

AccelrysWorld 2005



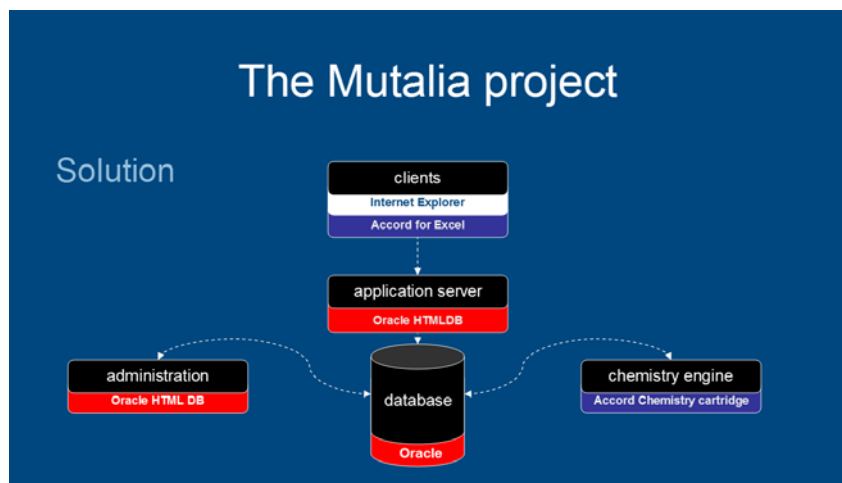
Building 'Mutalia', a Lead Discovery System, in 60 Days Dr Eric le Roux, DiscNgin

Located in the Biotech technology Park near Paris, DiscNgin is a young company founded in 2004 to provide professional services to biotechnology and pharmaceutical companies involved in drug discovery and research. Their already impressive client list includes names such as Sanofi-Aventis, Euroscreen, Mutabilis and Cytomics systems.

In a presentation at AccelrysWorld 2005 in London, Dr Le Roux summed up their philosophy as a drive to assist companies in catalyzing their innovation by providing resources to integrate technologies into the Discovery process in three areas:

- Controlling the introduction of technologies and increase the return on investment
- Reinforcing the expertise in scientific IT applied to discovery research
- Preserving scientific resources for innovation.

DiscNgin has business expertise in screening technology, chemical design & optimization, material management, pharmacological characterization, process automation and drug discovery workflow, and combines this with IT expertise in database and application development (especially using Oracle®), visualization and data pipelining – they have recently become an ISV partner for PipelinePilot™ development.



A schematic of the Mutalia solution created by DiscNgin.

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Recently, DiscNgin were retained by Mutabilis (a French biopharmaceutical company, founded in 2001 and specializing in antibacterial drug discovery) to create a lead discovery IT platform to support their newly-created medicinal chemistry department across biology, chemistry and inventory databases. The challenge was to create an effective platform in 3 months that was cost-effective (costing less than €60,000), could deal with several thousand molecular structures and associated biological data being used by 20 people, did not require the hiring of specialized IT staff and had minimal training requirements for those using and administrating it.

The discovery process workflow requirements on this platform were similarly stringent. Researchers had to be able to access all the necessary information across Mutabilis' extensive chemistry and biology databases as well as manipulate that data, analyze it, visualize it and add to it quickly and efficiently. Mutabilis also took the step of linking their data flow to their inventory requirements; this ensures that, as a small company, they would neither run out of nor waste reagents - enabling them to keep control of their stock rooms.

By using the Accord™ Chemistry Cartridge to 'chemistry-enable' Mutabilis' Oracle databases, Oracle's HTML DB and a mixture of Internet Explorer and Accord for Excel as clients, DiscNgin were able to meet all of these challenges easily in the 90-day timeframe, creating a tailor-made solution (Mutalia) and saving Mutabilis significant expenditure on an 'off-the-shelf' solution.

High-level feature-set		
Chemistry	Biology	Inventory
<ul style="list-style-type: none"> Compound registration Molecular descriptors calculation Substructure, exact, similarity, text searches SAR table generation Compound list management SD Files import/export 	<ul style="list-style-type: none"> Assay definition Data capture Data summarization Biological data export Assay list management 	<ul style="list-style-type: none"> Plate description management Plate list management Reagent management

The comprehensive list of top-level features were demanded - and were easily delivered using Accord

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