



**2007 Elsevier MDL  
US User Conference  
La Jolla (San Diego), April 30 – May 1, 2007**

## Agenda:

The US User Conference is an open forum for scientists and research information system developers and managers to share their own experiences with MDL products and network with other customers about product rollouts and implementation, migration and functionality/usability. Attendees at the 2007 conference include: Professor Dr. Kurt Wüthrich, 2002 Nobel Prize for Chemistry Laureate and keynote presenter for the European Users' Group Meeting, representatives from numerous Isentris Alliance partners, including ACD/Labs and Spotfire as well as representatives from Pharma, BioPharma and Academia.

Master of Ceremonies will be Dr. Phil McHale, V.P of Solutions Product Management, Elsevier MDL.

### Monday, April 30

7:30 **Breakfast**

7:30 **Registration opens**

8:30 **Demo** – Dr. Pieder Caduff of Elsevier MDL presents the registration of metabolic transformations and its conditions, the subsequent dynamic generation of metabolic networks using corporate metabolite data and MDL<sup>®</sup> Metabolite and how toxicity information is associated with these metabolites using a prototype MDL<sup>®</sup> Isentris<sup>®</sup> application developed by Elsevier MDL Consulting.

Additionally, Pieder will show a decision support application enabling scientists to associate pharmacological effect and side effect with generic compound classes by analyzing molecules based on their topological similarities.

Dr. Pieder Caduff is responsible for identification of New Technologies to achieve content Integration at Elsevier MDL. Pieder has been with Elsevier MDL for over 12 years and has been involved in the creation of Compound Index and DiscoveryGate<sup>®</sup> from the beginning of these projects.

Prior to joining Elsevier MDL, Pieder worked as a development chemist at Orgamol (a BASF company) in Switzerland, a contract synthesis scale-up company. Pieder holds a Ph.D. in Bio-organic Chemistry from the ETH Zurich.

9:00 **Meeting opens – Welcome and Introductory Remarks**

*Delivering innovation on a solid foundation*

Lars Barfod, President and CEO, Elsevier MDL

9.25 **Conference Information and Logistics**

Jean Holt, Sr. Director, Marketing and Communications, Elsevier MDL

9:30 **Keynote address**

**Joseph Cerro, Bayer**

Joseph Cerro has contributed to the development of Bayer's High-Tech Platform as a scientist and technologist since 1997. As Head of Informatics, he is responsible for striking the proper balance among business, scientific, and information technology demands in order to discover innovative drugs as efficiently as possible.

In recognition of his contributions as a Pharma industry thought leader, Mr. Cerro received the 2005 Albert Einstein Award for Outstanding Achievement in the Life Sciences from the State of Israel and Global Capital Associates.

10:15 **Break** – Learning Lab available

10:30 **How to meet the Scientist needs when delivering desktop solutions**

Dr. Christine Humblet, Wyeth

Dr. Christine Humblet recently joined Wyeth Research to head the Computational Chemistry & Cheminformatics group in the Chemical & Screening Sciences department. She is responsible for delivering discovery solutions supporting drug discovery in close partnership with the scientists.

Christine has more than 25 years of experience in the pharmaceutical industry, particularly in computer-assisted design and drug discovery and holds a Ph.D. in Chemistry.

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Agenda subject to change.

## Agenda (continued):

- 11:15 **Reagent Logistics at Boehringer Ingelheim – Migrating from BICIMS to BIRMA**  
Dr. Gerhard Mihm, Boehringer Ingelheim

Dr. Gerhard Mihm is group leader of the Screening Support Group in the Lead Discovery Department at Boehringer Ingelheim. Gerhard is responsible for the sample management operations in Germany supporting Boehringer Ingelheim's worldwide screening activities as well as the synthetic activities in MedChem and Combichem. He is, in addition, project leader for several of Boehringer Ingelheim's worldwide activities in the area of laboratory data management systems such as electronic laboratory notebooks and reagent inventory management applications.

Gerhard has over 20 years experience in the pharmaceutical industry. After 10 years as a team leader in the Medicinal Chemistry Department of Boehringer Ingelheim in Germany working on lead optimization projects, he took over responsibility for the sample management activities at the Biberach research site of Boehringer Ingelheim. In this function he established an automated, fully integrated system for the storage, handling and shipment of samples for BI's international screening activities.

- 12:00 **Lunch**

- 12:45 **Demo** – MDL<sup>®</sup> Logistics: Mary Beth Walsh of Elsevier MDL will explain how MDL Logistics addresses reagent identification, selection, procurement and disposal; 'cradle-to-grave' inventory management and full integration with a research organization's business rules and discovery processes. See how MDL Logistics optimizes scientists' workflows through integration with MDL<sup>®</sup> Notebook, MDL<sup>®</sup> Registration and external systems like SAP.

Mary Beth Walsh is responsible for the product management of Elsevier MDL's Sourcing and Logistics solution area, including MDL<sup>®</sup> Available Chemicals Directory, MDL<sup>®</sup> Screening Compounds Directory, MDL Logistics and MDL<sup>®</sup> Reagent Selector. She has been with Elsevier MDL for 5 years and holds an M.S. in Biophysical Chemistry from Yale University.

- 1.15 **Demo** – Hit profiling using MDL<sup>®</sup> Assay Explorer<sup>®</sup>: Debra Toburen of Elsevier MDL will explain how MDL Assay Explorer can help scientists prepare for statistical analysis, select appropriate models and parameters for curve fitting, interpret the results of regression analysis and finally optimize the results for the best fit of their data.

Debra Toburen has over 10 years of experience in research conducting assay development and high-throughput screening at both MDS Pharma (previously Panlabs) and Amgen. After a brief stay at IDBS, she has been with Elsevier MDL for over 7 years in the marketing department working on product development and marketing of solutions for biology data management.

- 2:00 **Eats, shoots and leaves...**  
Dr. Simon Smith, Johnson & Johnson

Dr. Simon Smith is Head of Bioinformatics Software Development for Johnson & Johnson Pharmaceutical Research and Development. At PRD, he is responsible for general global drug discovery and bioinformatics, related software acquisition and internal software development.

Simon has worked in the health care and pharmaceutical areas for over 20 years. His focus has always been on the use of information technology in new and emerging areas, from medical device companies to drug discovery. Simon holds a Ph.D. in Biomedical Computing from London University.

- 2:45 **State of informatics in Pharma**  
Dr. Yvonne Martin, Consultant

A Symposium Honoring Dr. Yvonne Martin will be held at the recent 233rd ACS National Meeting, Chicago, IL, March 25-29, 2007 – "Computer Assisted Drug Design: Reminiscing about the Future"

Retired Senior Research Fellow, Volwiler Society, Abbott Laboratories. Dr. Yvonne Martin's research interests include strategies for increasing the molecular diversity of compound collections; to triage hits from HTS; to predict the potency, binding affinity, or ADME properties of small molecules from their molecular structures; and for the computer design of novel compounds including 3D database searching, *de novo* design, and pharmacophore mapping.

Yvonne holds a Ph.D. in Chemistry (focusing on physical biochemistry) from Northwestern University.

- 3:15 **Break** - Learning Lab available

## Agenda (continued):

- 3:30 **High-throughput screening data management automation using MDL Assay Explorer & Microsoft Excel**  
Thuan Tran, Siga Technologies, Inc

Thuan Tran is the Associate Director of Bioinformatics at Siga Technologies, a small Oregon biotech developing biodefense countermeasures. Following his arrival in 2006, he implemented a high-throughput screening program to identify these small molecules. He is currently responsible for managing a cohesive and integrated bioinformatics program that enables scientists to rapidly and efficiently take the compounds identified from the HTS program from bench top to clinic to market.

- 4:15 **So what do we do now? Challenges for IT in early Discovery**  
Dr. Jay Gill, Bristol-Myers Squibb

Dr. Jay Gill leads the Applied Biotechnologies Informatics group within the Discovery Informatics and Automation department at the Bristol-Myers Squibb Company's Pharmaceutical Research Institute. Jay has more than 25 years experience developing scientifically oriented hardware and software solutions primarily for early drug discovery. The Applied Biotechnologies Informatics group supports the software needs of scientists across early discovery with a focus on software development and data management for array synthesis, analysis and purification, registration, compound inventory, HTS and Lead Evaluation and High Content Screening. Jay began his career as a neurobiologist studying signal transduction and encoding in the central nervous system, focusing on the sense of taste and received his Ph.D. from Duke University.

- 5:00 **Wrap-up** – Jean Holt, Elsevier MDL

- 5:15 **Demo** – MDL Isentris: Dr. Albert Crescenzo of Elsevier MDL will explain how to use Isentris to access biological and chemical information. Researchers require easy ways to transfer data between applications and share results with colleagues. See novel ways to make searching, browsing and sharing data easier through decision views, data drill down, *ad hoc* calculations and reporting.

Dr. Albert Crescenzo has been with Elsevier MDL since 1997. He first worked as a Senior Trainer in Educational Services, writing training materials and providing instructor lead workshops for MDL products and databases within the user community. For the past five years he has been a Consultant, creating product demonstrations and implementing software solutions for Elsevier MDL's customer base. Albert has a Ph.D. in Biophysics and Biochemistry from Yale University.

- 6:30 **Conference Dinner**

# Agenda (continued):

## Tuesday, May 1

7:30 **Breakfast**

8:00 **Registration opens**

8:15 **Demo** – MDL<sup>®</sup> Draw: Dr. Albert Crescenzo of Elsevier MDL will explain how to extend MDL Draw to include calculators from ACD/Labs, an Isentris Alliance partner. Andrew Anderson, Director of Sales with Advanced Chemistry Development, Inc (ACD/Labs) will also be available for Q&A.

9:00 **Elsevier MDL's technology vision**

Dr. Trevor Heritage, Senior V.P and Chief Scientific Officer, Elsevier MDL

Dr. Trevor Heritage joined Elsevier MDL in May 2005 as Senior Vice President of the Workflow Business Group. Trevor brings extensive scientific and pharmaceutical research experience to the Elsevier MDL management team as well as knowledge of BioPharma workflows and computational modeling. Prior to joining Elsevier MDL, Trevor was a Senior Vice President, Corporate Officer and General Manager of Tripos Inc.'s discovery informatics business. Trevor holds a Ph.D. in Organic Chemistry from University of Reading, England.

9:45 **Chemistry informatics at Pfizer: Past, present and future**

Dr. Chris Waller, Pfizer

Dr. Chris Waller is Director of World-wide Chemistry Informatics at Pfizer. Chris is responsible for setting the strategic direction and resource management for chemistry informatics at Pfizer Global Research and Development.

Prior to joining Pfizer, Chris worked as Head of Cheminformatics at Sphinx Pharmaceuticals, a division of Eli Lilly and Company. Chris holds a Ph.D. in Medicinal Chemistry from the University of North Carolina at Chapel Hill.

10:30 **Break** – Learning Lab available

10:45 **Implementation of MDL Assay Explorer and MDL<sup>®</sup> Report Manager into the Drug Discovery ADME workflow**

Edith Richter, Boehringer Ingelheim

Edith Richter is a Systems Analyst responsible for all IT-related tasks of their DDS department. The DDS department has for the past 5 years been implementing a platform that integrates in-house and purchased applications, responsible for supporting the whole workflow and all assays.

11:30 **Microsoft .NET and developing scientific applications using .NET controls**

Joint Presentation: Hong Choing, Microsoft and Dr. Jim Barstow, Elsevier MDL

Hong Choing is an Industry Architect Advisor in the Health & Life Sciences Industry Architecture Team at Microsoft Corporation. Hong is responsible for helping customers and partners solve business challenges with Information Technology (IT) solutions by providing guidance to business decision makers, architects and developers building enterprise solutions.

Hong has 16+ years of business and technology implementation experience with proven results in small and Fortune 100 companies. Prior to joining Microsoft in 2004, he was the Manager and Solutions Architect for a business unit of Merck & Co., Inc. At Merck, he was instrumental in evangelizing and implementing new technologies and solutions to help optimize the way clinical trials were conducted achieving cycle time reduction and reducing costs.

Dr. Jim Barstow has been with Elsevier MDL since 1982. Jim started at MDL working on all terminal based applications and designed the graphics and printing libraries. Jim has been the developer/architect of ChemTalk and much of ChemText in the CPSS series, MDL<sup>®</sup> ISIS/Base, ISIS Object Library and recently the Isentris datasource service, IDS and Isentris controls. Jim holds a Ph.D. in Chemistry from the University of California.

12:15 **Lunch**

12:30 **Demo** – MDL Isentris controls: Dr. Jim Barstow of Elsevier MDL will explain what the Isentris controls are, show the implementation concepts of the Isentris controls and also demonstrate how to build a query/browse application from scratch using the controls in Microsoft<sup>®</sup> Visual Studio<sup>®</sup> 2005.

## Agenda (continued):

- 1.00 **Demo** – MDL Notebook: Dr. Matthew Sage of Elsevier MDL will explain how to set up a simple discrete or parallel synthesis experiment using MDL Notebook.

Dr. Matthew Sage is an Advisory Consultant with over 7 years of experience working with Elsevier MDL. Matthew's role at Elsevier MDL encompasses presales demonstrations and evaluations, post sales implementation and training, as well as data migration consulting projects.

Prior to joining Elsevier MDL, he worked as a post doctorate at UC Davis, CA with Prof. T. Molinski working on Marine Natural Products and at the University of Sheffield with Prof. V.K. Aggarwal, developing Oxaziridinium catalysts for Asymmetric Epoxidation of Alkenes. Matthew holds a Ph.D. in Organic Chemistry from the University of Bath.

- 1.30 **MDL Iseptris – Responding to the scientist**  
Dr. Dominic John, Elsevier MDL

Dr. Dominic John is Group Manager at Elsevier MDL for Iseptris and has spent the last 7 years working on Discovery Informatics projects. Dominic holds a Ph.D. in biochemistry from Cardiff University and spent time as a post doctorate researching prokaryotic proteins and genes.

- 2.15 **Proof of concept implementations using MDL Iseptris – Dynamically generated synthesis schemes and metabolic networks**  
Dr. Pieder Caduff, Elsevier MDL

- 2:45 **Break** – Learning Lab available

- 3:00 **Recent and ongoing advances in chemical representation and searching**  
Dr. Jim Nourse, Elsevier MDL

Dr. Jim Nourse joined Elsevier MDL 22 years ago from Stanford University. At Stanford he worked on the DENDRAL project in computer-assisted structure elucidation. Jim holds a Ph.D. in Organic Chemistry from California Institute of Technology.

At Elsevier MDL Jim has been responsible for chemical structure representation, perception algorithms and structure searching, both as an individual contributor and as a manager of the CHRP group (CHemical Representation Project) that maintains and enhances these capabilities which are used in MDL products such as MDL<sup>®</sup> ISIS/Host, MDL<sup>®</sup> Direct and MDL<sup>®</sup> Cheshire.

- 3:45 **Integration supporting visualization and data access workflows**  
*Joint Presentation:* David Mosenkis, Spotfire and John McCarthy, V.P of Consulting, Elsevier MDL

David Mosenkis is an Application Specialist at Spotfire, with a focus on advanced visual analytics for chemistry. David has over twenty years experience leading the development and application of software and informatics systems for drug discovery. David has managed software development at Tripos, where he pioneered innovations in protein modeling and structural analysis, established and managed the East Coast office of DoubleTwist (formerly Pangea Systems) a bioinformatics software and services company, and managed software development and informatics at Locus Pharmaceuticals. David has also served as a consultant for organizations including Sanofi-Aventis and the Greater Philadelphia Bioinformatics Alliance.

John McCarthy is the head of consulting services at Elsevier MDL leading a talented technical team responsible for the demonstration, evaluation and deployment of MDL solutions to our customers. His area of interest is in understanding how scientists can efficiently capture, manage and integrate information within the discovery process transforming their raw data into information and knowledge.

Prior to joining Elsevier MDL he was part of the discovery informatics organization at American Cyanamid and Wyeth Laboratories and has worked for Symyx Technologies as a consultant in their Discovery Tools business.

- 4:30 **Ask Elsevier MDL Executives**

- 5.00 **Closing statements – Meeting concludes**  
Jean Colombel, Senior V.P of Sales and Services, Elsevier MDL