

DEDICATED RESOURCES FOR PTM IDENTIFICATION

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Proteomics experiments through mass spectrometry data together with bioinformatics analysis have greatly improved the identification and characterisation of post-translational modifications (PTM). In this talk, some of our contributions to this field will be presented. Among our bioinformatics tools, QuickMod is an MS/MS search tool that takes full advantage of the speed and accuracy of a library search while exploring the experimental data for modified variants of peptides in the library. QuickMod is part of our identification workflow, which enables a more complete annotation of MS/MS datasets providing a better understanding of the biological system under investigation. All software in our identification workflow is open source, implemented in Java based on the Java Proteome Library (JPL), available at <http://sourceforge.net/projects/javaprotlib/>.

The group has a long standing experience in data integration, data management and storage (SWISS-2DPAGE and the ExPASy server are just two examples). Lately, special attention is devoted to the functional role of sugars whether added enzymatically (glycosylation) or non-enzymatically (glycation) to proteins.

A heterogeneous range of bioinformatics databases and tools is now available on the web for glycomics studies. But as pointed out in a recent review [1], the landscape looks “like disconnected islands”. Connecting islands is an urgent task that can be undertaken while selecting and inserting existing resources in workflows.

Linking resources is a solution to dealing with an ever-increasing data flow and to extracting useful information. Previous experience in proteomics can benefit glycomics studies. These different disconnected resources need to be collected in a single virtual space and linked together to allow knowledge of the structure and function of the glycosylation of proteins to be determined in much the same way as the structure and function of proteins has been facilitated by the integration of proteomics knowledge

into UniProt (<http://www.uniprot.org/>). We are collecting as much data on the glycosylation of proteins that is available to us and are attempting to create a UniCarb equivalent for the integration of glycomics knowledge. The project is becoming concrete through the cross-linking of three resources developed in collaboration between SIB and groups in Australia, Ireland and Sweden (GlycosuiteDB, SugarBind and UniCarb-DB).

[1]. Lütteke T. *Chembiochem* 9(13):2155-60, 2008