Division.

"With ISENTRIS," Riva says, "we've been able to retain our critical ISIS functionality, while moving to a system with much improved integration and ease-of-use. The new system is demonstrating its power, enabling scientists to access new assay types and related experimental data as soon as they are created."

The upcoming release of ISENTRIS 2.0 brings even more power to researchers' desktops—and developers' toolkits.

Dr. Dominique Swinnen, Senior Scientist at Serono, got an early look at the new release. "ISENTRIS 2.0 looks very promising," says Swinnen. "I was really impressed with how user-friendly it was and especially with the reaction planning functionality. The ability to explore precursor reaction steps and quickly build reaction plans looks very useful and could save us a lot of time during our synthesis preparation."

What's new?

Single search across databases

The new MDL[®] ISENTRIS[®] client saves researchers' time by integrating commercial data into their workflow. For instance, while browsing reactions from multiple sources, researchers can view and collate lists of commercially available compounds and lists of reaction citations. They can explore and build custom reaction pathways from the available data sources, and link to external citations and compound safety data. The result is less leg work for the researcher, faster answers to questions and better support for decisions.

¹ Health Industry Insight, Q2 2006, "Leading Indicators IT Spending Survey."

Visual synthesis planning

Reaction planner functionality automatically generates synthesis pathways for products or reactants of interest (Figure 1).

The system investigates multiple reaction databases and suggests appropriate reaction steps for creating the product or reactant of interest. A synthetic chemist can then decide which path to take using data such as citation, yield, reagents, condition and reactant availability.

"It's very satisfying to preview the reaction planning features to customers in the field and see their response," said Albert Crescenzo, a consultant with Elsevier MDL. "I've had people literally ask me to hold on while they dashed out and came back with more colleagues."

Expanded power to use Excel

Scientists frequently rely on Microsoft® Excel® for sorting and manipulating data. ISENTRIS for Excel functionality lets scientists manage and share data in spreadsheets in ways not possible with ISIS for Excel and other applications (Figure 2).

Beyond managing data in a spreadsheet, ISENTRIS for Excel makes it easy to search corporate and proprietary sources for relevant information. Scientists can preview and try different searches before placing the data in a spreadsheet, so when they begin collating and sorting they have the precise data they want.

When you save a list in ISENTRIS for Excel, the system saves any filtering information you've applied too. When

ISENTRIS offers a superior approach to essential tasks and gives organizations the chance to create comprehensive scientist-centered information systems today.

you recall that list, you immediately get the specific data you want.

Presentation-quality drawing with sketch support

MDL® Draw makes drawing chemical structures and reactions simple with an all-purpose tool that lets scientists draw an entire structure, including query options.

The new 2.0 release of MDL Draw adds support for common workflows. For example, chemists can draw reactions and quickly annotate them with text and arrows. Biochemists can create a peptide or nucleotide sequence where individual residues can be expanded to full structure to show modifications.

Importantly, MDL Draw 2.0 adds ISIS-compatible sketch file support, so scientists can access legacy, ISIS-drawn structures stored in Microsoft Word documents or presentations and style the font, color and line thickness directly from the toolbar. The new release also supports publication-quality graphics, so researchers can insert structures into reports and presentations.

Chemistry searching in Oracle® databases

ISENTRIS 2.0 substantially improves performance for searching large reaction databases. A boost to fast reaction search in MDL® Direct 6.0, the database-tier component of MDL ISENTRIS, has been

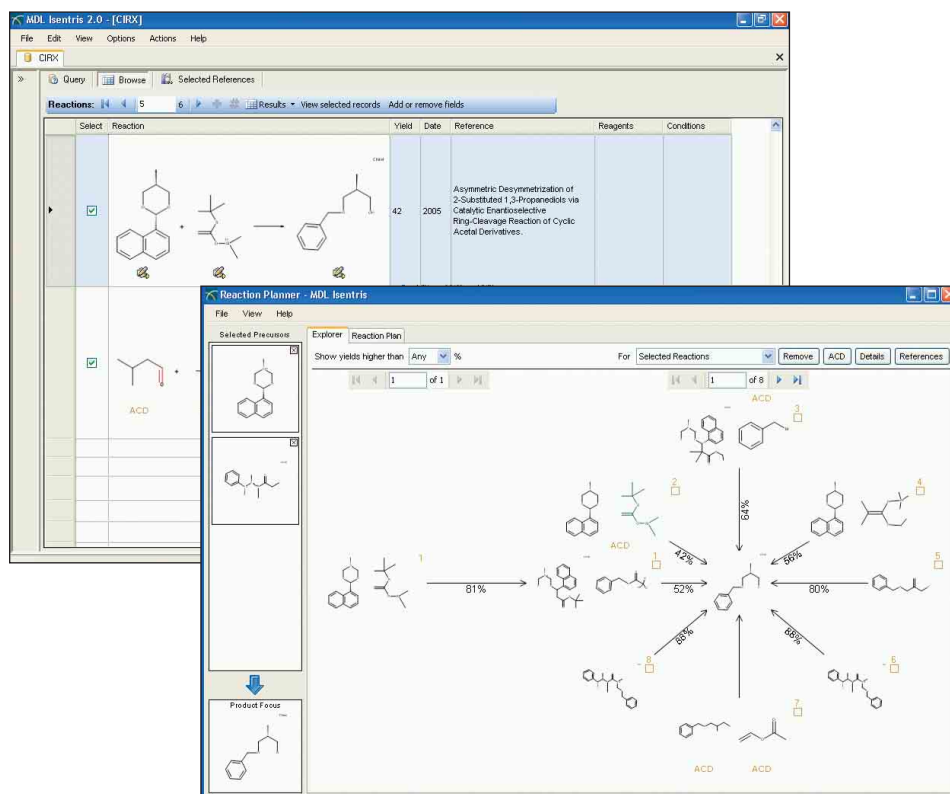


Figure 1: Chemists can enter a target structure in ISENTRIS and immediately view preparations of the structure gathered from reaction and synthetic methodology databases.



A new generation of applications built on ISENTRIS gives researchers easy access to essential information in the context of their work.

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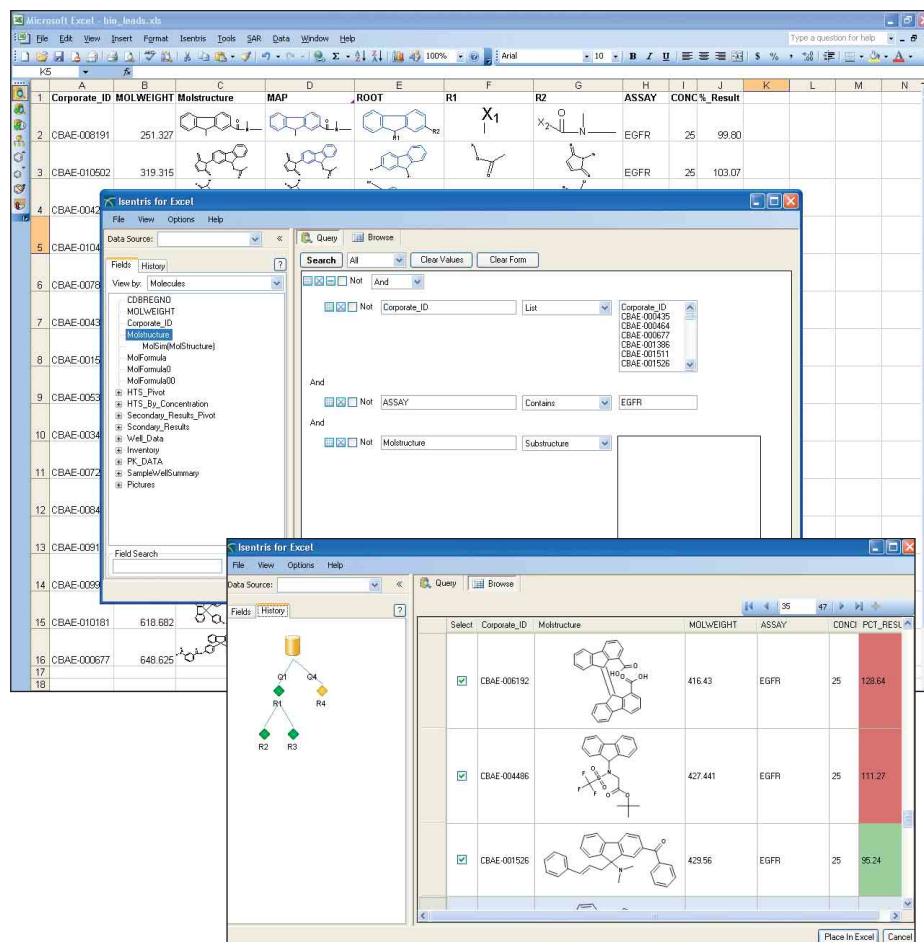


Figure 2: With ISENTRIS for Excel, scientists can collate data, perform analysis, annotate and share information with colleagues.

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Head of Chemical Synthesis,
Pharmaceutical R&D Division
Recordati

The MDL ISENTRIS client and ISENTRIS for Excel were created using ISENTRIS controls and provide an example of how organizations can achieve a consistent look-and-feel within their research desktop environment. Reusable, standard controls reduce development and maintenance costs and give applications similar behavior, making it easier for researchers to learn how to use them.

Capitalizing today

The combination of innovative out-of-the-box functionality and development-friendly design in ISENTRIS is helping scientists accomplish tasks that were previously time-consuming or impossible. Advances in the latest 2.0 release make the case even more compelling.

MDL ISENTRIS offers a superior approach to essential tasks and gives organizations the chance to create comprehensive scientist-centered information systems today. Organizations taking the ISENTRIS initiative today stand to generate a substantive business advantage.

tested and proven on databases with over five million reactions and at least 20 million molecules.

Combine this performance with unsurpassed chemistry capabilities, such as full reaction transformation searching and enhanced stereochemistry support (including non-tetrahedral stereochemistry of biaryls and allenes), and ISENTRIS assures researchers of immediate, anytime access to correct, consistent chemistry data.

MDL Direct 6.0 is now independent of ISIS and fully integrated with Oracle technology. A migration infrastructure enables existing ISIS-based customers to migrate from 5.1 to 6.0 in a measured and uninterrupted manner. MDL Direct 6.0 also offers Linux support.

"We're looking forward to this release of MDL Direct as a major step in our

roadmap to a clean Linux environment," said Karsten Linneberg, Head of Section in R&D IT at Leo Pharmaceuticals. "It will also provide a clean Oracle setup by eliminating the need for maintenance components of MDL ISIS/Host."

Simplified development

MDL ISENTRIS includes a set of .NET controls that developers can use in the familiar Microsoft Visual Studio environment to rapidly build, extend and integrate new and existing applications.

The ISENTRIS controls provide discovery-specific ISENTRIS functionality for the .NET developer's toolbox. Developers can combine the out-of-the-box, documented and supported ISENTRIS controls with third-party controls and standard .NET controls from Microsoft to accelerate application development.



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