

## Warr Zone Revisited

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Greetings, new readers!

This should be the first of about eight columns I will contribute to this exciting new portal over the next twelve months. By coincidence rather than by design, this month's column comes to you direct from the Elsevier MDL European Users' Group meeting in Strasbourg, France. How might this be relevant to you, scientists who are probably more aligned to computational chemistry than to corporate databases and inventories? Agreed MDL (<http://www.mdl.com/>) is not in the business of producing innovative QSAR methodologies, but it is the market leader in the pharmaceutical industry when it comes to "data on demand; power for decisions", to quote the slogan for its ISENTRIS 2.0 platform.

The take home message from this meeting was that the uphill struggle of the establishment of the ISENTRIS 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 ISENTRIS includes a set of .NET controls for rapid application development that developers can use in the Microsoft Visual Studio environment. The MDL ISENTRIS client and ISENTRIS for Excel were built using these controls.

ISENTRIS 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 to the current readership 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.

Many more Elsevier MDL solutions were discussed at this two-day meeting but I don't want to devote too much space to any one vendor. In the middle of March I hope to attend the CambridgeSoft User Meeting and in June I will be in Budapest for the ChemAxon user meeting. I hope to incorporate some ideas from those meetings (and others) in later columns. I also hope to devote one column to business and strategy issues in the cheminformatics and molecular modeling industries. If any interesting new players enter the field I would certainly hope to feature them and their technologies in another article. Maybe I will also produce an analysis of pipelining/workflow technologies for prototyping cheminformatics applications. Another topic I am considering is an analysis of emerging markets in India and China, for example. Finally, I might cover PubChem and the IUPAC International Chemical Identifier (InChI), but I do want to encourage readers to send me ideas for what they would really like me to write about in future.

Please bear with me while I explain a little about my own interests and ventures: some of the hyperlinks that follow may well interest you. You can read the lowdown on the Warr business and Warr Zone on our Web site (<http://www.warr.com>). The marketing message is outlined there (<http://www.warr.com/whatwedo.html>) but you will probably find David Bradley's interview of me more interesting ([http://www.reactivereports.com/55/55\\_0.html](http://www.reactivereports.com/55/55_0.html)). I am proposing to do occasional interviews myself in *this* column: I welcome suggestions for your favorite gurus and the questions I might use when I grill them. Hugo Kubinyi has already volunteered to be my first victim. Hugo received the 2006 Herman Skolnik Award of the Chemical Information Division (<http://www.acscinf.org/>) of the American Chemical Society (ACS) at the Fall 2006 National ACS Meeting in San Francisco and I had the pleasure of attending the symposium (<http://acscinf.org/dbx/mtgs/232nm/232cinfprogram.asp>) he organized to mark the occasion. Send me an email if you would like to know more. My second interviewee will probably be in industry: watch this space.

Over the last year or two, I have done some work on the history of cheminformatics. Back in 2000 I looked at cheminformatics as an emerging discipline (<http://www.warr.com/warrzone2000.html>) and in 2005 I researched two talks on *Twenty Five Years of Progress in Cheminformatics*, one as a tribute to Peter Willett (<http://www.warr.com/25years.html>) and the other in honor of Johnny Gasteiger (<http://www.warr.com/yearprog.pdf>). I gave a more light-hearted tribute to Johnny at the 2<sup>nd</sup> German Conference on Cheminformatics in November.2006: the slides are online ([http://www2.chemie.uni-erlangen.de/people/Johann\\_Gasteiger/WendyWarr\\_Presentation\\_Goslar2006.pdf](http://www2.chemie.uni-erlangen.de/people/Johann_Gasteiger/WendyWarr_Presentation_Goslar2006.pdf)).

Many more open access publications appear in Warr Zone (<http://www.warr.com/warrzone.html>) or elsewhere (<http://www.warr.com/epubs.html>) on the Warr Web site. Our links page (<http://www.warr.com/links.html>) and events listings (<http://www.warr.com/meetings.html>) have proved particularly popular. As an Associate Editor of the *ACS Journal of Chemical information and Modeling*, I clearly have a great interest in the peer review process and my experience (<http://www.warr.com/warrzone2004.html>) is on open access.

At the Spring ACS National meeting in 2008, I will be organizing a symposium on the cheminformatics challenges of collaborations between the big, global pharmaceutical companies and smaller enterprises (including academic groups). I welcome suggestions for topics that I might include. The symposium will be jointly sponsored by the Chemical Information Division of ACS and the Chemical Structure Association (CSA) Trust (<http://www.csa-trust.org/>).

The CSA Trust is an internationally recognized organization established to promote the critical importance of chemical information to advances in chemical research. In support of its charter, the Trust has created a unique Grant Program, renamed in honor of Professor Jacques-Émile Dubois who made significant contributions to the field of cheminformatics. The Trust is currently inviting the submission of grant applications for 2007 (<http://www.csa-trust.org/awards.htm>). I will conclude by inviting you all to pass on this announcement to any potentially worthy researchers.