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*Discovery Partners  
International*

Saving time with  
MDL<sup>®</sup> Report Manager

*Speedel Experimenta and MDL<sup>®</sup> Select*  
Streamlining workflows in a start-up lab

*DiscoveryGate<sup>SM</sup> for academia*  
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*MDL<sup>®</sup> Plate Manager*  
Accelerating biology workflows

*MDL<sup>®</sup> Open Library*  
Optimizing the value of  
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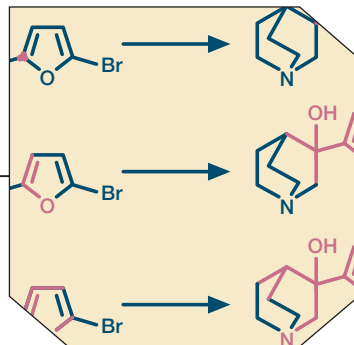
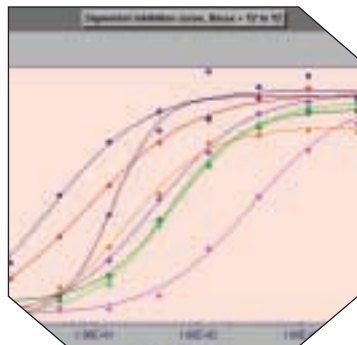


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# C M O L E C U L A R N E W S M A G A Z I N E

2004 • Vol 22 No 2



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Cover image courtesy of Discovery Partners International. DPI offers integrated services, products, and systems spanning the drug discovery continuum.

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*John McCarthy, director of Global Corporate Consulting*



*Aleksandar Ruzicic, director of Global BioPharma Consulting*

*MDL pre-sales support and consulting are now consolidated into two groups. Global Corporate Consulting, under the direction of John McCarthy, focuses on defining and delivering informatics solutions for MDL's largest corporate customers. Global BioPharma Consulting, under the direction of Aleksandar Ruzicic, concentrates on all other life science customers and prospects worldwide (with the exception of Japan and South Korea). Molecular Connection talked to John and Aleks about how their organizations will help customers take full advantage of the latest discovery informatics strategies.*

## John McCarthy and Aleksandar Ruzicic

### Delivering integrated discovery informatics strategies

#### What is the particular focus of Global Corporate Consulting?

**John:** Our group focuses on delivering global projects to large pharmaceutical companies with worldwide operations. We help large enterprises analyze their current R&D information systems, assist with developing new strategic concepts for global applications, and offer integrated solutions. MDL® Isentris™, the next-generation, three-tier discovery informatics architecture from MDL, is the platform on which we're building this new integrated approach to discovery informatics.

My team is heavily involved in transitioning global clients to the Isentris platform. This entails understanding each client's specific informatics needs and developing, with the client, appropriate application and system transition strategies to ensure that they get the greatest value from Isentris as they come on board. After analyzing the systems and architectures currently in place, we help clients assess what informatics projects they should take on—and when and how they should implement projects to take full advantage of Isentris.

Technology integration is the bottom line in everything we do, and this goes beyond a consideration of data alone to include a company's underlying business processes and the workflow applications used by scientists. By leveraging the metadata that customers collect—the data about their data—we can set up systems that help scientists “self-serve” when it comes to accessing data. Instead of relying on data specialists, scientists can use MDL integration technology to access the data they need, thereby accelerating and streamlining their workflows.

To assist in delivering globally- and regionally-based integration projects, the Corporate

Consulting team has representatives in both Europe and the United States. While speaking local languages and supporting local evaluations, we do concentrate on the global picture, however, because that is the primary perspective of our customer base.

#### What is the focus of Global BioPharma Consulting?

**Aleks:** Our clients are the biotechnology companies that use recombinant genetic engineering to develop products and the biopharmas that are using biology and chemistry together to develop products for human therapeutics, diagnostics, drug delivery, and cell and gene therapy. Our customers encompass many diverse market segments, including drug developers, Contract Research Organizations, HTS/combichem companies, and proteomics/genomics specialists.

We support customers worldwide, excepting only MDL's largest corporate customers (which are the responsibility of John's group) and customers in Japan and South Korea (where MDL Information Systems Japan KK offers full sales and service support). Our customers range from large, global enterprises through small to mid-sized companies, all the way to the smallest start-ups. The needs of our larger clients are similar to those of John's group, obviously with somewhat less complexity, because the companies we serve may not have such extensive global operations. Our smaller customers, on the other hand, tend to have distinct requirements. They typically want out-of-the-box solutions, very well integrated across all their research informatics needs, and the ability to deploy new technology quickly and to measure immediate productivity improvements.

*(continued on page 4)*

(continued from page 3)

To meet these objectives, we have teams in Europe and the United States that deliver both small, local projects and larger international projects across multiple sites with the same responsiveness, attention to detail, and reliance on high industry-standard practices.

### Why has MDL brought pre-sales and consulting into the Global Corporate and BioPharma Business groups?

**John:** To deliver successful integration projects, it's essential to present a consistent face to the customer during initial discussions, requirements gathering, solution design, and all the way through to implementation, testing, and training, whether the final project is a highly customized system or the simple installation and configuration of out-of-the-box software.

**Aleks:** Right... this unified approach helps MDL consultants to focus on and understand the unique technical and business needs of each customer—and to build a stronger relationship with the customer, in tandem with the Account Manager in charge. This continuity is critical to the accomplishment of yet another ongoing goal, which is to optimize the benefits customers receive from our products. We want scientists and developers alike to make better use of our products internally. By consolidating our technical experts into a single customer-facing organization, we gain a much better understanding of customers' needs, ensure smooth project implementations, and help customers identify effective ways to measure the value of their new systems on an ongoing basis.

**John:** Customers migrating to ISENTRIS will benefit from this enhanced relationship management team and the expanded technical advisory role it fosters. The most important aspect of any transition is implementing the new technology and eliminating old systems in as non-disruptive a manner as possible. The answer to each organization's transition puzzle depends on its unique structure and needs—and MDL consultants are much better equipped to assess and address these items by virtue of our unified organization.

**Aleks:** For mid-size and smaller customers, our new, integrated organization will also help us better understand our customers' needs

for out-of-the-box solutions. For example, MDL® ChemBio AE was originally a consulting application, which we developed in direct response to customer needs for storing and retrieving chemical and biological data. We'll continue bringing solutions like this to market in the future.

### What are the key products driving MDL informatics solutions for both your groups?

**John:** MDL ISENTRIS is a crucial component of the discovery informatics strategy we are recommending for MDL's largest corporate customers. This technology is poised to take discovery informatics to the next level, and my team is eagerly awaiting the launch of the MDL® Base desktop application, which will complete the ISENTRIS offering this year. We're also very interested in helping customers make better use of DiscoveryGate<sup>SM</sup>, the Web-based discovery environment from MDL. Our focus here is to make sure that the right people have access to the right data on DiscoveryGate, to ensure that research scientists are getting full value from this continually expanding and diversifying resource. Finally, we're also looking closely at developing synergies with other Elsevier products and technologies for the life science market. All of our customers depend on the primary scientific journals in their research, and Elsevier's ScienceDirect® digital library, EMBASE™ bibliographic database, and tailored EMSCOPES service can greatly enhance access to these critical resources.

**Aleks:** The biology solutions offered by the BioPharma group are particularly flexible, enabling customers to implement a wide range of assays, from high-throughput *in vitro* screening to highly complex and less standardized *in vivo* experiments. For example, MDL® Select offers an integrated workflow solution for smaller companies, which can include MDL ChemBio AE for chemistry registration, MDL® Plate Manager, and MDL® Assay Explorer with its new Partek statistical visualization tool. Our mid-sized customers have already started migrating to the ISENTRIS technology. Actually, one of our largest ISENTRIS-based consulting projects is with a biopharma customer that is leveraging the power of the MDL chemistry registration domain service (*Molecular Connection*, Vol. 22, No. 1, pg. 7). Customers also appreciate the advantages of our hosted

DiscoveryGate solution for accessing MDL® Available Chemicals Directory, the CrossFire Beilstein database, ChemInform Reaction Library, and the MDL® Metabolite and Toxicity Databases, to name just a few content products. They welcome the reduced need for equipment and IT support for constant database, software, and operating system upgrades, but are even more interested in improving productivity, making better decisions, and shortening discovery timelines. MDL consultants can assist all our customers in building informatics infrastructures that manage data and discovery workflows optimally, using high industry-standard practices. Working with MDL colleagues in Educational Services, we also ensure that scientists are fully trained, which is a critical success factor when rolling out information technology that affects day-to-day routines. (For more on this, see the article on MDL® Open Library on page 14 of this issue.)

### What differentiates the solutions provided by your teams from those offered by other informatics providers?

**Aleks:** MDL and Elsevier provide a breadth of discovery informatics capabilities and a depth of experience that is unmatched in the industry. Collectively, our consultants offer many hundreds of years of experience in an industry that essentially began with the founding of MDL just over twenty-five years ago. Today we offer virtually everything a life sciences company needs to build an effective, integrated discovery operation, from underlying informatics infrastructure through scientific content to advanced experiment management and predictive science applications.

**John:** Combining MDL's expertise in capturing in-house experimental data with Elsevier's ability to deliver public information is really quite a unique advantage that no other company provides. The goal of ISENTRIS is to bring these two key data sources to scientists in a unified way by fostering an integrated approach to content, applications, and technologies. Our consulting teams tap the wealth of a large and diverse organization to bring the most comprehensive solutions to customers—solutions based on MDL's proven expertise in discovery informatics, on Elsevier's abundant scientific content resources, and on powerful, integrated third-party technologies. ■

## Speedel Experimenta accelerates discovery with MDL solutions

*“Our experience is that MDL software is very easy to use... Because of the flexibility of the ISIS product, we’ve been able to build in a lot of useful customization...”*

*Robert Mah, senior scientific expert, Speedel Experimenta*

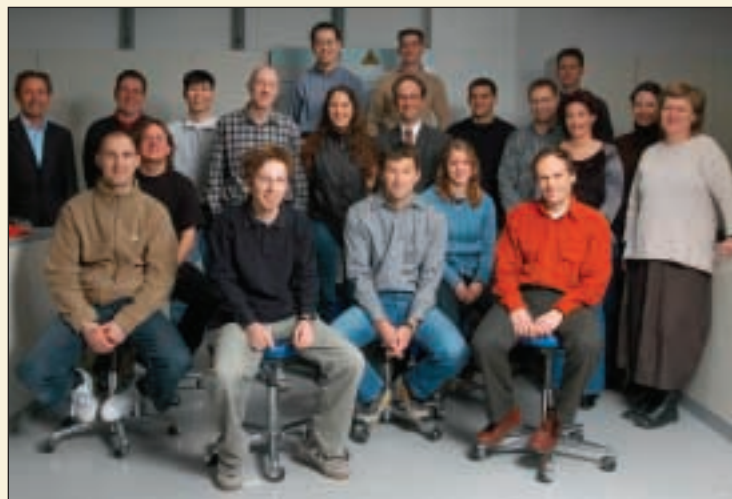
**B**iopharma companies—especially start-up and small-to-medium enterprises—are driven by cutting-edge science and technology, but many lack the deep informatics infrastructure required to power their R&D needs. A customized information and experiment management solution is critical to the success of these companies. MDL® Select is a flexible suite of products and services for managing discovery workflows and a great value for biopharmas that need to get up and running quickly.

One company benefiting from this tailored solution is Speedel Experimenta AG, the medicinal chemistry research unit of the Speedel Group. Founded in 1998 in Basel, Switzerland, Speedel is a biopharmaceutical company with a predominant focus on cardiovascular and metabolic diseases. The company is already a world-leader in the development of renin inhibitors.

“Speedel Experimenta AG was created in 2002 to support the Speedel Group in the areas of medicinal chemistry, pharmacology, and galenical formulation,” says Nick Miles, director of communications and investor relations for the Speedel Group. “We now have approximately 20 scientists and technicians optimizing the synthesis of development compounds.”

Speedel Experimenta selected MDL® ISIS as the underlying informatics environment for representing and searching chemical structures, reactions, and 3D models. For ordering and inventory of chemicals, Speedel's scientists use MDL® Available Chemicals Directory and MDL® CIMS, a chemical inventory management system developed by MDL consultants. They use MDL® Reaction Browser for reaction searching and a number of MDL synthetic methodology databases for selecting and evaluating synthetic methods. Speedel scientists also use an electronic lab notebook built on the MDL® ISIS/Base desktop application.

Robert Mah, senior scientific expert, explains that Speedel opted for MDL technology “because we wanted a single solution, and many of our scientists were familiar with MDL products from their previous jobs at major pharmaceutical companies.” Hitting the ground running was a



*Speedel Experimenta team members rely on MDL solutions in their daily efforts to optimize synthetic routes and pharmacologically active molecules.*

top priority for Speedel Experimenta as they established their new, state-of-the-art lab in the Allschwil Innovation Center. “Since our lab is located very close to MDL’s Allschwil office, we simply dropped our hardware off, and MDL technicians quickly installed all the products, including the necessary Oracle® software. As well as training us in the optimal use of the system, MDL was very helpful in fine-tuning the system to archive products and commercial reagents and transfer data between the lab notebooks and CIMS.”

MDL products play a critical role at every stage of the discovery process at Speedel Experimenta. Scientists begin by brainstorming for new molecules and approaches to cardiovascular therapies, capturing new ideas in MDL ISIS/Base. After the modeler has prioritized the ideas, the most pressing targets are assigned to individual chemists who consult reaction databases like ChemInform Reaction Library, which provides information about new synthetic methods, and ORGSYN, which covers proven compound preparations. They turn next to MDL Available Chemicals Directory and CIMS to assess the availability of building blocks and starting materials.

Speedel scientists document ongoing experiments in their MDL electronic lab notebooks and transfer new product information into another ISIS database. After compound testing, the scientists record the biological and chemical results in the same database, so that all structure and associated information is together in one place, ready for yet another brainstorming session that completes the discovery cycle—and frequently launches another one. ■

*“Technology like MDL’s that helps us accelerate and better manage research workflows is crucial in reliably demonstrating the safety and efficacy of drugs.”*

*Nick Miles, director of communications, Speedel Group, [www.speedelpharma.com](http://www.speedelpharma.com)*

# Discovery Partners International

## Charting success after success with MDL<sup>®</sup> Report Manager

### **D** DISCOVERY PARTNERS INTERNATIONAL

DPI (NASDAQ: DPIL) offers integrated services, products, and systems that span the drug discovery continuum, including target characterization, targeted and screening-library design and synthesis, high-throughput and high-content screening, lead generation and optimization, gene expression analysis, and protein crystallization.

The company is headquartered in San Diego, California and has operations in the United States, Europe, and Japan.

Tel: (858) 455-8600

[www.discoverypartners.com](http://www.discoverypartners.com)

As an active player in the drug discovery market, Discovery Partners International, Inc. (DPI) has contributed to dozens of successful collaborations, complementing the internal capabilities of pharmaceutical and biopharmaceutical companies.

To maintain its position as a leading drug discovery company, DPI continually seeks to improve efficiency and better deliver collaborative solutions for customers. At its South San Francisco location, the company's Discovery Chemistry unit (formerly ChemRx) recently employed MDL<sup>®</sup> Report Manager to cut hours and even days from the time required to prepare detailed reports for customers.

Paul Barnes is a quality assurance associate for the Discovery Chemistry unit. The unit delivers custom, novel libraries of drug-like compounds to pharma and biotech companies. "Apart from delivering compounds to our clients, we also provide detailed synthesis protocols in Microsoft

Word format," says Barnes. "The protocol reports enable our clients to reproduce the compounds in their own laboratories."

The majority of the compounds are made in a combinatorial fashion, with building blocks added to rows and columns of 96-well plates. The synthesis protocol contains a plate scheme and building blocks listed in the order they are put in the plates. The building block information is placed in a Microsoft Word table that contains not only the name and structure for each compound, but also the "ACD" number (from MDL<sup>®</sup> Available Chemicals Directory), the molecular weight, and the weight of compounds used in the reaction (see Figure 1).

#### Fast, error-free reporting

Recently DPI began using MDL Report Manager to automate the generation of these tables.

"Before employing Report Manager, we created the tables by hand," says Barnes. "Since each table can have up to 200 building blocks, not only was creating the tables very time-consuming, but it allowed the possibility of introducing errors into the tables."

Report Manager allows researchers to rapidly produce a wide range of preformatted reports including data and live structures from multiple databases. Using Report Manager, chemists at DPI are able to submit a list of numbers to the Available Chemicals Directory database, and obtain a list of building blocks to complete the synthesis protocols for customers.

"Now, not only is the table 100% accurate," says Barnes, "but what once required up to several hours to generate only requires a minute or two."

Barnes customized the report output so that the building block lists are printed in a pre-determined order and product names are formatted to the company's specifications.

"We created a fairly simple macro to convert the output to the standard format we include in synthesis protocols," he says.

#### Making chemists happy

The training process on the new system was simple, according to Barnes. "I set up a



*DPI production chemists transfer solutions to 96-well microtiter plates. The company offers integrated services, products, and systems spanning the drug discovery continuum. DPI's Discovery Chemistry unit in South San Francisco recently accelerated its production of synthesis protocol and scaffold documentation using MDL Report Manager.*

*“[Report Manager] has saved Ph.D. level chemists and other chemists in our company hundreds, and maybe thousands, of hours of work in the past year alone. I wouldn’t be surprised if the ROI is 100 times the purchase price of Report Manager.”*

*Paul Barnes, quality assurance associate, DPI*

demonstration for the development chemists at their department meeting, passed out a page or two of written instructions, and made myself available to answer their questions whenever they needed help,” he says. “The chemists were able to learn quickly and I didn’t have to provide very much support after the initial training.”

How has the new process been received by researchers at DPI? “Incredibly well,” says Barnes. “They were very receptive to it because it saved them tons of time, it was quick and easy to access, and the information obtained from Report Manager was error-free.”

#### Compounding benefits

Once Report Manager became a hit, Barnes created another time-saving application, this time for the production of scaffold tables in synthesis protocol reports (see Figure 2). “These tables have between 48 and 150 entries,” Barnes says. “Again, our chemists were generating these tables by hand.”


“The structures and all other information in the table are generated by our informatics group when they enumerate a library. However, the output from informatics is in Microsoft Excel. I was able to use Report Manager to achieve the desired output in Microsoft Word.”

In the case of the scaffold tables, DPI chemists saw an even larger efficiency gain with Report Manager, according to Barnes. “The time savings with the automation of creating scaffold tables was immense. What was once taking hours and even days is now accomplished in under 5 minutes.”

#### Beyond time savings

In addition to the efficiencies mentioned above, Barnes points to other benefits of Report Manager’s automation of reporting at DPI: “Scaffold tables that are error-free eliminate downstream errors that existed when tables were made by hand. Error-free tables save informatics, development, production, and QA many hours of troubleshooting and can save the company from costly mistakes.”

As chemists at DPI realized the advantages of using Report Manager, they began using

Entry No.	ACD No.	Name	Structure	MW	Amount (g)
1	5249	Pyrrolidine		71.1	.75

*Figure 1: The synthesis protocols that DPI provides to customers can have up to 200 building blocks. The adoption of MDL Report Manager has fully automated production of the report, eliminating countless hours of chemist production and the possibility of errors.*

it in more situations. “Chemists ended up using Report Manager not just twice, but rather several times per project,” Barnes says. “They got into the habit of using Report Manager since it was easy to use, reliable, and gave them the information they needed.”

No.	DPI Lot No.	Building Block ACD Nos.	Structure	MW	Amt. (g)
1	5152-XYZ-94	6931 1301 5926	Proprietary	289.14	19.88

*Figure 2: A typical excerpt from a DPI scaffold table communicates to clients the building block ACD numbers, structure, molecular weight, and amount of scaffold compounds incorporated in the reactions. Report Manager now generates the tables automatically.*

#### Return on investment

All of this has amounted to a boon for both Barnes and DPI. Though the company hasn’t specifically calculated a return on investment (ROI), Barnes estimates the figure to be high.

“[Report Manager] has saved Ph.D. level chemists and other chemists in our company hundreds, and maybe thousands, of hours of work in the past year alone,” he says. “I wouldn’t be surprised if the ROI is 100 times the purchase price of Report Manager.”

More importantly, “our chemists can spend more time doing what they are paid to do, instead of generating paperwork.”

As for Barnes, the benefits are personal. “I am able to trust that information generated by Report Manager is error-free and I don’t have to spend as much time reviewing and troubleshooting documents,” he says. On top of that, Barnes received three employee recognition awards in 2003 for his successes with Report Manager. ■

#### The information you need, quickly

MDL Report Manager is an easy-to-configure reporting tool that uses MDL® ISIS chemical structure searching and live structure reporting to integrate and extract data from multiple databases into prefformatted reports.

The latest release features capabilities that make corporate-wide reporting even easier, including Web reporting, curve fitting for biologists, and PowerPoint reporting.

Share your company's experiences with MDL solutions.  
Submit an article idea at [www.mdl.com/news](http://www.mdl.com/news).

# Accelerating biology workflows: Coordinating dose-response testing with MDL® Plate Manager

The dynamic, collaborative nature of the discovery process makes effective communication and project management integral to success.

In lead generation workflows, research teams must often coordinate iterative processes that involve scientists of different disciplines working from remote locations. Chemists submit compounds to be plated and tested by biologists, who in turn request active compounds to be replated for dose response studies. Inventory scientists, meanwhile, ensure the quality of the library, store the plates and samples, and make them available to biologists. Throughout, researchers feel the ever-present burden to accelerate discovery.

How can project teams minimize the time between the chemists' sample registration and biologists' assay testing, accurately track sample histories, and maintain sufficient availability of compounds at all times? MDL® Plate Manager offers a solution that systemizes the record keeping, communication, and processes that are vital to this collaborative workflow environment.

Plate Manager is a central repository for plate and sample information that integrates with MDL data management and chemical registration tools. It provides comprehensive sample and container management to accommodate varying workflows and the specific needs of IT managers.

The following case study examines the workflow of requesting active samples to be plated for dose response studies, and illustrates how Plate Manager and the biological data management system MDL® Assay Explorer provide an integrated solution that saves researchers' time, protects integrity of samples, and provides teams the best opportunity for successful discovery.

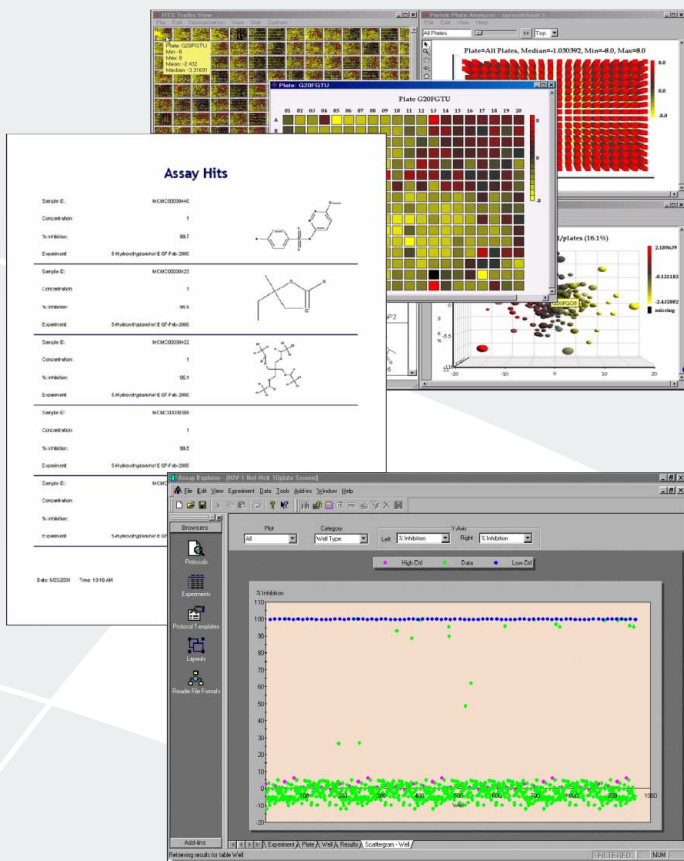


Figure 1: Biologists easily identify compounds meeting specified criteria in assays by using visualization features in Assay Explorer.

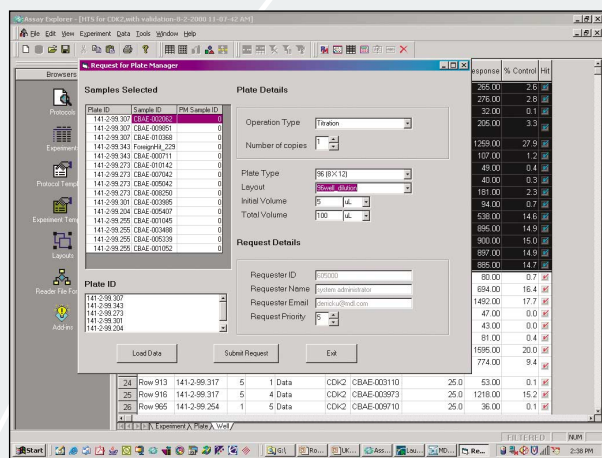


Figure 2: A biologist can initiate the replating of compounds for a dose response test by selecting active compounds in Assay Explorer and clicking a button; once completed, the request is sent directly to the inventory scientist.

## A workflow solution

MDL Plate Manager is part of a complete experiment management solution for chemistry and biology workflows. Plate Manager integrates with MDL® ChemBio AE for compound registration and chemical information storage, MDL Assay Explorer for managing biological data including *in vivo* data, and MDL® Report Manager for comprehensive reporting of research data.

Using Plate Manager, scientists can perform management tasks from their desktop, including:

- Importing plates and samples
- Requesting and creating new samples and plates
- Cherry-picking samples
- Reformatting plate layouts
- Browsing and searching for plate and sample information
- Tracking sample volumes, concentrations, genealogy, and location
- Viewing and searching by chemical structure and custom properties

## Identifying hits

In this scenario a biologist has tested a set of plates and is using Assay Explorer to capture and analyze the data. The biologist selects active compounds from the set based on specified criteria, e.g. compounds showing results three times the standard deviation from the mean, above or below 50% inhibition or percent of control, etc. (Figure 1).

## Getting dose response plates quickly

To request active compounds, or hits, to be replated for dose response testing, the biologist simply selects the filtered or identified hits. A single click in Assay Explorer generates the request form. After the biologist completes the form, the system routes the order directly to a queue in Plate Manager for the inventory scientist managing the plate and samples (Figure 2).

## Managing the request queue

The inventory scientist has a complete set of tools to manage incoming requests in Plate Manager efficiently. The scientist can evaluate and filter requests based on the date they were submitted, the biologist submitting the request, or the priority level specified by the requestor. The inventory scientist can then create or build the plates directly from the request (Figure 3).

Plate Manager checks sample volumes automatically and decrements the source plates. If samples do not meet established volume criteria, Plate Manager alerts the inventory scientist. (Samples with insufficient volumes can be stored in the database and the inventory scientist can use the lists to order more compounds.) Plate Manager will also notify the inventory scientist if the source has expired based on established business rules prescribing a permissible number of freeze-thaw cycles.

Plate Manager maintains a location hierarchy, so inventory scientists can manage plates and samples rationally by selecting samples from local sites. The system also maintains a complete genealogy for samples and plates so scientists always know the parent plate and the original sample that created subsequent assay plates.

This array of automated controls and tools in Plate Manager allows inventory scientists to maintain a high-quality plate library, assuring researchers access to the right samples at the right time.

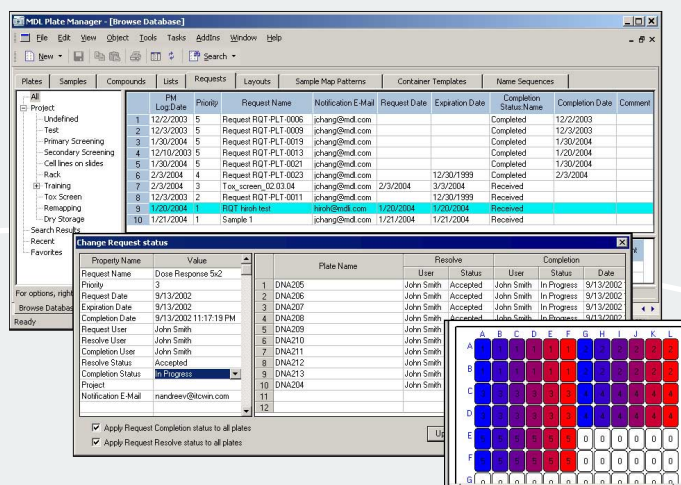
## Automated notification

Once the request has been fulfilled, Plate Manager sends an email to notify the biologist who requested the plates that the plates have been created and are ready for testing (Figure 4). In the case of a partially filled request, Plate Manager will also notify the biologist of the plates or samples that could not be created.

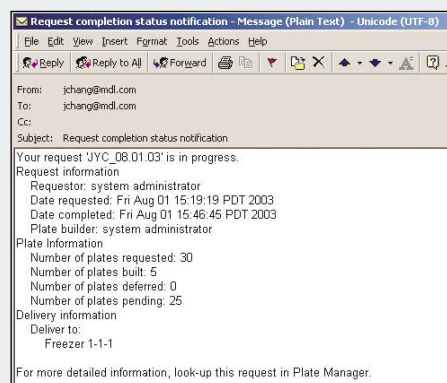
## Accelerating workflow

With systematic coordination and automated communication, Plate Manager speeds the process of requesting and fulfilling plate requests. Biologists are able to test for dose response sooner, in turn accelerating the results to chemists and the project team (Figure 5). The system's effective monitoring of inventory quantities and freeze-thaw cycles ensures library integrity, and management tools allow inventory scientists to maintain precise records and efficiently utilize local samples.

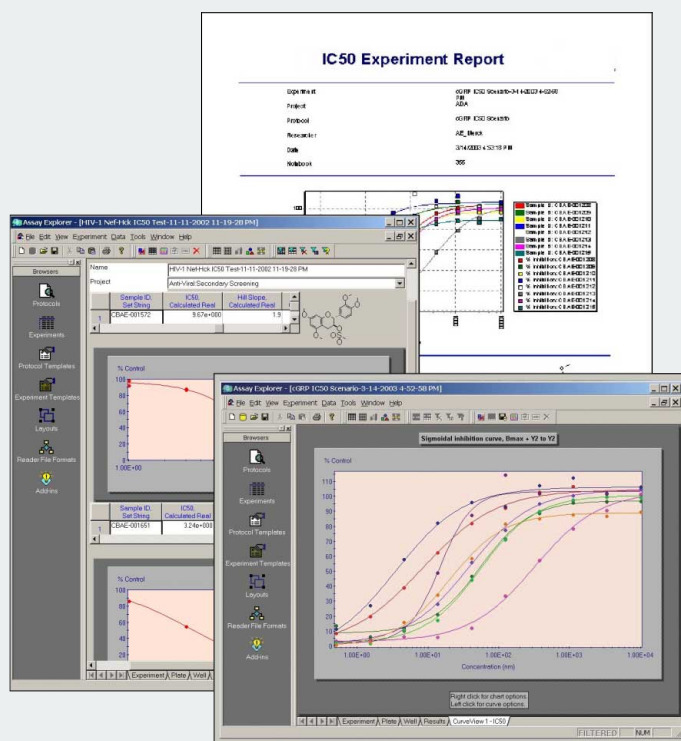
Plate Manager helps scientists complete the screening cycle quickly and efficiently with high-quality compounds, allowing high-quality leads to move forward in the drug discovery process. ■



**Figure 3:** Inventory scientists can efficiently manage plate requests using built-in features in Plate Manager to prioritize requests, build plates, track inventory volumes, monitor freeze-thaw cycles, and manage plates and samples by location.



**Figure 4:** An automated email advises biologists on the status of their plate requests



**Figure 5:** After receiving plates of samples from the inventory scientist, a biologist conducts dose-response tests and analyzes the results in Assay Explorer.

## DiscoveryGate<sup>SM</sup> opened to academic community

For many corporate scientists, DiscoveryGate is the first stop for scientific information and answers to discovery questions.

Thanks to a new initiative by MDL, this vital structure-searchable resource is now available and affordable for the academic community, enabling students, faculty, and academic researchers around the world to experience the dramatic power of the Web-based DiscoveryGate research environment.

DiscoveryGate provides richly excerpted information from the areas of chemistry, synthesis, ADME, toxicology, and pharmacology. The service gives researchers access to more than 13 million chemical structures, 10 million reactions, and over 200 million associated calculated and reported properties, including synthesis, bioactivity, metabolism, toxicology, and physical property data.

DiscoveryGate for academia (<https://gateway.discoverygate.com>) features a campus-wide access model: When an institution licenses DiscoveryGate, any number of eligible faculty members, students, or researchers at the institution may simultaneously use it—access is not limited to a few people at a time.

Academic researchers can access 14 databases such as CrossFire Beilstein, MDL<sup>®</sup> Available Chemicals Directory, MDL<sup>®</sup> Drug Data Report, and MDL<sup>®</sup> Toxicity, authoritative reference works, and links to over 20,000 journal titles including Elsevier's premier full-text database, ScienceDirect (appropriate subscriptions/licenses required to access third-party content in their environments).

"This offering is a tremendous boost for academic librarians, chemistry students, and faculty researchers," said Tim Hcctor, product manager for MDL. "DiscoveryGate is affordable for institutions, management is simple, and availability to researchers is assured." ■

## Introducing xPharm<sup>SM</sup>: Better pharmacological decisions, earlier in discovery

A new information resource from MDL and Elsevier is the equivalent of an expert, on-call pharmacologist.

xPharm<sup>SM</sup> is a unique online database of pharmacological information that provides a comprehensive set of records on topics of interest. The database provides detailed information on molecular targets linked to pharmacological agents (compounds), disorders, and principles to make it easy for researchers to understand the context and relationships between them.

By providing highly structured and indexed information that is interlinked and easy to navigate, xPharm helps scientists make better decisions earlier in the discovery process. Not only are connections among targets, disorders, agents, and principles evident in the database, but the topics are linked hierarchically to allow researchers to obtain general overviews or specific information depending on their prior knowledge of the topic.

Featuring greater detail than any other pharmacological source, xPharm is the most comprehensive pharmacological data source available. Records are written by the most recognized and respected names in pharmacology and the life sciences. External links from xPharm to related data provide a seamless network of extended pharmacological information, and the

The screenshot shows the DiscoveryGate xPharm interface. At the top, there are navigation tabs: Home, Contents, Search, Agents, Targets (highlighted), Disorders, and Principles. Below the tabs is a search bar with the text 'Quick Search' and a dropdown menu set to 'within All xPharm'. The main content area displays 'Search Results within Targets' for the search term '13 polymorphism'. It shows 'Viewing 1 result' and lists '1. Monoamine Oxidase B'. Underneath, there is a section for 'Target Structure' and 'Protein Information' describing MAO-B, including its structure and function. At the bottom of the screenshot is a 3D molecular model of the MAO-B protein structure.

*xPharm is a fully interactive database covering molecular targets, agents, related disorders, and the principles that govern their interactions. The content includes summaries for non-specialists and detailed views and data for experts. Records are written by recognized experts in pharmacology and life science.*

database integrates directly with complementary data such as full text articles, protein and gene sequences, and PubMed (appropriate subscriptions/licenses required to access third-party content in their environments).

The combination of xPharm's comprehensive, authoritative pharmacological information with

researchers' ability to specify and tailor search results greatly improves decision making in early drug discovery.

xPharm is now available. For more information visit [www.mdl.com](http://www.mdl.com) or contact your MDL Account Manager to arrange for a demonstration. ■

# MDL extending reaction-linking capability

Linking reactions in MDL databases to reactions and other references in third-party electronic sources gives you a fast and efficient way to browse, query, and manage discovery data. This critical linking capability, achieved through reaction classification code technology licensed from InfoChem GmbH, has been available to MDL customers using MDL® ISIS Reaction Browser and Integrated Major Reference Works™ for some time. In 2004 MDL is extending this powerful linking functionality and integration tool to include:

- Summary reactions in MDL® Compound Locator
- MDL's complete line of synthetic methodology databases available via MDL® Database Browser
- Over ten million reactions in CrossFire Beilstein (accessible via MDL® CrossFire Commander)

## Managing and querying reaction data

Reaction classification codes help you manage and query reactions more efficiently by categorizing reactions according to the type of transformation they represent. As shown in Figure 1, the codes categorize reactions at broad, medium, and narrow constraint levels—with each level specifying varying amounts of structural information about the reaction center. The broad classification level only considers atoms and bonds at the reaction center, resulting in a large hit list. The medium level extends outwards to encompass the immediate neighboring atoms within one bond length of the reaction center, resulting in a medium-sized hit list. The narrow level takes the description another bond length further, resulting in a much smaller, more selective hit list.

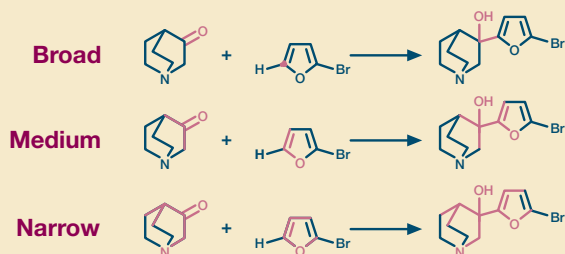


Figure 1: Reaction classification codes generated by an algorithm that MDL licenses from InfoChem GmbH classify reaction queries into broad, medium, and narrow levels based on the structural features surrounding the reaction center.

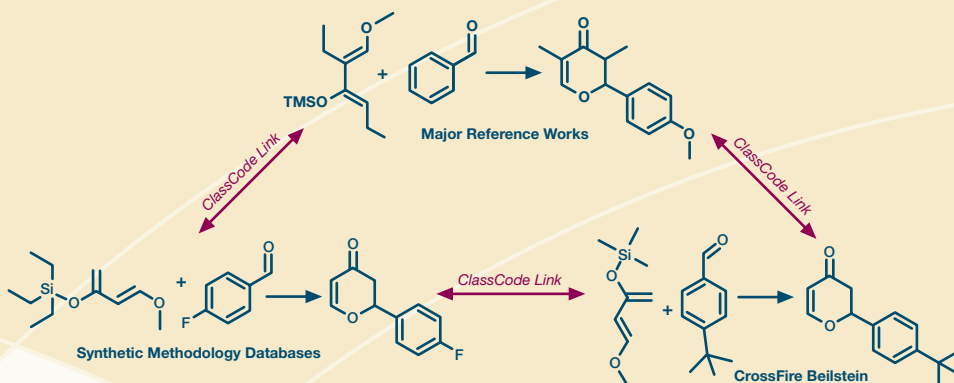


Figure 2: This example, starting with a search in synthetic methodology databases, is only one way to approach a synthesis problem. Since the reaction linking is bidirectional, you can start in any type of reaction data source, and quickly link to relevant reactions from the other sources.

## Accelerating the selection of synthetic routes

The ability to link to similar reactions from various complementary data sources greatly simplifies synthesis planning. With a single search, you can find reactions for preparing a molecule in one data source, and then link directly to relevant reactions in other data sources.

For example, you are trying to develop an efficient route to a library of phenyl dihydropyranones. One way to begin is to search MDL's synthetic methodology databases. These databases include extensive information on reactions that help chemists predict the success of a particular method of synthesizing novel molecules.

A substructure search for the target structures retrieves 196 reactions, of which 71 use a hetero Diels-Alder reaction with a  $\text{Eu}(\text{fod})_3$  catalyst (see Figure 2). Several of these look useful for your purpose, but you want to know more about the scope and limitations of the methodology.

You can link directly to similar reactions in various major reference works in synthetic chemistry for extensive reviews on this methodology. This search retrieves 24 very similar (narrow classification) reactions. Figure 2 shows an example from the *Encyclopedia of Reagents for Organic Synthesis* using a specialized boron alkylated CAB catalyst that is stable to moisture and air.

Having decided that this methodology is useful, you can link directly to similar reactions in CrossFire Beilstein to find another 152 specific examples of reactions using your chosen synthetic methodology. The reaction shown in Figure 2 describes a very high yield reaction using a metallocerium complex. The combined results from these various reaction sources, obtained from a single query, provide the information you need for fast, efficient design of synthetic routes.

By enabling easier linking between reaction databases and more straightforward access to information about reactions of interest, MDL's extension of reaction class code technology to encompass all of MDL's reaction databases represents a significant step towards a more integrated life science research environment.

For additional information on how MDL's expanded reaction linking capabilities can accelerate your reaction clustering and searching activities, contact your MDL Account Manager or submit a request for information at [www.mdl.com](http://www.mdl.com). For more information on synthesis planning, visit [www.mdl.com/promos/synthetic.methodology](http://www.mdl.com/promos/synthetic.methodology).

# MDL<sup>®</sup> Isentris<sup>™</sup>—Sharpening your focus on research targets

Building an integrated discovery informatics environment for the biopharma industry is a challenge matched by MDL's technology and experience. It requires nothing less than providing life scientists with the right information, at the right time, in the right format and context, and giving them the right tools to process the information productively. The challenge is further complicated by today's increasingly complex and competitive global R&D environment in which disparate project teams must collaborate effectively to fill product pipelines under extreme time and cost constraints.

Meeting these industry challenges is MDL<sup>®</sup> Isentris<sup>™</sup>—an open, scalable, and extensible n-tier discovery informatics architecture that improves the efficiency of life science researchers by integrating business processes, data, and workflow applications.

Isentris consists of four core products: MDL<sup>®</sup> Core Interface, the middleware platform that handles server processing and integrated business logic, workflow applications, and data; the MDL<sup>®</sup> Draw client application for chemical structure rendering and viewing; MDL<sup>®</sup> Direct (data cartridges) for searching chemical databases in an Oracle environment; and the MDL<sup>®</sup> Base desktop application, an extensible environment for enhanced data access and workflow support. With the release of MDL Base in 2004, the full Isentris n-tier solution will be complete.

## Working more efficiently

The task-centered MDL<sup>®</sup> Base desktop application mirrors the way scientists work. By supporting *in situ* data re-orientation and sorting, cherry-picking, automatic form creation, search histories, and the sharing of data between applications and colleagues, MDL Base ensures that data are utilized more efficiently and with greater productivity. The Isentris open API enables developers to easily integrate other MDL, in-house, and third-party applications that have the same "look and feel," share the same resources, and use the same technology. With applications sharing a common appearance and functionality, scientists can effectively collaborate and pursue discovery without having to learn new user interfaces or understand the differences in applications' underlying technologies.

## Knowing more

MDL Isentris streamlines the storage, retrieval, integration, and sharing of public and proprietary information, including chemical structures, reactions, biological activity, and related property data. MDL Base and MDL Draw constitute the Isentris user interface. Together they deliver dynamic and transparent database access to the scientist. This self-service data access enables scientists to retrieve the information they want in a format and context that facilitates hypothesis exploration and decision-making. Utilizing middle tier services within MDL Core Interface to integrate and share data, scientists are better able to communicate their research findings and collaborate effectively. MDL Direct powers this data access with Oracle<sup>®</sup> data cartridge technology for storing, searching, and retrieving molecules and reactions.



*Integrating business processes, workflow applications, and data, MDL<sup>®</sup> Isentris<sup>™</sup> is a three-tier architecture supporting vertical chemistry and biology discovery informatics solutions while offering opportunities to leverage existing horizontal technologies already in use at research organizations.*

## Improving data management

The Isentris three-tier architecture is the ideal environment for managing the rules governing how data are stored, integrated, and retrieved. Isentris implements these rules in the middle tier where MDL Core Interface provides standard query and database services (e.g., session/task management, database access, object storage, user management, etc.). Core Interface's open, scalable, Java-based development environment is also a solid foundation for building custom domain services to support chemical registration, warehousing, calculations, combichem, workflow management, and procurement. In conjunction with MDL Base and MDL Draw, MDL Core Interface manages the crucial intersection between scientists and data, ensuring that all project team members are "on the same page" in terms of the business logic governing data access and analysis.

## Enabling integration

In today's challenging research environment, global research organizations with highly specialized investigational interests need the capability of selecting "best of breed" informatics and workflow management solutions that integrate across research and enterprise boundaries. MDL Isentris is an effective informatics solution because it works alongside other vendor applications and architectures. With its research focus, openness, flexibility, scalability, and extensibility, MDL Isentris complements and enriches other informatics technologies, supporting enterprise-wide business, data, and application integration spanning chemistry and biology research.

For additional information on MDL Isentris, or on the carefully planned technology transition strategies that support the new architecture, contact your MDL Account Manager or submit a request for information at [www.mdl.com](http://www.mdl.com). ■

## Tetrahedron journals— Global access to essential research

Molecular Connection asked Iain Craig, senior publishing editor of Elsevier's organic chemistry group, to provide an overview of Elsevier's Tetrahedron journals and the upcoming Tetrahedron Symposium.

The Tetrahedron family of journals constitutes an essential resource for organic and medicinal chemists. The five leading international journals are *Tetrahedron* (published weekly), *Tetrahedron Letters* (weekly), *Tetrahedron: Asymmetry* (biweekly), *Bioorganic & Medicinal Chemistry* (biweekly) and *Bioorganic & Medicinal Chemistry Letters* (biweekly). These journals are a key part of Elsevier's portfolio of publications and services in chemistry and the life sciences.

The journals publish state-of-the-art research centred on the disciplines of synthetic organic chemistry, medicinal chemistry, and bioorganic chemistry and are continually striving to offer the best services to authors and readers.

### Fast, responsive peer review

Twenty-two editorial offices around the globe ensure fast, responsive peer review, and electronic submission and online publication enable even faster publication—in fewer than 10 weeks for many papers.

### Easy access via ScienceDirect

ScienceDirect, Elsevier's comprehensive electronic collection of science, technology, and medical full-text and bibliographic information, offers global access to all papers in the journals. The journals are read in over 63 countries, with over 2 million full-text articles downloaded from *Tetrahedron Letters* during 2003. *Tetrahedron Letters* is the most cited chemistry letters journal in the world, with over 60,000 citations in 2002 (Source: Institute for Scientific Information®).

### The Tetrahedron Prize

The annual Tetrahedron Prize is awarded by the Executive Board of the Tetrahedron publications. First presented in 1981 to Professor Albert Eschenmoser, the prize is considered one of the top awards in the field. The prize consists of a gold medal, a citation, and \$10,000. In 2003 Professor Robert H. Grubbs and Professor Dieter Seebach were jointly awarded the prize.



### The Tetrahedron Symposium

This year's annual Tetrahedron Symposium will be held in association with *Drug Discovery Today*, and will take place in New York on June 18, 2004. The theme is the interaction of chemistry and biology, with a particular focus on drug discovery. The speakers are: Dale Boger (Scripps Research Institute), Samuel Danishefsky (Sloan-Kettering Institute and Columbia), William Jorgensen (Yale), Christopher Lipinski (formerly Pfizer), Cynthia Maryanoff (Johnson & Johnson), Gary Posner (Johns Hopkins), Stuart Schreiber (Harvard) and Edward Scolnick (Merck).

For further information on the 2004 Tetrahedron Symposium, including how to register, go to [www.tetrahedronsymposium.elsevier.com](http://www.tetrahedronsymposium.elsevier.com). ■

## The Biopendium™ database—The world's premier proteome annotation resource

MDL has become a promotional agent of Inpharmatica, Ltd. for the sale of the Biopendium™ database. Biopendium plays a key role in accelerating drug discovery by enabling the high-throughput annotation of genomic data for target prioritization, target mining, and microarray analysis. The database gives researchers instant access to 10 billion pre-calculated protein relationships derived from more than 1.4 million sequences from 150 different genomes, integrating structural and ligand information. The agreement enables MDL to offer both installed and hosted versions of Biopendium for sale to interested organizations worldwide (with the exception of Japan).

"Inpharmatica's Biopendium enables Elsevier to bring comprehensive protein sequence and structure data to researchers, complementing MDL's extensive chemistry, synthetic methodology, pharmacology, metabolism/toxicology, and sourcing/logistics content," says Lars Barfod, executive vice president and chief business officer of MDL. "This agreement will help accelerate drug discovery research across the chemistry and biology domains."

For additional information on how the Biopendium database promotes fully informed decisions on the value of proteins as candidates for drug targets, contact your MDL Account Manager or submit a request for information at [www.mdl.com](http://www.mdl.com). ■

## MDL® Open Library—Supporting increased, more effective use of MDL solutions



When companies license powerful informatics, content, and workflow solutions from MDL, they clearly see the value of the investment. To realize a full return on the investment, however, company employees must adopt the technology and take full advantage of its functionality. A comprehensive training program that recognizes the complex human factors involved in database and software implementation is an essential component in optimizing the adoption and utilization of new technology.

Are you planning a rollout of new MDL database or software products? Are you transitioning to a new version of an application? Are you taking full advantage of MDL software functionality? Do you need more in-depth training in specific products? If questions like these sound familiar, then you will want to explore the new Open Library offering from MDL Educational Services.

Developed in response to customer interest, MDL® Open Library is a comprehensive package of educational materials and delivery options that is designed to increase the value of MDL databases and software by increasing their utilization. Available on an annual subscription basis, Open Library provides open and unlimited access to MDL's entire courseware catalogue for scientists—an extensive collection of over 35 titles. In addition, the package includes Web-based, self-paced training modules and a library of quick reference guides that cover most MDL products.

Customers have complete flexibility to construct a curriculum and in-house library that best supports their MDL solution profile, making training materials available 'anytime, anywhere' to all eligible employees worldwide and on-demand. The system promotes both centralized content control and decentralized learner access. Customers determine how employees access their MDL course catalogue and library (e.g., they may be controlled by an in-house coordinator and managed on an internal server or intranet Web page). The self-paced courses, indeed all training materials, courses, and events, can be hosted through the customer's own in-house Learning Management System. This simplifies enterprise-wide distribution of courseware and integration with other in-house training operations.

Open Library includes 10 service days, which may be used for face-to-face classroom instruction, train-the-trainer programs, Web Workshops,

or custom course development. The program also enables customers to purchase additional training/service days at a discounted fee and acquire hard-copy courseware (training manuals, quick reference guides, etc.) at cost through a Web-based ordering system.

Peg Renery, director of educational services at MDL says: "Open Library's blended approach to curriculum design and flexible, open-access delivery options help customers establish a 'just-in-time' training capability that accommodates a wide range of personal learning styles. Customers can build a training program that is relevant to their needs by cherry picking materials from instructor-led courses, quick reference guides, Web Workshops, and self-paced modules. MDL will even create custom documentation as part of the Open Library program."

The potential benefits of the Open Library extend all the way to a company's bottom line. By making high quality, up-to-date MDL courseware available to all eligible employees worldwide via the customer's own intranet, the program eliminates internal training development and maintenance costs. The annual license for a bundled training package customized to each client's needs offers the opportunity for substantial savings over picking courses and materials *à la carte*. In addition, a renewable subscription for content and services is easier to administer and a more effective channel for disseminating training materials on continually evolving database and software products within a global enterprise. All designated employees have the right to use the training materials, anytime, anywhere, once the content is accessible in the customer's environment.

Life science companies interested in creating a tighter linkage between their software technology purchases, employee development investment, and bottom line results should investigate the possibilities of MDL Open Library. Improved education will result in the wider adoption of new technology, enhanced productivity, accelerated performance, better research, and a greater competitive advantage.

For a detailed assessment of how MDL Open Library can maximize the value of MDL database and software solutions at your site, contact your MDL Account Manager or Peg Renery at [p.renery@mdl.com](mailto:p.renery@mdl.com) or 800-955-0051, ext. 1377. ■

For complete, up-to-date listings of all courses included in MDL® Open Library, go to [www.mdl.com](http://www.mdl.com), click on **Education**, then on **Classroom Training** and **Web-delivered Training**.

# Mark your calendars!

You can find MDL at the following events over the next few months:

## MDL US USER CONFERENCE

Boston, MA, May 2-6

## BIOLOGY DATA MANAGEMENT EXCHANGE

Boston, MA, May 6-7

## SPECIAL LIBRARIES ASSOCIATION NATIONAL MEETING

Nashville, TN, June 5-10

Look for us in the Elsevier booth to see DiscoveryGate<sup>SM</sup> and xPharm<sup>SM</sup> in action.

## DRUG DISCOVERY TECHNOLOGY

Boston, MA, August 8-12

Booth 2204

## ACS 228th NATIONAL MEETING

Philadelphia, PA, August 23-25

Booth 302

## SOCIETY FOR BIOMOLECULAR SCREENING

Orlando, FL, Sept 11-15

For more details, go to [www.mdl.com](http://www.mdl.com). Click on **Company Info** and **Events**.

## New email address for product support questions

Customers in Europe, the Middle East, Africa, and the Americas can now submit all product support questions to a single email address: [support@mdl.com](mailto:support@mdl.com).

MDL Technical Support Specialists (TSSs) will continuously monitor this address 16 hours per day (9:00 AM Central European Time to 4:00 PM Pacific Time). While our TSSs will continue to focus on providing high quality support to customers in their respective regions, this change also enables them to quickly respond to critical customer needs during these business hours, regardless of a customer's physical location. All previous MDL customer support email addresses remain in effect.

The email address for submitting customer support questions in the Asia Pacific region remains the same: [jsupp@mdl.com](mailto:jsupp@mdl.com). This site is monitored from 9:00 AM to 5:00 PM Japan Time during business days.

## MDL Web Workshop Schedule

MDL offers 2-hour, interactive Web Workshops for small groups of up to eight participants. These short, 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](mailto:edservices@mdl.com) or 800-955-0051, ext. 1326.

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

For more information on MDL training programs, click on **Education** at [www.mdl.com](http://www.mdl.com).



## Developer and Administrator Classes

MDL<sup>®</sup> Draw Enterprise Edition

MDL<sup>®</sup> Cheshire

Hview Design, Development, and Optimization

Application Development with MDL<sup>®</sup> Core Interface

Application Development with MDL<sup>®</sup> Direct

Application Development with MDL<sup>®</sup> ISIS

Application Development with MDL<sup>®</sup> ISIS Object Library

MDL<sup>®</sup> ISIS/Host Administration

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

Date	AM SESSION (09:00-11:00 Eastern Time)	PM SESSION (13:00-15:00 Eastern Time)
May 11	MDL <sup>®</sup> ISIS for Excel for the current ISIS user	Creating reports with MDL <sup>®</sup> Report Manager
Jun 8	Exploring DiscoveryGate <sup>SM</sup>	Exploring DiscoveryGate <sup>SM</sup>
Jun 22	Transition to MDL <sup>®</sup> CrossFire Commander 7.0	Transition to MDL <sup>®</sup> CrossFire Commander 7.0
Jul 13	Transition to MDL <sup>®</sup> CrossFire Commander 7.0	Exploring MDL <sup>®</sup> Metabolite and MDL <sup>®</sup> Toxicity Databases
Jul 27	Drawing basics in DiscoveryGate <sup>SM</sup>	Structure searching in CrossFire Beilstein using DiscoveryGate <sup>SM</sup>
Aug 10	Drawing structure queries with MDL <sup>®</sup> Draw	Exploring Integrated Major Reference Works <sup>TM</sup>
Aug 11	Locating compounds in DiscoveryGate <sup>SM</sup>	Reaction searching in CrossFire Beilstein using DiscoveryGate <sup>SM</sup>
Sep 13	Transition to MDL <sup>®</sup> CrossFire Commander 7.0	Transition to MDL <sup>®</sup> CrossFire Commander 7.0
Sep 14	MDL <sup>®</sup> ISIS for Excel for the current ISIS user	Creating reports with MDL <sup>®</sup> Report Manager

# MDL® Isentris™

## The new shape of integration

Spanning and integrating business processes, data, and workflow applications, MDL Isentris is the first out-of-the-box, n-tier informatics architecture designed specifically for life science researchers. Isentris bridges chemistry and biology workflows, consolidates knowledge within and across projects, encourages collaboration, eliminates barriers, and fosters creativity.

Built on an open, scalable, and extensible informatics platform, Isentris enables IT groups to develop and deliver robust, high quality, integrated applications—helping researchers save time, reduce costs, focus on science, and make better decisions.

MDL is launching Isentris at Drug Discovery Technology in Boston, August 8-12, 2004. *Visit booth 2204 to learn more about how Isentris integrates and energizes life science discovery.*



*Powering the  
Process of Invention™*

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