GlycoVault: A Bioinformatics Infrastructure for Glycan Pathway Visualization, Analysis and Modeling

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GlycoVault

- Integrated bioinformatics infrastructure that can serve as a resource to end users, other programs and applications
- Collects data and knowledge from different resources
- Supports glycan data analysis
- Provides foundation for integration and visualization of knowledge and data
Motivation
Why Not Just a Simple Database?

- Including ontologies allows greater flexibility
- Complex relationships often stored across many relational tables
- Complexity increases as the number of properties to be stored increases
- Querying is often complex and involves many tables
Application Support

- GlycoVault supports data retrieval in different formats that can be used by other applications instantly.

- Some of the applications supported include:
  - GlycoBrowser
    - Ontology based visualization tool that supports glycan pathway analysis
  - GlyMpse
    - Ontology driven simulation tool for biochemical pathways
System Architecture

Glyco Browser
GlycoVault Gateway
GlyMpse

REST Web Services (Remote Access)

GlycoVault API (Local Access)

XPath,XQuery
Java Methods
SPARQL

Glyde-II
GOM
GlycO

XML
Java Object Model
OWL

Structures and Pathways

Experimental Data

ApachePOI
JDBC/SQL

Spread sheets
Relational Tables
Example for Contents in GlycoVault

Gene -> Transcribes -> Transcripts

Transcribe -> Translate -> Protein

Protein -> Enzyme | Structured Protein

Protein -> Catalyze

Catalyze -> Reaction

Reaction -> Consists

Consists -> Produce | Consume

Asn -> Asn -> Asn -> Asn
How It Is Populated?

- Workflow engines
  - rt-PCR workflow
  - Glyco Analysis workflow (under development)

- Ontology Population
  - GlycO Qrator

- Administrators would be able to upload files using the GlycoVault API
GlycoVault API (Local Access)
Web-based User Interface

- Supports data retrieval from GlycoVault
- Aggregation of services designed to support efficient usage of available data
- Supports different users
  - pure biologists
  - professional computer scientists
A mockup home page for GlycoVault Gateway
Conclusions and Future Work

- Multi-faceted approach provides flexibility in utilizing content
- API supports data retrieval in different formats to support various applications
- A user friendly interface called “GlycoVault Gateway” is being developed
Thank You

Questions