Case Study

MASCOT *Integra*

Ludwig Institute for Cancer Research relies on Mascot Integra for data management and process automation in proteomics research

The Proteomics Facility of the **Ludwig Institute for Cancer Research** (LICR) is led by **Professor Mike Waterfield**. Three research groups are located in the Cruciform Building on the University College London campus: Bioanalytical Chemistry, Cancer Proteomics, and Translational Cancer Proteomics.

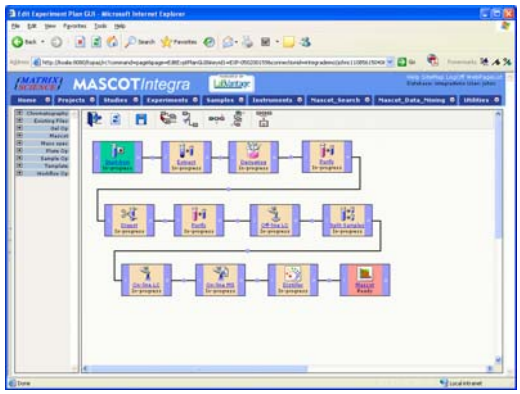
The aim of the **Bioanalytical Chemistry Group** is to develop bioanalytical tools, specifically within the field of mass spectrometry, to address important biological questions. Research interests include derivatisation and affinity chromatography as an alternative to gel electrophoresis, with the objective to create an integrated reliable and easy-to-use automated mass spectrometry based system for medium- to high-throughput characterization of proteomes.

Over the last two years, the **Cancer Proteomics Group** has optimized Fluorescence 2D-DIGE (2D-difference gel electrophoresis) for the rapid, sensitive and accurate detection of differential protein expression across multiple biological samples from different sources. The 2D-DIGE workflow is integrated with downstream identification and characterisation of proteins by mass spectrometry through a close

collaboration with the Bioanalytical Chemistry Group. Research is focused on cancer cell signalling, cancer biomarker identification, cellular stress responses and the integration of protein and mRNA screening data.

To accomplish their research objectives, best-of-breed instrumentation and software from many different manufacturers has been selected. With such diverse hardware, data management and process automation present a particular challenge. LICR selected Mascot Integra for this purpose because it offers a unique combination of capabilities:

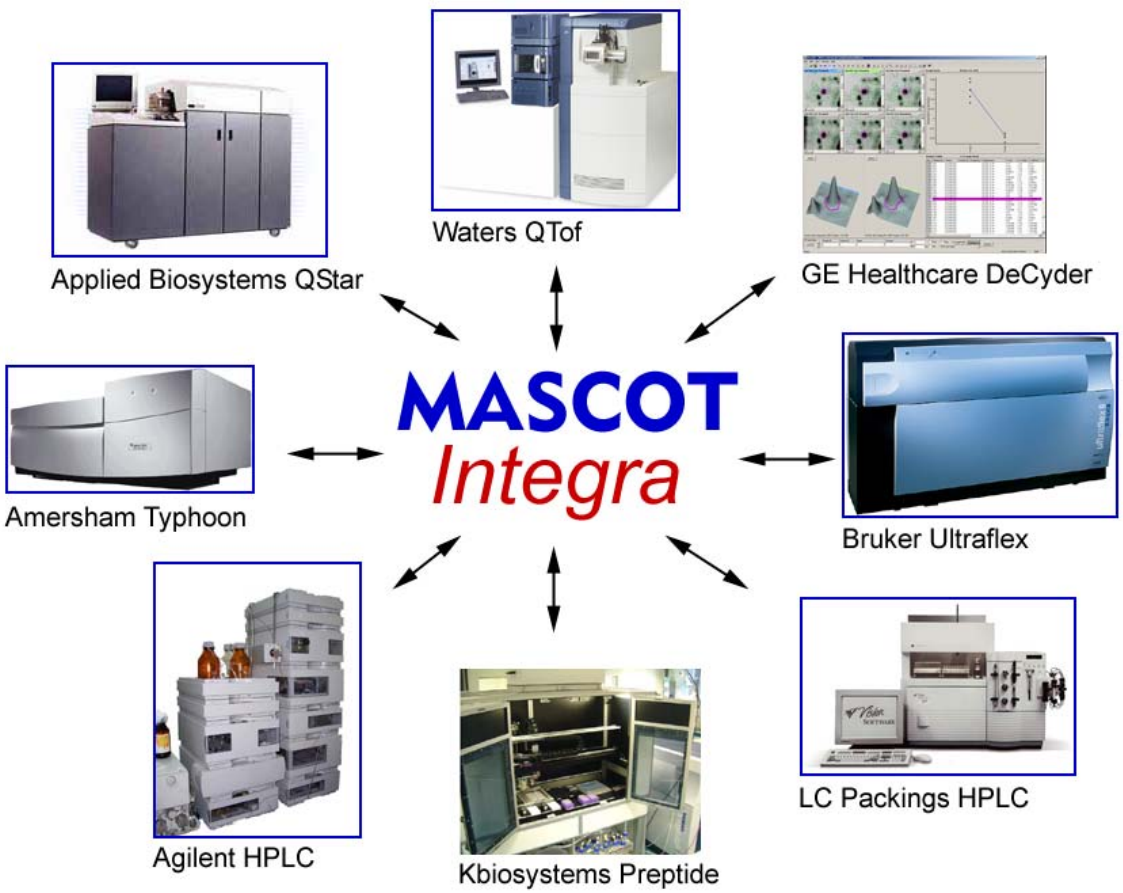
- Mascot Integra supports all of the experimental protocols used in proteomics research, including 1D gels, 2D gels, multi-dimensional chromatography, and both on-line and off-line mass spectrometry
- An intuitive drag & drop interface is used to model the experimental workflow
- Flexible and customisable integration based on file exchange for complex instruments, such as mass spectrometers, robotics, and chromatographs
- Complete automation of processing of raw mass spectrometry data into optimized peak lists and Mascot search submission
- Comprehensive reporting and data mining of Mascot search results



Mascot Integra has a true multi-tier architecture, allowing all of its functionality to be accessed through a standard web browser. The underlying database engine is Oracle®, ensuring that the system will scale to the largest and most demanding requirements. Role-based security allows access to certain projects, pages and functions to be restricted to project members.

Professor Waterfield describes the issues associated with proteomics data management:

"Our cell and molecular biologists are engaged in many complex collaborative experiments in cancer research, often interacting with clinicians, which makes a reliable informatics infrastructure essential. Mascot Integra is a key component of this infrastructure, managing the data associated with our proteomics programs. Virtually all of our instruments come with a dedicated data system, often of great sophistication. The challenge is to integrate these disparate data sources in a way that is flexible enough to cope with the rapid evolution of the individual tools. For the scientist, trying to answer difficult biological questions, it is paramount that all of the relevant information is consolidated into a single database, which can be managed and queried efficiently."



Selected recent publications from the Bioanalytical Chemistry Group at LICR:

Cutillas, P. R., Chalkley, R. J., Hansen, K. C., Cramer, R., Norden, A. G., Waterfield, M. D., Burlingame, A. L. and Unwin, R. J. (2004). The urinary proteome in Fanconi syndrome implies specificity in the reabsorption of proteins by renal proximal tubule cells. Am J Physiol Renal Physiol, 287, F353-64.

Barnouin, K. N., Hart, S. R., Thompson, A. J., Okuyama, M., Waterfield, M. and Cramer, R. (2005). Enhanced phosphopeptide isolation by Fe(III)-IMAC using 1,1,1,3,3,3-hexafluoroisopropanol. Proteomics, 5, 4376-88.

Chan, H. L., Gharbi, S., Gaffney, P. R., Cramer, R., Waterfield, M. D. and Timms, J. F. (2005). Proteomic analysis of redox- and ErbB2-dependent changes in mammary luminal epithelial cells using cysteine- and lysine-labelling two-dimensional difference gel electrophoresis. Proteomics, 5, 2908-26.

Weeks, M. E., Sinclair, J., Jacob, R. J., Saxton, M. J., Kirby, S., Jones, J., Waterfield, M. D., Cramer, R. and Timms, J. F. (2005). Stress-induced changes in the Schizosaccharomyces pombe proteome using two-dimensional difference gel electrophoresis, mass spectrometry and a novel integrated robotics platform. Proteomics, 5, 1669-85.

Cutillas, P. R., Biber, J., Marks, J., Jacob, R., Stieger, B., Cramer, R., Waterfield, M., Burlingame, A. L. and Unwin, R. J. (2005). Proteomic analysis of plasma membrane vesicles isolated from the rat renal cortex. Proteomics, 5, 101-12.

Home page: **www.ludwig.ucl.ac.uk/licr_html/welcome.htm**

For more information about Mascot Integra, including over 45 minutes of Flash movies, visit **www.matrixscience.com**/integra.html

The sample tracking and workflow technology that underlies Mascot Integra has been developed by LabVantage Solutions, Inc. This ensures that Mascot Integra is compatible with and upgradeable to LabVantage's range of enterprise LIMS products. For more information visit http://www.labvantage.com/integra

Publication 2006-02-07