



2007 Elsevier MDL European Users' Group Meeting Strasbourg, France February 26-27, 2007

The **2007 European Users' Group Meeting** was a great success. Thank you to all the speakers and attendees who made this one of the best gatherings in years.

Comments from attendees:

"The UGM is always a good opportunity to meet with people, exchange experiences and discuss ideas. It was interesting this year to see the progress made with Isestris and I hope this will encourage more end users to attend this event in the future."—**Dr. Gerhard Mihm, Boehringer Ingelheim**

"The EUGM has been very useful in terms of understanding new Elsevier MDL directions and the evolution of its main product, MDL Isestris. The latest release seems indeed very promising in terms of User Interface design and new capabilities. From a broader perspective, it was also encouraging to see the continuing integration of MDL content and workflow applications."—**Dr. Luca Sartori, Genextra**

"At the EUGM it was very interesting to learn which products are used to make scientific research and development more efficient. The Keynote address of Professor Dr. Kurt Wüthrich was very impressive and even for a non-specialist very understandable. The meeting was very useful for the informative and inspiring discussions with colleagues and especially with MDL staff about possible new developments and their applicability to practical problems."—**Geert Pauwels, European Patent Office**

"The take home message from this meeting was that the uphill struggle of the establishment of the Isestris platform is a thing of the past and we, the users, can now concentrate on building scientific solutions based on this solid platform. Indeed, out-of-the box solutions have already appeared on schedule. MDL Isestris includes a set of .NET controls for rapid application development that developers can use in the Microsoft Visual Studio environment. The MDL Isestris client and Isestris for Excel were built using these controls.

Isestris for Excel is altogether more powerful and efficient than ISIS for Excel. It allows SAR tables to be built in five minutes; R-group decomposition is much simpler; and there are pivoting features that were impossible with ISIS for Excel. Another solution of particular interest...is integration of ACD/Labs calculations (and others) into MDL Draw, the tool that allows users to enter structures, reactions and queries. I also watched a demonstration of the use of the technology to cluster compounds based on MDL keys and then, for each cluster, look for the maximum common substructure (MCSS) within result sets. This enables scientists to find a scaffold of relevance, quickly, in a set of results and then further analyze the data based on substitution patterns and bioactivity. There are also links to Spotfire for visual analytics."—**Dr. Wendy Warr, Wendy Warr & Associates**

"For a small drug discovery organization like ours, it is important to provide a broad spectrum of scientific information directly to the scientist. Elsevier MDL's DiscoveryGate® platform gives us easy access to various databases of great relevance for our medicinal chemists and biologists. A convenient way for us to stay informed about new services and developments in the field is to attend the Elsevier MDL Users' Group Meetings."—**Dr. Guido Kurz, CNIO**