GlycoVault: An online storage and visualization system for glycan structures

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Abstract

Glycans are complex chains of monosaccharides that play critical roles in several structural and modulatory functions in cells. Despite the deficiency in informatics tools for glycans, high throughput technologies have led to the production of ever increasing amounts of glycan data [1]. Glycobiology labs are currently using several different technologies to produce many different types of data. Unfortunately this diversity in data makes it difficult to create a central storage system and information is saved as a jumble of spreadsheets and text files. Further compounding the problem is the visual nature of glycan data, with many labs resorting to storing structure information as hand-drawn annotation on printouts of spreadsheets.

In order to address the need for a centralized storage and visualization platform for glycan data we developed the web-based GlycoVault system. GlycoVault allows users to upload and store experimental glycan data such as GlycoMod [2] files along with some annotation data. These files can be later retrieved and used to generate visual reports listing figures of glycan structures observed in an experiment. GlycoVault also contains several interactive tools to visually explore glycan structures. A drawing tool is available to interactively draw and store glycan structures. In addition, GlycoVault allows users to create networks of glycan structures and then visualize pathways connecting different structures. Users can also determine what reactions are necessary to convert one glycan structure into another.

GlycoDigit

GlycoVault uses the GlycoDigit [3] format to represent glycan structures internally. GlycoDigit is a fixed-length alpha-numeric code for representing glycan structures commonly found in secreted glycoproteins. The code uses a pre-assigned alpha-numeric index to represent the monosaccharides attached in different branches to the core glycan structure. The numeric nature of the code makes it ideal for the development of a mathematical operators and algorithms to compare glycan structures.

GlycoDigit Code

0x 3g 1a 3a 0x 0x 2c

Overview of Glycan Data Workflow
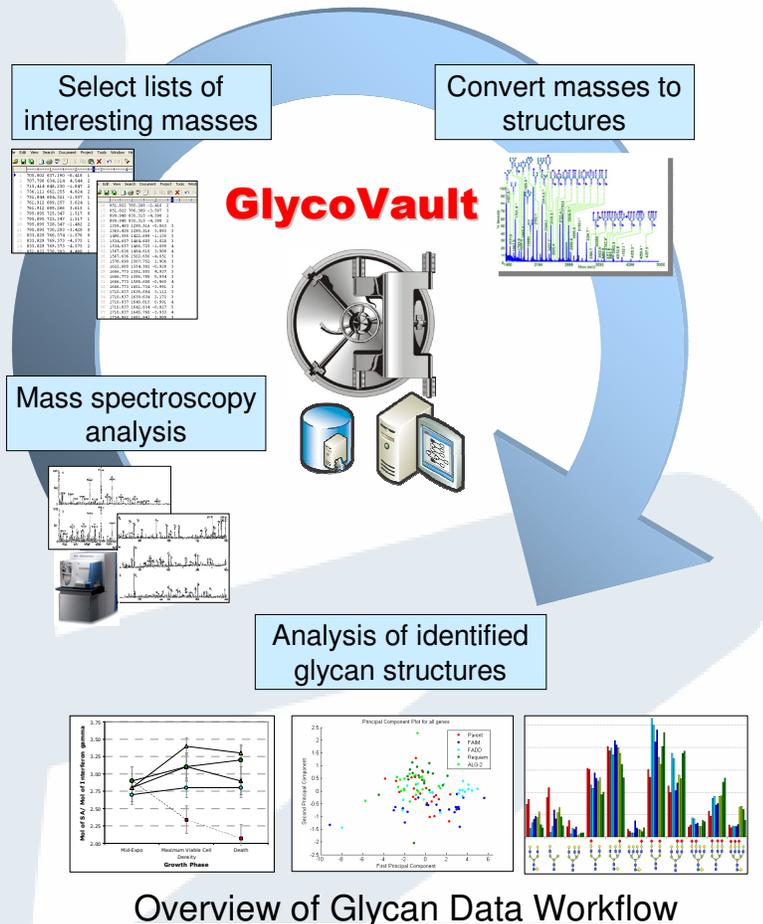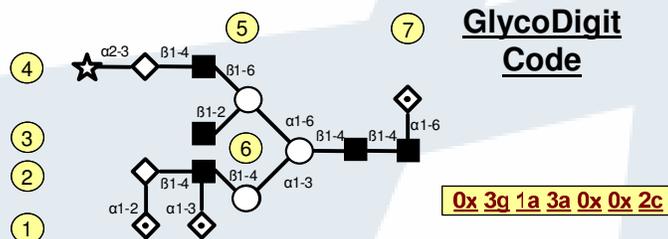
Interface and Features

Glycan Mapper

Report Generation

Interactive Visualization

Glycan Pathway Analysis

MS Analysis

Features of GlycoVault:

• GlycoVault acts as a storage and management system for glycan data.

• Users can upload GlycoMod files and automatically generate reports of glycan structures obtained.

• Based on GlycoDigit representation system, GlycoMod output is converted to pictorial representation.

• While uploading GlycoMod files users can also enter experimental conditions such as cell line, culture type, pH, temperature, etc.

• Users can later search for glycan data either through name of experimenter or date the experiment was conducted.

• GlycoVault also provides tools to visually explore glycan structures through an interactive drawing interface.

References

[1] Pérez, S. and Mulloy, B. 2005. Prospects for glycoinformatics. *Curr. Opin. Struct. Biol.*, 15:517-524.

[2] Cooper C.A., Gasteiger E. and Packer N. 2001. GlycoMod - A software tool for determining glycosylation compositions from mass spectrometric data. *Proteomics*, 1:340-349.

[3] Yusufi F.N.K., Park W., Lee M.M. and Lee D.-Y. 2008. An alpha-numeric code for representing N-linked glycan structures in secreted glycoproteins. (submitted)