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MDL[®]
ISENTRIS[™]

*Where drug discovery
and informatics meet*



MDL[®]

an Elsevier company

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As the director of MDL® Discovery Framework, Tom Blackadar is responsible for the technology underlying the critical integration of MDL, customer, and third-party content and workflow applications. Since joining MDL in 1985, Tom has acquired an in-depth knowledge of MDL framework technology through successive positions in product development and marketing.

As Tom has been the voice of MDL Isentris from its inception, it was only natural that Molecular Connection would go one-on-one with him to understand how Isentris integrates and energizes life sciences research... especially as Isentris is officially unveiled this summer at Drug Discovery Technology in Boston.

Tom Blackadar on MDL® Isentris™

Integrating and energizing life sciences discovery

What is MDL Isentris?

MDL Isentris is a new informatics platform for discovery research. It is the only fully supported, three-tier architecture specifically designed for research that also facilitates the integration of an organization's business processes, data, and workflow applications. This three-way integration enables organizations to develop and deploy applications that let chemists and biologists better access and manage their data. Isentris also promotes better decisions and research outcomes by streamlining workflows and improving collaboration amongst global, multidisciplinary project teams.

Isentris is built on modern, mainstream technologies; it offers an open architecture for application development and adoption and, most importantly, it promotes a self-service research model, making scientists much less dependent on IT professionals for real-time support.

For all of these reasons, Isentris will contribute to the achievement of tangible, bottom-line returns including more innovative, successful research, improved productivity, and increased profitability. The Boston Consulting Group has estimated the potential savings from a truly integrated IT environment to be over \$280 million with a one third reduction in R&D expenditure for each new drug, and savings of nearly \$160 million resulting from data integration alone.

What was the motivation behind Isentris?

The life sciences industry needs a flexible, broadly applicable discovery informatics platform. Customer requirements are incredibly varied in this regard. On the one hand, customers need scientific applications quickly and cost-effectively, which makes them turn to out-of-the-box solutions. But the discovery space is very

complex, and equally compelling requirements for extensibility and customizability can tip the balance towards a do-it-yourself solution.

Informatics vendors typically take one approach or the other. They'll either build an application that meets all the requirements but can't be integrated into an infrastructure, or they'll develop technology that's highly customizable but doesn't deliver a broad solution. Both approaches fail.

Isentris provides the best of both worlds. It's an enterprise solution that works admirably out-of-the-box while also being highly extensible for do-it-yourself organizations that need to customize and extend the system to meet specific requirements.

Because MDL's technology needs are similar to those of its customers, we gain similar benefits from Isentris. Building applications on an open, scalable, reliable, and proven technology platform lets MDL focus on developing solutions that offer high-value functionality for customers.

What is revolutionary about Isentris?

Isentris is both an integration engine and a total workflow solution. R&D organizations today depend on many electronic data sources and software tools for data acquisition, record searching, and workflow management. These different tools all have their own "look and feel." They can be difficult to learn and expensive to maintain. What's more, they often provide overlapping functionality, which is not cost-effective, and their lack of interoperability impedes communication and collaboration, both within and between organizations.

An integrated informatics and workflow solution is essential for successful, enterprise-wide

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discovery, but no single vendor can provide this complete solution. Global research organizations need the capability of selecting “best of breed” applications from leading-edge suppliers. For this reason, integration and interoperability are supremely important.

Isestris is revolutionary because it works alongside other architectures rather than competing against them as just another proprietary system. With its openness, flexibility, scalability, and extensibility, Isestris complements and enriches other database and software technologies from MDL and other vendors, providing a powerful, integrating framework for researchers and IT developers alike.

While revolutionary, Isestris is also proven. It's been tried and tested in a truly large-scale environment, DiscoveryGate®, MDL's hosted service that provides single-query access to a wealth of discovery data.

How will Isestris help scientists?

Isestris enables scientists to make better decisions by improving and simplifying access to consistent data, by enhancing project team collaboration, and by supporting global organizations. With improved data integration and easy-to-use software, chemists and biologists can share lists, queries, and results. They can experiment with different ways of examining data. They can look for interesting patterns, relationships, and trends—and they can do all of this without repeated trips to IT support. When data are consistent, reliable, and easy to search, global project teams can quickly work with new approaches and hypotheses to develop successful products more efficiently. And Isestris enabling technology is designed for researchers. Scientists can pursue discovery unhindered, without having to think about, or be distracted by, the powerful technology underlying the process.

How will Isestris help developers?

To assist the development community, Isestris uses the latest industry programming standards and a wide range of methods for integrating new functionality. Developers can build or extend applications using C#, VB.NET, Java, or new visual wiring concepts. The published API supports an open environment for integrating in-house and third-party tools that share the same resources and use the same technology. Isestris also provides plug-and-play functionality in the middle tier, database, and

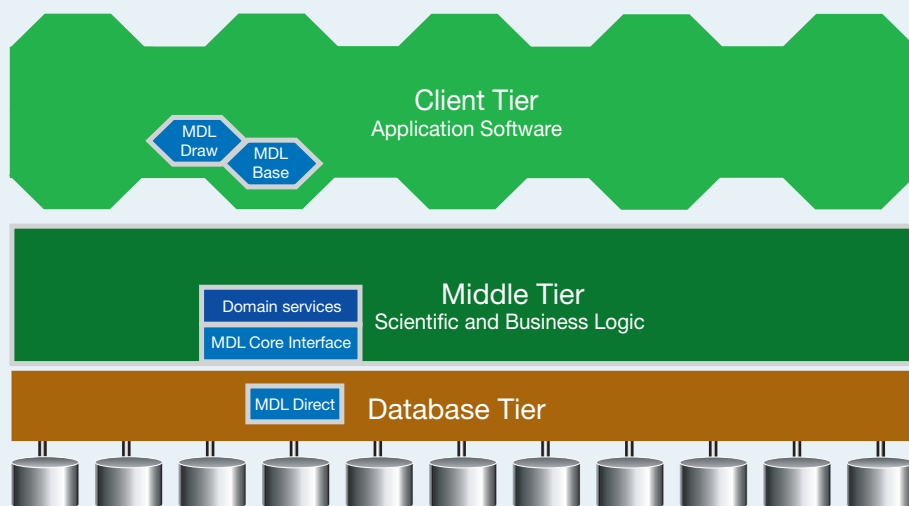


Figure 1: Isestris distributes discovery informatics functionality across a three-tier architecture that combines business processes, data, and applications.

even in the client tier. This open, centralized, plug-in environment makes it much easier for IT groups to develop, deploy, and share new custom and commercial applications that meet researchers' needs—and to do so quickly, cost-effectively, and with scalability for the future.

What are the components of Isestris?

As shown in figure 1, the MDL® Base desktop application and MDL® Draw structure-rendering tool together constitute the user interface. MDL Base gives chemists and biologists access to multiple information sources in a single view, and in real time. Easy-to-use query, list logic, filtering, and history tracking features let scientists acquire, manage, and share critical discovery data in a collaborative environment.

In the middle tier, MDL® Core Interface provides the integrating “nuts and bolts” of the system. Here a common set of business rules defines how structures and data are registered and searched, how applications connect to the system, and how information is managed.

As well as defining standard query and database services, Core Interface also hosts a variety of domain services for handling discovery logistics, calculations, compound registration, reaction management, and similar domain-specific logic.

The underlying database tier enables scientists to access a broad range of public and proprietary information stored in industry-standard relational and non-relational databases. MDL® Direct facilitates this data access by utilizing Oracle® data cartridge technology for

storing, searching, and retrieving molecules and reactions.

What is the migration strategy for transitioning customers to Isestris?

With over 25 years as an informatics provider, MDL has extensive experience migrating organizations to new platforms and systems—and MDL is committed to providing customers with a smooth, well-thought-out transition to Isestris. Existing molecule and reaction data cartridges provide a clean migration route for existing ISIS customers, because both MDL® ISIS/Host and MDL Direct (data cartridges) read and write to the same database. This means that customers can introduce new applications based on Isestris without disturbing existing ISIS data or disrupting project workflows.

What was involved in bringing Isestris to market?

The Isestris development project has been a five-year undertaking involving a huge investment. Over 80 MDL employees from numerous disciplines and departments around the world are currently assigned to the Isestris project team. As the world's leading life sciences publishing and discovery informatics specialists, Elsevier and MDL are uniquely positioned to deliver a project of this magnitude.

Isestris is built on a thorough understanding of the need to integrate business processes, data, and workflow applications. MDL has designed Isestris to offer researchers and developers unsurpassed power, openness, and flexibility in the pursuit of a superior discovery informatics environment. ■

The Integrating Data Source

Blazing a data trail to discovery

MDL[®] Isestris[™] organizes and searches chemical structures and alphanumeric data using a revolutionary new way of accessing and presenting data called the Integrating Data Source (IDS)¹. Part of MDL[®] Core Interface, the IDS provides a rich, flexible foundation for connecting and integrating information from relational and other data sources into a network model while still presenting information in the hierarchical format that scientists prefer for storing and querying data.

The result is a much more powerful Isestris system that lets scientists access and search complex, integrated data in a flexible, straightforward way. In the new self-service research environment created by the IDS, scientists can take the initiative in acquiring, searching, and managing data, even to the extent of accomplishing data transformations that would previously have required time-consuming and costly IT support. Tom Blackadar, director of MDL Discovery Framework, says: "The network focus of the IDS helps to break down information silos, brings the chemistry and biology domains together, and enables researchers to pursue discovery workflows more efficiently."

Moving beyond hierarchies

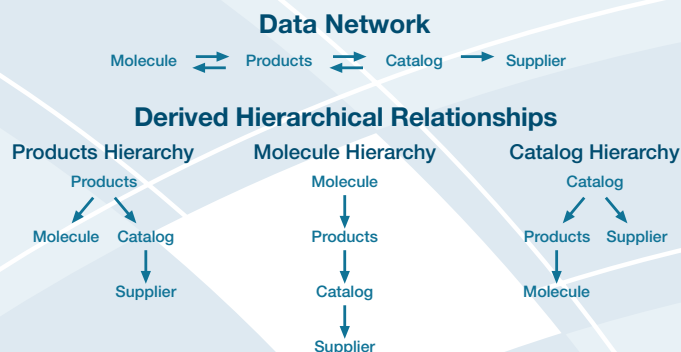
MDL[®] ISIS was launched in 1991 to help research organizations deal with the explosion of complex data resulting from automated techniques and high-throughput screening. ISIS makes it possible to present data from one or more relational databases in unified, static, tree-structured views for storing, accessing, and searching content. The views present data hierarchically, they are server-based, and they are fairly successful in hiding underlying complexity from the researcher. The problem is that the complexity of today's research environment is outstripping the technology of concealment.

With the volume and complexity of data continuing to increase geometrically, today's research environment requires a radically new approach to database management. Data models are no longer simple hierarchies, but large, complex networks consisting of multiple interlinked hierarchies. Each researcher has different questions to ask and different entry points into the network for accessing data. MDL Isestris addresses this situation by providing an integrating data source that works off a single description of an entire data network to build hierarchies on the fly.

Building the network view

In the IDS scheme, the data network consists of nodes linked by connectors. A node can be any source of data—a relational database table, a chemical database like MDL[®] Available Chemicals Directory (ACD), ChemInform Reaction Library, or another integrating data source. A node can even be something as simple and useful as a calculation (LogP, toxicity predictor, etc.). A connector describes the relationship between two nodes, pulling nodes together pair-wise into the network and specifying how they are linked, what the output fields are, and how queries are handled. Connections can be one-to-one or one-to-many and can even represent calculations or data pivoting functions.

Networks and Derived Hierarchies



The Integrating Data Source enables researchers to orientate and query data according to their needs. For example, researchers can browse and query MDL[®] Available Chemicals Directory by product, molecule, or catalog. When browsing or querying molecules, researchers wishing to see all related structures from a single supplier can simply change the view from molecule to catalog.

For example, a "tall and skinny" table used for storing data is not the preferred format for presenting information to a researcher. The IDS includes a standard data-pivoting connector, which, when linked to a tall and skinny table, exposes the table for browsing and querying as if it were pivoted, making the data far easier to locate and view.

"The critical value of connectors is that once they are specified, they can be used over and over again in many different hierarchies," says Jim Barstow, research fellow with MDL Research and Development. "This makes it relatively straightforward to create and expand the network on the fly by the simple addition of new connectors for accessing proprietary databases, image processing software, third-party calculations, or other applications." The connector concept translates into very real benefits for IT administrators and researchers. If an organization uses a particular table with great frequency—for example, an ACD or products table—it is possible to create a base-level connector to link to the table from one node in the network and then to access the same table from other nodes by reusing the base-level connector to derive additional pathways. "The benefit to researchers is that they can easily move a successful query from one domain to another to look at the same data from a different perspective," says Barstow. "It's very easy to query from one hierarchy and retrieve from another, connecting molecules to products, packages, catalogs, and companies in a dynamic, networked view that streamlines and accelerates discovery research."

For IT professionals, the IDS replaces the time-consuming, labor-intensive management of static data files with the much more interesting and rewarding effort of building dynamic, integrating data networks that reflect today's discovery workflows. By enabling project teams to access and transform complex chemistry and biology data from a variety of different sources, the IDS is also the cornerstone of the Isestris self-service model for researchers. ■

¹ U.S. and other patents pending.

MDL[®] ISENTRIS[™]—Enhancing project team

The project team is the core working unit of discovery. Do your project teams have immediate access to the vast amounts of data generated across disciplines and departments? Are they in a position to make research-advancing decisions quickly, confidently, and with the best results?

MDL[®] ISENTRIS[™] brings project scientists and data together, supporting data integration, streamlined workflows, and best-of-breed applications to help chemists and biologists collaborate more effectively and make better decisions.

Sharing project results

Enabling scientists to explore electronically captured information and share results with colleagues is critical to the collaborative process. However, this transfer often occurs at meetings, via e-mail, or through other informal channels, which can jeopardize data integrity and result in project delays.

With ISENTRIS, project team members can log in to a home page that guides them to new results or to a specific point in the project workflow. History tracking helps researchers follow and re-create their thought processes as they ask questions, cherry pick results, add and subtract data, change forms, and build hypotheses (Figure 1).

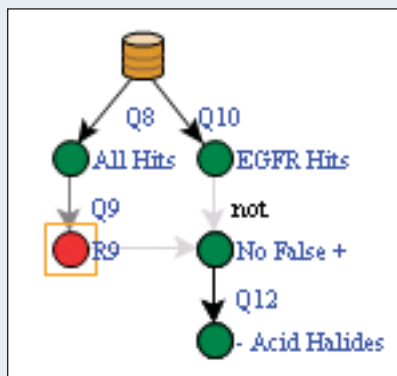


Figure 1: The history tree tracks and preserves the valuable train of thought behind a scientist's results and conclusions.

By bringing life scientists and information together, supporting the self-service model, and promoting a more collaborative work environment, ISENTRIS enables superior decisions and better outcomes in moving candidate compounds through the pipeline.

Facilitating access to project data

Chemical and biological experimentation across multiple projects amasses hundreds of variables in many different contexts including protocols, projects, experiments, and biological assays. This confluence of diverse data makes thorough investigation challenging. To further complicate the issue, data are often difficult to access, because they are not typically stored in a way that lets scientists query and view results intuitively. The bottom line is—most scientists do not care to study or explore database table structures or underlying data storage methodologies. They just want answers to their questions quickly and easily.

To hide the complexity of chemical and biological data storage from the scientist, ISENTRIS automatically generates innovative, abstract data presentations using metadata stored during data capture by biological data management systems such as MDL[®] Assay Explorer. With ISENTRIS processing information such as storage

location, units, and relationships, scientists can quickly determine their query and browsing options on the fly (Figure 2).

Accessing real-time project data

Multidisciplinary scientists working in project teams contribute daily to a wealth of project information. These results might be PK/PD or ADME/Tox results on a compound they hope will be the next blockbuster drug. To ensure productive, timely workflows, data stored in discipline-based silos must always be available for analysis, collaboration, and decision-making. Resource- and time-intensive data marts or data warehouses are often created to optimize search and retrieval performance, eliminate inconsistencies among source systems, and provide a high-level view that can aid data interpretation, collaboration, and decision-making. The down side is that researchers must sometimes wait for considerable periods of time while data are made accessible in these formats.

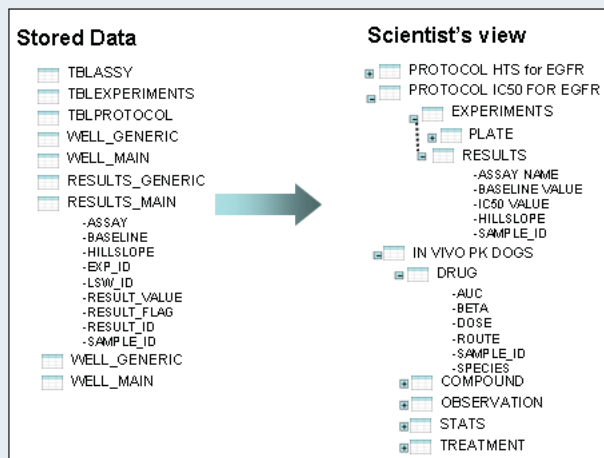


Figure 2: ISENTRIS automatically presents integrated chemical and biological data to the researcher in a hierarchical format that is easy to search and manage.

productivity by improving access to data

Advanced integration tools in ISENTRIS enable project teams to access and share data immediately after storage by greatly reducing the back-end data management required to format and structure the data for scientific analysis. While not realistically eliminating all data warehouses, especially for large data collections, ISENTRIS will minimize the effort and expense of creating warehouses in many instances. As described in the previous article on the Integrating Data Source, abstract data pivoting and metadata-driven views available with ISENTRIS greatly improve the integration and presentation of project data (Figure 3).

Building queries autonomously

The large number of experimental variables in scientific research necessitates the use of many complex and specific forms for browsing project data and results. Scientists are typically faced with the choice of creating hundreds of individual forms or a single large, composite form for accessing project data across research domains. Both solutions are difficult to maintain, inflexible, and result in crowded or unfocused data presentation.

ISENTRIS promotes self-service data access and eliminates the static forms and queries that restrict scientific inquiry. Instead, auto-generated database views present data in the desired context for browsing and querying (Figures 4 and 5).

Presenting ISENTRIS to customers at a recent user conference, Dr. Dominic John of MDL Marketing stated: "It's essential for scientists in the lab to be able to just get their job done, and the software should aid them in this. Software should not be something that requires time and effort to master." ISENTRIS is an integrating discovery informatics architecture that has positive implications for project teams and research organizations alike. By bringing life scientists and information together, supporting the self-service model, and promoting a more collaborative work environment, ISENTRIS enables superior decisions and better outcomes in moving candidate compounds through the pipeline. ■

	SAMPLE_ID	PKCa_IC50	CDK2_IC50	EGFR_IC50
1	DTSM96-06462			11.166
2	DTSM96-05103			11.451
3	DTSM96-00036			11.451
4	DTSM96-07843		3.531	20.875
5	DTSM96-00154			20.875
6	DTSM96-07877			21

Figure 3: Data stored in generic tables do not have to be physically pivoted into a warehouse or data mart. Instead, ISENTRIS uses descriptive metadata to create an abstract impression of a pivoted view that is intuitive for the scientist and easy to use.

Figure 4: The ISENTRIS query builder enables scientists to build and save queries on the fly.

	STRUCURE	CORPORATE_ID	MOL_WEIGHT	SAMPLE_ID	ASSAY	IC50	HILL_SLOPE	HIT	REPORT
1		DTSM96-10149	300.265	DTSM96-10149	EGFR	7.632	1.09	N	C:\report\exampl1.xls
2		DTSM96-10136	386.311	DTSM96-10136	EGFR	26.276	1.104	N	C:\report\exampl1.xls
3		DTSM96-08532	226.23	DTSM96-08532	EGFR	3.924	1.163	N	C:\report\exampl1.xls
4		DTSM96-08432	238.198	DTSM96-08432	CDK2	419	1.476	N	C:\report\exampl1.xls
5		DTSM96-08349	376.416	DTSM96-08349	EGFR	7.949	1.311	N	C:\report\exampl1.xls
6		DTSM96-08239	510.486	DTSM96-08239	EGFR	2.127	1.689	N	C:\report\exampl1.xls

Figure 5: Once a query is created, ISENTRIS automatically generates browse forms to display the results. Scientists can add and remove fields from these forms, so that they elicit only pertinent information. They can also autonomously change the presentation of data, filter data, dynamically create tables, and cherry-pick and sort results without requiring IT assistance.

MDL® Discovery Logistics

Chemically intelligent reagent sourcing and management on the Isentris platform

With lab automation and high-throughput screening turning biopharmaceutical research into a 24/7 operation, reagent procurement and management are becoming ever more crucial aspects of a successful discovery program. It's indisputable that the efficient procurement, distribution, management, and replacement of research materials can significantly enhance the productivity of scientists, minimize research costs, and streamline discovery workflows. Although the benefits of an effective materials management system are obvious to all, getting there is not a trivial undertaking.

What are the primary logistics needs of a life sciences research organization? For the scientist, the main requirement is to be able to search and order substances in a single, easy-to-use workflow. As scientists often do not know exactly what they need at the beginning of a research project, the logistics system must support flexible searching using intuitive structure and data queries. Scientists also need easy access to online sources and integration with high-throughput tools.

IT developers need logistics workflows that are adaptable to different sites. They also want dependable, round-the-clock operation. To satisfy regulatory requirements, managers need to know the location and quantity of regulated items in the inventory. Management also needs a system that is 21CFR-11 capable, that provides EH&S information to employees, and that integrates well with other systems in the company (compound registry, purchasing, robotics, barcode equipment, etc.).

The logistics challenge

Organizations faced with building or upgrading a logistics capability can choose to build their own solution, tailor a horizontal (multi-industry) product, or go with a vertical (niche) vendor. Companies sometimes opt for in-house development because they believe it gives them greater control over functionality and because of the perceived lower costs compared to outsourcing. The anticipated lower cost of ownership rarely accrues over time, however, as IT staffs often struggle to maintain and support complex, evolving inventory systems over the long term. Additionally, companies need to question the advisability of using limited internal resources for a project that the marketplace can readily deliver, especially when the project is targeting workplace efficiency as opposed to true competitive advantage. According to Dr. Frank Schaffer, director with MDL Marketing, "most large pharmaceutical companies prefer to buy an off-the-shelf logistics system instead of building and supporting it themselves. However, the system needs to be flexible enough to fit their workflow."

Horizontal solutions tend to follow a "one-size-fits-all" model, utilizing various configuration switches or templates to tailor a generalized system for specific industries. This approach may work well when moving, for example, from the garment to the automotive industry.



But the requirements for chemical structure handling, customization, and integration in the life sciences arena are not easily addressed by configurable software and industry templates. For this reason, highly generalized, horizontal inventory systems typically fail to meet the critical biopharma requirement for a chemically intelligent, integrated, and customizable logistics solution.

The vertical vendor approach

Logistics provides a compelling test case for integration, because it typically touches more employees and departments than almost any other discovery activity—everyone from R&D and operations management through project scientists and safety officers to purchasing agents and stockroom clerks. Drug discovery logistics presents unique integration challenges that are best addressed by an expert in the field. These challenges include managing dynamic workflows, connecting structural and catalog data, and handling restricted chemicals in accordance with regulatory requirements. An industry informatics expert is better equipped than a company's in-house developers or an external, horizontal vendor to provide a focused logistics solution that gets all the details right, including the key element of chemistry functionality.

MDL has over 20 years of experience providing logistics systems to the pharmaceutical and biotech market, and today over 60 companies and approximately 7,500 scientists are using MDL logistics solutions. These numbers do not include the innumerable companies and researchers using MDL® Available Chemicals Directory. This indispensable, structure-searchable database provides supplier and pricing information for a quarter million unique chemicals and approximately one million research-

grade and bulk products from over 600 suppliers. Other MDL® logistics products include:

- **MDL® Reagent Selector**—a set of integrated tools that enables combinatorial chemists to locate and select reagents quickly using chemical queries
- **MDL® SMART**—a Web-based sample management and reagent tracking system that helps organizations manage samples through the discovery process
- **MDL® CIMS**—a consulting application for ordering and managing reagent inventories. Built on MDL® ISIS, this modular system has been in use since 1995 at both large and small biopharmaceutical facilities.

Introducing MDL® Discovery Logistics

As an experienced vendor with a proven biopharma track record, MDL is taking reagent logistics to the next level by delivering it as one of the first multi-tier applications built on the new MDL® Isestris™ architecture. Schaffer calls MDL® Discovery Logistics “an integrated materials management solution that addresses reagent identification, selection, sourcing, procurement, and disposal; ‘cradle-to-grave’ inventory management; workflow optimization; and full integration with a company’s business rules and discovery research processes.” Built on MDL® Core Interface, the Java-based, middleware component of Isestris, MDL Discovery Logistics will model and power the central inventory and procurement processes used by organizations that select, buy, manage, and dispose of chemicals.

A shopping cart will provide a familiar mechanism for managing selections from inventories, catalogs, or other collections. A powerful procurement engine will serve as a standard interface for managing inventory and procurement data, handling business rules, and interfacing to corporate purchasing systems and e-commerce sites. With business logic and workflow functionality implemented in the middle tier, as opposed to being embedded in the client application, MDL Discovery Logistics will provide an open, flexible, extensible, and scalable inventory management solution. “While the initial product release scheduled for late 2004 or early 2005 will, of course, include access to MDL® Available Chemicals Directory,” says Schaffer, “near-term plans also call for the online procurement and management of life science articles and migration to the MDL® Base desktop application. MDL Discovery Logistics will eventually combine MDL Reagent Selector, MDL SMART, and MDL CIMS functionality into a single solution.”

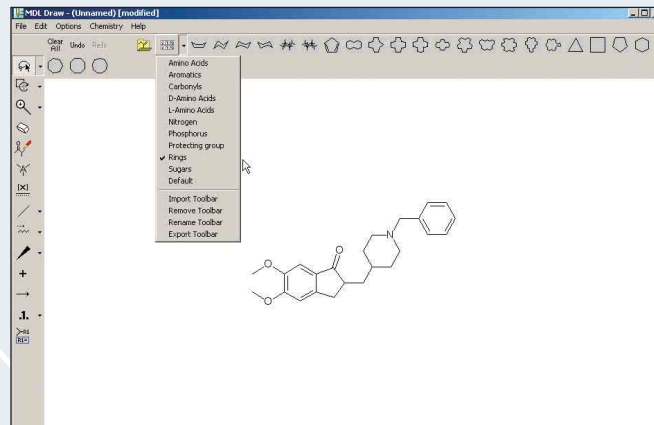
What this means for customers is time savings, as scientists are able to select and order materials and start experiments sooner using a common, integrated, enterprise-wide logistics system. Cost savings will result from up-front visibility of pricing details, including preferred suppliers and quantity discounts, and the reduction of unnecessary orders. Companies also reduce the risk of regulatory fines and workplace accidents by instituting tighter controls over hazardous/restricted materials and improving compliance with regulatory requirements.

An effective logistics solution can pay for itself in one to three years while providing significant quantifiable and qualitative benefits. MDL has leveraged its 20 years of experience in inventory management to create MDL Discovery Logistics, a complete solution for life sciences companies built on new generation technology provided by MDL Isestris.

For more information on this new materials management solution, contact your Elsevier Account Manager or submit a request for information at www.mdl.com. ■

MDL® Draw 1.2

Sharable structure templates in a .NET environment



Drawing structures is fast and easy with drag-and-drop customizable template toolbars that scientists can export to share with colleagues.

A new release of MDL® Draw offers striking enhancements that raise the standard in chemical structure drawing yet again. MDL Draw 1.2 offers developers new add-in capabilities and a Microsoft Visual Studio® .NET environment, while providing scientists with new abilities to create and import custom templates. Drawing complex structures has never been faster or easier.

The initial introduction of MDL Draw made waves with its unique all-purpose drawing tool that allows scientists to continuously draw a structure without changing tools. Now, new structure template capabilities in version 1.2 allow scientists to create countless customized templates for various chemical structures.

As scientists begin work on a new project they simply import a set of all the common structures or substructures they will be working with and place them on the MDL Draw toolbar. The drawing of complex structures is reduced to a few clicks! To extend the convenience, scientists can create multiple template toolbars and share them with colleagues.

Another aspect of MDL Draw 1.2 that will appeal to scientists is the ability to save drawn structures as images in gif, png, tif, bmp, or wmf formats.

For developers, MDL Draw 1.2 now provides all the chemical drawing capabilities that were available in the Java™ version in a .NET environment. The use of .NET means that it's now easier and faster to integrate chemical drawing into Microsoft and .NET applications. The new version is still XML-configurable, so developers can configure the chemical drawing look-and-feel according to company needs.

In addition, new add-in capability in version 1.2 boosts developers' toolkits with programming flexibility and ease. Applications like AutoNom for chemical structure naming or Cheshire scripts for structure normalization or calculations can be quickly integrated into MDL Draw and the corresponding menu items automatically appear. ■

Organon tames drug literature explosion with EMSCOPES

Customized bibliographic database solution keeps employees current, saves manpower

Research companies face a continual challenge in providing employees with access to relevant current literature. For pharmaceutical companies, the challenge isn't optional: screening scientific literature to assess regulatory compliance is a legal requirement.

Locating and organizing carefully selected, relevant drug information in a literature database is often challenging, expensive, and time-consuming. Organon, a global pharmaceutical company with operations in more than 60 countries, experienced this difficulty intimately when the volume of material handled by its in-house operation abruptly increased.

The drug literature database at Organon is handled by the Global Business Intelligence Center and Rene van den Bersselaar. "In the early years we had something like 1000 to 1500 articles indexed in our product literature database," Van den Bersselaar recalled. "But about five years ago that increased enormously—and increased year by year to such an extent that it became a consideration for us whether we should continue indexing the system in house, or look for external resources to do it for us."

Even though Organon's research focus is limited to core therapeutic fields (reproductive medicine, psychiatry, and anesthesia), the number of people required to tag, label, and index the articles related to their own or competitor compounds was growing significantly as more publications became available. Organon faced a cost-benefit decision, and Van den Bersselaar explored the options.

One alternative was an automated index system that could be loaded with full-text articles. Such systems generally pick up approximately 80% of the relevant articles. For purposes of regulatory submissions, however, a drug literature database must be

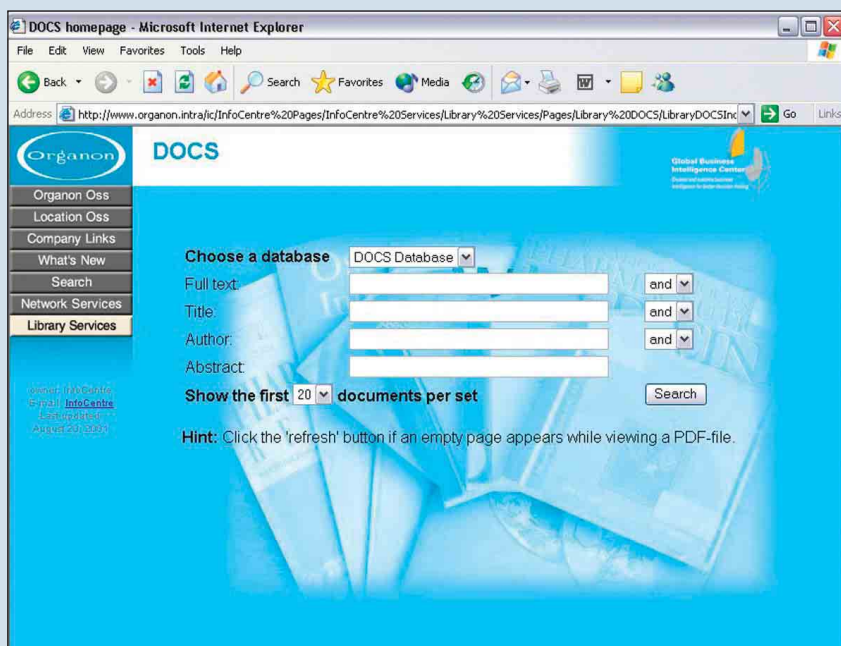
more precise. "In those days—and I believe it's still the situation—there wasn't a really good automated index system available," Van den Bersselaar said. "You introduce a degree of uncertainty with that type of system. The requirements in our company were such that we could not afford that."

Van den Bersselaar turned his attention to providers who managed the service the way Organon did it in house: with a team reading the abstract, result, and experiment sections of articles, and assigning the right indexing terms. Organon considered three candidates, including EMSCOPES, which Van den Bersselaar was familiar with but had never closely investigated. "This provided a reason to sit around the table and explore the possibilities," he said.

Bibliographic solutions

In addition to checking compliance, pharmaceutical and biotechnology companies use drug literature databases for monitoring products after launch, tracking competitor companies and drugs, and discovering novel uses for existing products. Some companies use their database when preparing new drug applications or answering customer inquiries. To address their own unique agendas, companies need access to a variety of in-house and external information sources.

Elsevier established EMSCOPES to meet the need for customized drug literature databases. Designed with a modular approach, EMSCOPES allows customers to choose which services meet their specific



Articles indexed by EMSCOPES are regularly added to the Organon literature database and made available to employees on the intranet via DOCS, the company's product literature system

needs for drug literature information. The EMSCOPES services include:

- **EMBASE™ search service** Based on a customized client profile, EMBASE (the most current biomedical database, well known for extensive global coverage of pharmaceutical research literature) is searched for relevant new abstracts, with fully indexed records sent to the customer weekly.
- **Multiple database search** Unique records from other databases, such as Thomson ISI BIOSIS® or Derwent Drug File, are added to the search, de-duplicated against the EMBASE records, re-indexed, and structured in the EMBASE record format.
- **Client submitted material** In-house material from the customer (grey literature, reports, conference material, etc.) is processed into the standard EMBASE record format.
- **Customized indexing** For clients needing a greater level of detail, customized drug-specific indexing can be added to selected abstract records, whether from EMBASE or other sources.

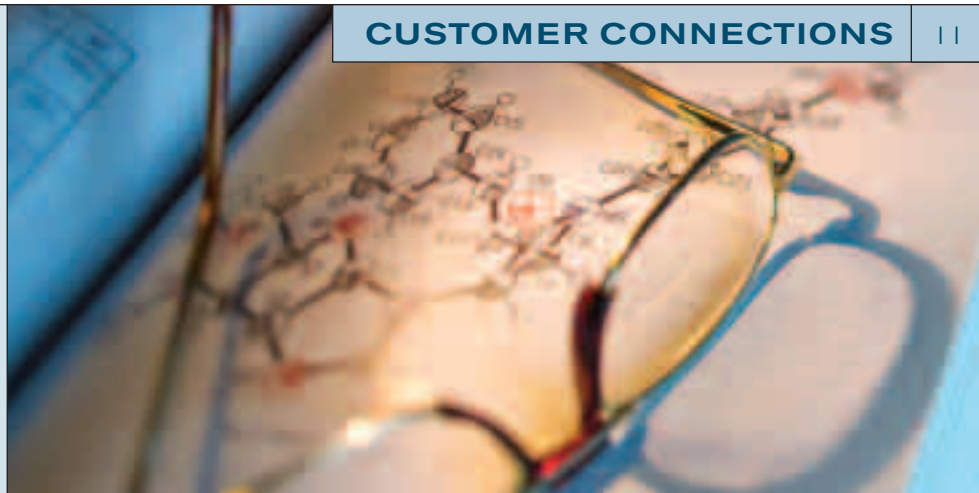
As the owner of EMBASE, Elsevier has extensive searching and indexing expertise in-house and can offer a cost-effective solution, including the most up-to-date version of EMBASE and perpetual archiving rights. All records are de-duplicated and consistently formatted, making records easy to search and yielding relevant results.

An easy transition

Van den Bersselaar was optimistic following the discussion with EMSCOPES, and Organon moved into a trial period. Soon the company adopted all of the EMSCOPES modular services.

Now indexed articles are regularly added to the company's database and made available to employees on the intranet via DOCS, the Organon product literature system. Because indexed materials are integrated into the existing system, there was no need to re-train employees.

"We were able to work together with Elsevier, with EMSCOPES, to get a formula that seamlessly transferred into our existing database," said Van den Bersselaar. "For the end users it was not really a change—it's still the same interface, still the same database. The searching and indexing is outsourced to Elsevier, but it can still be searched on the same indexing terms, because EMSCOPES



was flexible enough to deal with our precise indexing requirements."

The simplicity of the Organon product literature system makes it ideal for the broad range of users that includes regulatory affairs specialists, product managers, medical advisors, sales representatives, and researchers. The Elsevier customized indexing makes scanning the literature efficient: often the drug information that is needed is available in the customized index, so in many cases it is not necessary to consult the full text article.

"If people are not very skilled index users, they just type in the words—the product names—they are looking for, and they get the information," noted Van den Bersselaar. "People with more experience, like medical literature information specialists, can use the full depth of indexing of those articles."

Realizing benefits

After adopting EMSCOPES, Organon saw immediate improvements. "What is very clear is that we had an enormous decrease in the internal data handling and maintenance," recalled Van den Bersselaar. "With the dramatically increasing number of articles, we weren't able to deal with all the articles ourselves. So there were big savings in headcount with this system."

The benefits of migrating to a professional service weren't limited to manpower and maintenance. The EMSCOPES quality control team helped Organon set up clear, well-defined indexing rules. "Another great benefit for us is that we are able to provide a more constant quality of index articles and a more continuous feed of data," Van den Bersselaar said. "When we were doing everything in house, our indexers sometimes had their own interpretation of how an article should be indexed. With EMSCOPES we do a much better job because it is more

constant, more defined, and more explicitly described."

Van den Bersselaar summarized the overall advantage: "We suffered from the pressure to keep up to date, and to have the expertise and the backups in house in case people were not available. Those risks are now outsourced by giving EMSCOPES the responsibility to deliver indexed articles according to our needs, our definitions, and our requirements."

The next step: Literature linking

As employees search the database and find relevant articles, they will want to go to the full-text articles. To simplify that step, Organon is implementing literature-linking software from Elsevier, which can link desktop applications to full-text articles, patents, and other types of documents.

"Late last year we introduced MDL® LitLink in the CrossFire Beilstein environment, connecting the reference work to full-text journals. Now we are also linking the product literature database to our library catalog so the full-text articles can be interlinked directly within the system."

The bottom line

For Organon, the transition to EMSCOPES for the delivery of high-quality indexing of current literature has been a success. In the face of dramatically increasing numbers of articles and growing costs for maintaining the drug literature in house, outsourcing was clearly the right choice.

"If you figure in manpower or headcount, then I think the ROI is very clear," Van den Bersselaar said. "And by having a limited or calculated risk in combination with much less maintenance and manual involvement, it was very easy for me to explain to management that this was the way we had to go."■

Share your company's experiences with Elsevier solutions.
Submit an article idea at www.mdl.com/news.

Customers meet training objectives with MDL Web Workshops



"It's very, very useful. It's almost like having the teacher right there with you. I absolutely got what I needed out of the training."

*Dr. Marcos L. Sznajdman,
Norak Biosciences*

A variety of MDL customers are using innovative, hands-on Web Workshops to satisfy diverse training objectives. From biotechs to major universities, from small companies to large distributed organizations, customers are finding interactive Web Workshops to be an effective way to teach valuable skills.

What is an MDL Web Workshop? Web Workshops are a leading-edge training format that features hands-on, skill-based instruction. Superior to passive "webinars" (which are limited to listening), Web Workshops allow students to learn by doing. Interactive Web Workshop sessions are led by MDL education specialists and follow the same classroom instruction model that MDL has proven in countless iterations worldwide.

The convenience of scheduling Web Workshops makes them ideal for reaching dispersed audiences and delivering focused content in shorter sessions. This flexibility allows organizations to use the training in the way that best meets their needs. For example, the University of Arkansas recently gathered a dozen students for a group-training Web Workshop on CrossFire Beilstein and CrossFire Web organized by Physics and Chemistry Librarian Usha Gupta.

"We opted to train undergraduate chemistry majors...to expose them to Beilstein early because it is useful in completing class assignments," said Gupta. "The Web Workshop enabled us to train students in a relatively cost-effective, hands-on forum where experts could answer their questions. The MDL trainers did an excellent job. They even worked some examples we sent them into the Workshop, which was especially helpful for the participants."

Another university system used a "train-the-trainer" approach, thereby avoiding the expense of bringing people together from outlying locations. Key participants at different sites took part in a single Web Workshop before they trained other students and faculty at their respective campuses.

In a recent case, a scientist at a Research Triangle Park, NC biotech company found that a one-on-one Web Workshop offered the best way for him to get up to speed quickly on DiscoveryGate®.

Dr. Marcos L. Sznajdman is the associate director of chemistry at Norak Biosciences, a privately held company that is becoming a world leader in the discovery and development of drugs that regulate G protein-coupled receptors (GPCRs). "I was the only person from this company taking that class," Sznajdman said. "If we had 15 or 20 people to train, like in big companies, then bringing a person here would make sense, but for one person I think the MDL Web Workshop was the best format."

Sznajdman was initially attracted to the convenience of the format: "I liked the flexibility of the Web Workshop, and the fact that it only took two hours was great for my schedule."

In the end, however, the quality of training made the strongest impression. "I think it's very effective because you have hands-on training and you can also see what the teacher is doing at the same time," Sznajdman said. "It's very, very useful. It's almost like having the teacher right there with you. I absolutely got what I needed out of the training."

That the workshops are highly effective is no surprise to Peg Renery, the director of educational services at MDL. "We modeled the Web Workshops on the same principles as classroom training," Renery said. "It's a three-step process: Tell me, show me, let me do."

With participants at workstations, actively participating in the lesson, the Workshops are an effective means of distributing knowledge and skills. "This type of hands-on learning duplicates the best elements of classroom training and delivers comparable success," said Renery. "It's the next best thing to classroom training."

For more information on MDL training programs or Web Workshops, contact your Account Manager or Peg Renery (p.renery@mdl.com, 1 800-955-0051 ext. 1377). See page 15 for a list of upcoming Web Workshops. ■

Elsevier's *Current Opinion* and *Trends*

Required reading for life sciences researchers

Molecular Connection asked Claire Moulton, publishing manager of *Current Trends* Editorial, to provide an overview of the Elsevier *Current Opinion* and *Trends* journals. Anthony Li of the editorial team produced the following summary.

From plant biology to immunology and pharmacology, the review-based *Current Opinion* and *Trends* journals keep readers abreast of the latest developments in their fields. Each review summarizes the work of numerous primary papers, removing the need to trawl through reams of primary literature, and their easy-to-read format means that they are accessible to a wide audience.

Since the launch of the first *Trends* journal in 1976, the series has expanded to 14 *Trends* and 10 *Current Opinion* titles. This growth has been accompanied by increasing popularity and rate of citation in the life sciences. The success of both series continues online and the journals now also boast high levels of readership within ScienceDirect®, Elsevier's electronic compilation of science, technology, and medical full-text and bibliographic information.

Current Opinion and *Trends* journals bring informative, well-illustrated review articles to the life sciences researcher, but there are some characteristic differences between the two series.

The *Current Opinion* format

The bi-monthly *Current Opinion* journals constitute a series of themed issues, covering the field systematically over the course of a year. In essence, this means that each area is given its own special issue every year, and the editors ensure that the themed sections continue to be relevant and important.

Each themed issue is headed by prestigious guest editors, who are chosen for their expertise within the subject area and are positioned to suggest hot topics and identify suitable field leaders as authors. For example, Nobel Laureate Peter Doherty recently co-edited a section on host-pathogen interactions for *Current Opinion in Immunology*.

The reviews themselves concentrate on recent research in rapidly progressing or emerging areas where findings are set in the context of the whole field. The reference lists include recommended reading, directing readers to primary papers of particular interest.

A typical *Trends* journal

Trends journals are published monthly. They focus on reviews but also feature two other types of main article—the opinion and research focus. An opinion represents a personal viewpoint on a research-related topic with the aim of stimulating debate. Research focus articles report on exciting topics that have just hit the primary literature, with an emphasis on the importance of the paper within the context of the field.

Trends review articles are lively and topical, but have also been through peer review to ensure a balanced representation of the literature. Careful editing enhances accessibility to the non-specialist without compromising depth or quality for the specialist.

In April 2004, *Trends in Pharmacological Sciences* celebrated its 25th year as the top monthly review journal in toxicology and pharmacology. The special anniversary issue looked at topics including the potential for personalized medicine 51 years after the structure of DNA was solved and asked whether technological advances are improving the drug discovery process.

This year, *Trends in Biotechnology* will review a broad range of subjects, from the immunogenicity of human embryonic stem cells to the application of RNAi in improving the nutritional value of plants. ■



Current Opinion in

- *Biotechnology*
- *Cell Biology*
- *Chemical Biology*
- *Genetics & Development*
- *Immunology*
- *Microbiology*
- *Neurobiology*
- *Pharmacology*
- *Plant Biology*
- *Structural Biology*



Current Trends in

- *Biochemical Sciences*
- *Biotechnology*
- *Cell Biology*
- *Cognitive Sciences*
- *Ecology & Evolution*
- *Endocrinology & Metabolism*
- *Genetics*
- *Immunology*
- *Microbiology*
- *Molecular Medicine*
- *Neurosciences*
- *Parasitology*
- *Pharmacological Sciences*
- *Plant Science*

Lars Barfod new CEO; Bernard Aleva to S&T Board

This summer MDL offered a fond farewell to one chief executive while welcoming a familiar figure into this key position.

Bernard Aleva, who has been president and CEO since July 2003, has left MDL to assume the position of Managing Director of Engineering with Elsevier's Science and Technology (S&T) Division. Effective July 1, 2004, Bernard joined the S&T Board with responsibility for Elsevier's global Engineering businesses.

Arie Jongejan, CEO of the S&T Division, was effusive in his praise of Bernard's accomplishments during his three years in the US, first as CEO of Elsevier Engineering Information in Hoboken, New Jersey and during the past year as CEO of MDL. "(Bernard) has been instrumental in bringing these businesses closer to the overall Elsevier organization and in focusing the companies' business strategies. Now I'm very pleased to have him join my S&T team and look forward to working with him to expand Elsevier's Engineering businesses."

Lars Barfod has succeeded Bernard as president and CEO of MDL. Since joining MDL in March 2001, Lars has been executive vice president and chief business officer, most recently heading up Elsevier's global life sciences business organization.

Martin Tanke, managing director of life sciences, said: "Lars has played a key role in shaping MDL's marketing and sales strategies and has been responsible for the formation of a unified life sciences business organization. His industry knowledge and expertise in business and organizational development will be enormous assets to MDL and Elsevier's life sciences management team."

Addressing the company in San Leandro, Lars stressed that the executive reassignments do not imply any change in strategy with regard to MDL or Elsevier's life sciences offerings. "The focus we've



(Left to right) MDL President and CEO Lars Barfod; Elsevier Managing Director of Life Sciences Martin Tanke; Elsevier Managing Director of Engineering Bernard Aleva

established, the rollout of MDL® Isentris™, and the applications on top of that—all those things are unchanged... We remain committed to bringing innovative, robust MDL informatics and workflow solutions to customers, along with Elsevier's comprehensive life sciences offerings."

Jean Colombel has been appointed Senior Vice President of Life Sciences Sales & Services, replacing Lars in that position. Jean came to MDL in 1991 and has held several positions in Sales and Consulting management, including Vice President, European Business. Since 2003, he has served as Vice President, Global Corporate Business, Life Sciences. ■

User meetings get high marks

Customers gather in London, Seville, and Boston

MDL customers from around the world gathered this year for meetings to share experiences, discuss ideas, and learn about new solutions and upcoming offerings. This spring over 60 European customers from more than 30 companies gathered in London and in Seville, Spain for the UK and European user group meetings. More recently, 100 attendees from 60 companies assembled for the U.S. conference in Boston. An additional meeting is set for the Japanese user group in Tokyo, September 8-10.

The conference agendas were designed to give people a chance to meet in focused, interactive sessions with others who shared their interests. "One aspect of the user meetings that I most enjoy is the opportunity to engage in discussion with other people who are confronting similar challenges," said U.S. Steering Committee Chairman Rich Lawson of AstraZeneca. "It gives people a chance to exchange ideas and learn what approaches work and—sometimes just as usefully—what doesn't work."

Among the specialized offerings were a technical exchange for "gearheads" to share informatics tips, a panel discussion for librarians on meeting the needs of patrons, a small business forum for companies with limited IT budgets, and a session on handling large molecules and biopolymers.

For many people, the meetings provided a chance to see new MDL technology in action. In Boston, the MDL® Isentris session, featuring

(continued on next page)

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a live demonstration of the new MDL® Base desktop application, drew standing-room-only crowds as people clamored for a firsthand look at the immense power of ISENTRIS (see stories, pages 3-9).

Coordinated with the conference, MDL offered a technical training course for application developers to familiarize themselves with ISENTRIS capabilities. "I found the ISENTRIS training class quite stimulating," said Steven Dietrich of Molecular Computing Systems, Inc., one of the many developers and system designers who benefited from the hands-on experience.

The Boston conference once again featured an Integration Showcase, allowing attendees to converse with vendors offering complementary technologies or services. Participating companies included Deltasoft, Inpharmatica, Intellichem, Kelaroo, Partek, and Scientific Software.

"This was the best conference in a number of years," added Dietrich. "The talks were interesting, the keynote speakers were stimulating... The conference truly was great this year." ■

**"This was
the best
conference in a
number of years."**

Steven Dietrich
Molecular Computing
Systems, Inc.

Mark your calendars!

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Boston, MA, August 8-12

Booth 2204—**Don't miss the launch of MDL® ISENTRIS™!**

ACS 228th NATIONAL MEETING

Philadelphia, PA, August 23-25

Booth 302

ISSX 2004

Vancouver, BC, August 29-September 2

Booth 217

JAPANESE USER GROUP MEETING

Tokyo, Japan, September 8-10

For information, contact Keiko Ogita (k.ogita@mdl.com)

SOCIETY FOR BIOMOLECULAR SCREENING

Orlando, FL, September 11-15

Booth 800

R&D LEADERS' FORUM

Geneva, Switzerland, October 4-6

ONLINE INFORMATION

London, UK, November 30-December 2

For more details, go to www.mdl.com. Click on **Company Info** and **Events**.

Developer and Administrator Classes

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MDL® Cheshire

Hview Design, Development, and Optimization

Application Development with MDL® Core Interface

Application Development with MDL® Direct

Application Development with MDL® ISIS

Application Development with MDL® ISIS Object Library

MDL® ISIS/Host Administration

MDL® Plate Manager Administration

For scheduling and registration information, contact Hannah Kauffman at 800-401-4321, ext. 2107 (h.kauffman@mdl.com) in the U.S. and François Culot at +33-1-45-36-80-23 (f.culot@mdl.com) in Europe.

MDL Web Workshop Schedule

MDL offers two-hour, interactive Web Workshops for small groups of up to eight participants. These focused sessions will quickly bring you up to speed with the MDL products listed below.

For general information on the Web Workshops including topic descriptions, or to register for a scheduled event, contact Veronica Zuniga at edservices@mdl.com or 800-955-0051, ext. 1326.

To schedule special sessions of any of the workshops below (which can be offered on different dates or limited to participants at your site alone), or to arrange custom workshops on topics of your own choosing, contact your Elsevier Account Manager or Peg Renery at p.renery@mdl.com or 800-955-0051, ext. 1377.

For more information on MDL training programs, click on **Education** at www.mdl.com.

Date	AM SESSION (09:00-11:00 Eastern Time)	PM SESSION (13:00-15:00 Eastern Time)
Aug 10	Drawing structure queries with MDL® Draw	Exploring Integrated Major Reference Works™
Aug 11	Locating compounds in DiscoveryGate®	Reaction searching in CrossFire Beilstein using DiscoveryGate®
Sep 13	Transition to MDL® CrossFire Commander 7.0	Transition to MDL® CrossFire Commander 7.0
Sep 14	MDL® ISIS for Excel for the current ISIS user	Creating reports with MDL® Report Manager
Oct 5	MDL® ISIS for Excel for the current ISIS user	Creating reports with MDL® Report Manager
Oct 6	Exploring DiscoveryGate®	Exploring DiscoveryGate®
Nov 9	Transition to MDL® CrossFire Commander 7.0	Transition to MDL® CrossFire Commander 7.0
Nov 10	Transition to MDL® CrossFire Commander 7.0	Exploring MDL® Metabolite and MDL® Toxicity Databases
Dec 7	Drawing basics in DiscoveryGate®	Structure searching in CrossFire Beilstein
Dec 8	Drawing structure queries with MDL® Draw	Exploring Integrated Major Reference Works™

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discovery and
informatics meet*

MDL Isestris brings true integration to discovery and empowers productivity by providing:

- A research environment that supports business process, data, and workflow integration
- Self-service access to integrated discovery data
- New pioneering methods for reducing data complexity
- An open, standards-based platform for application development

MDL is demonstrating Isestris at Drug Discovery Technology in Boston, August 8-12, 2004. Learn about improving access to chemistry and biology data and building discovery applications by attending the Isestris workshop, "Empowering Discovery Informatics," at 12:15 pm to 1:00 pm on Monday, August 9, or visit booth 2204 for more information on MDL Isestris.



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