

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

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NCRR

Integrated Technology Resource for Biomedical Glycomics



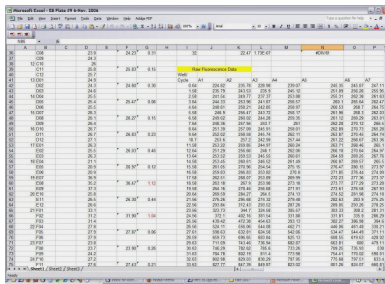


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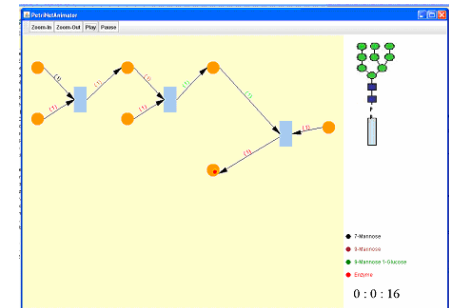
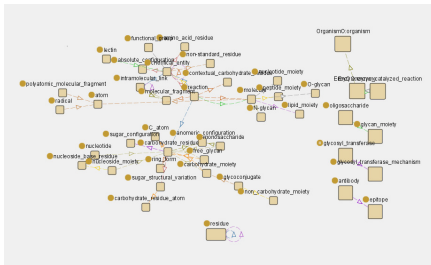
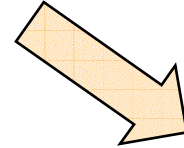
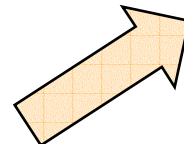
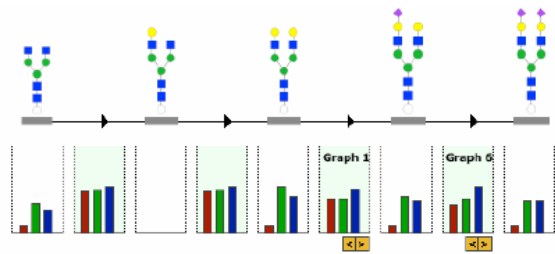
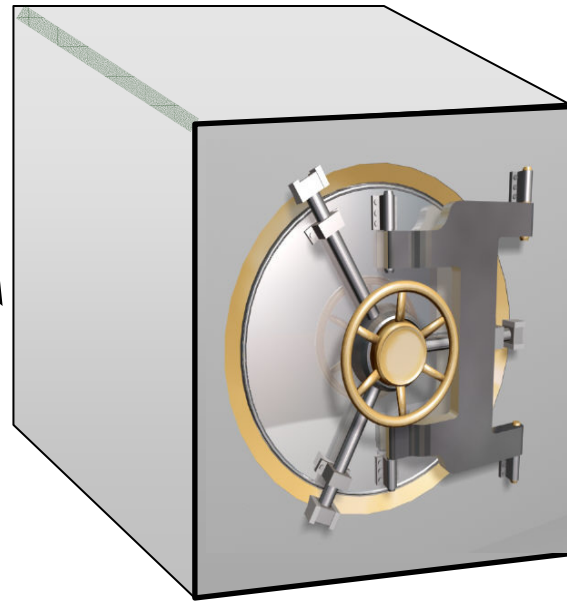
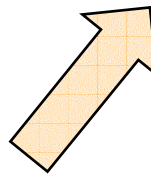
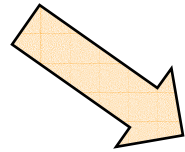
GlycoVault

- ❑ 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



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100





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

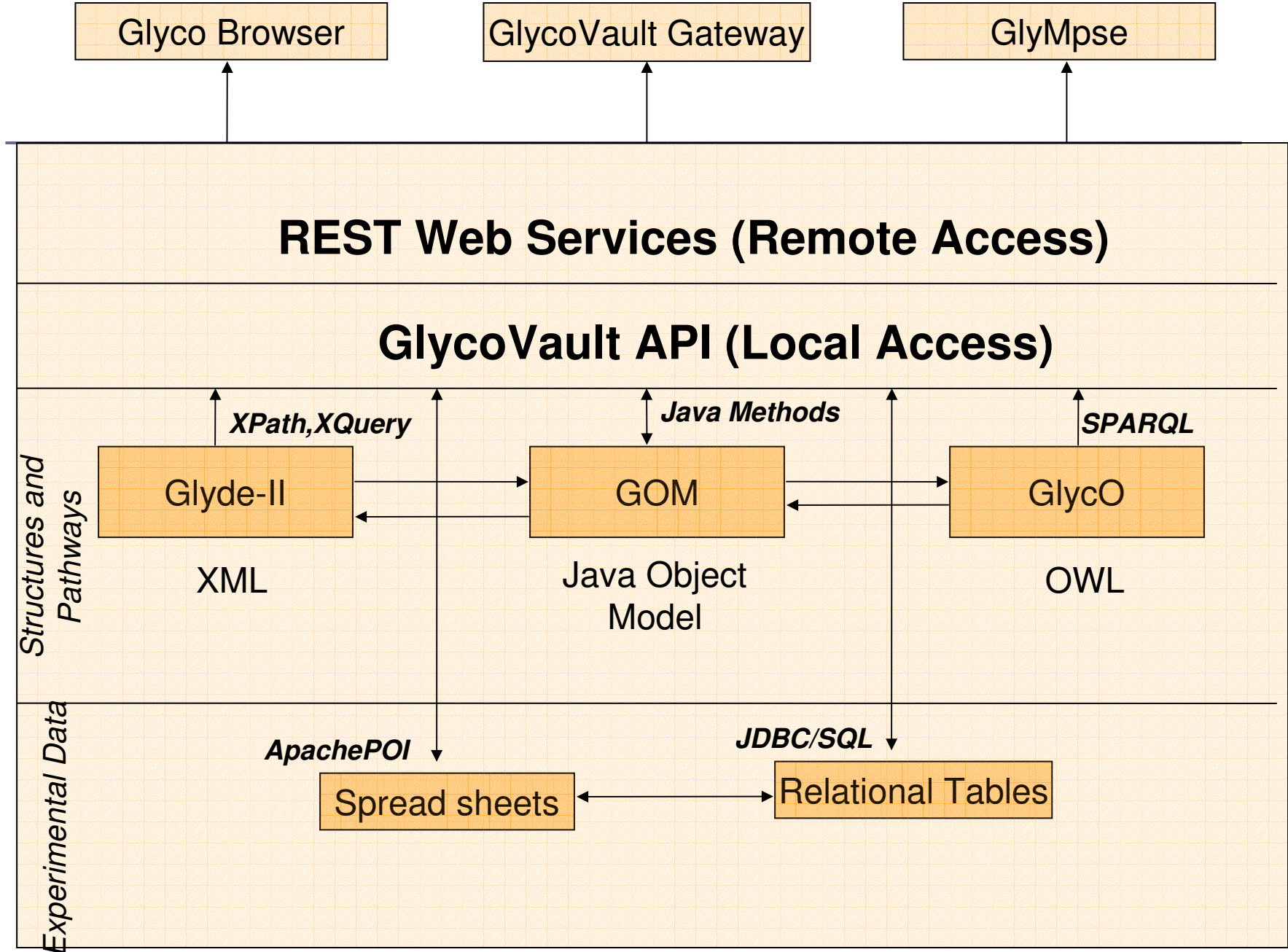


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Application Support

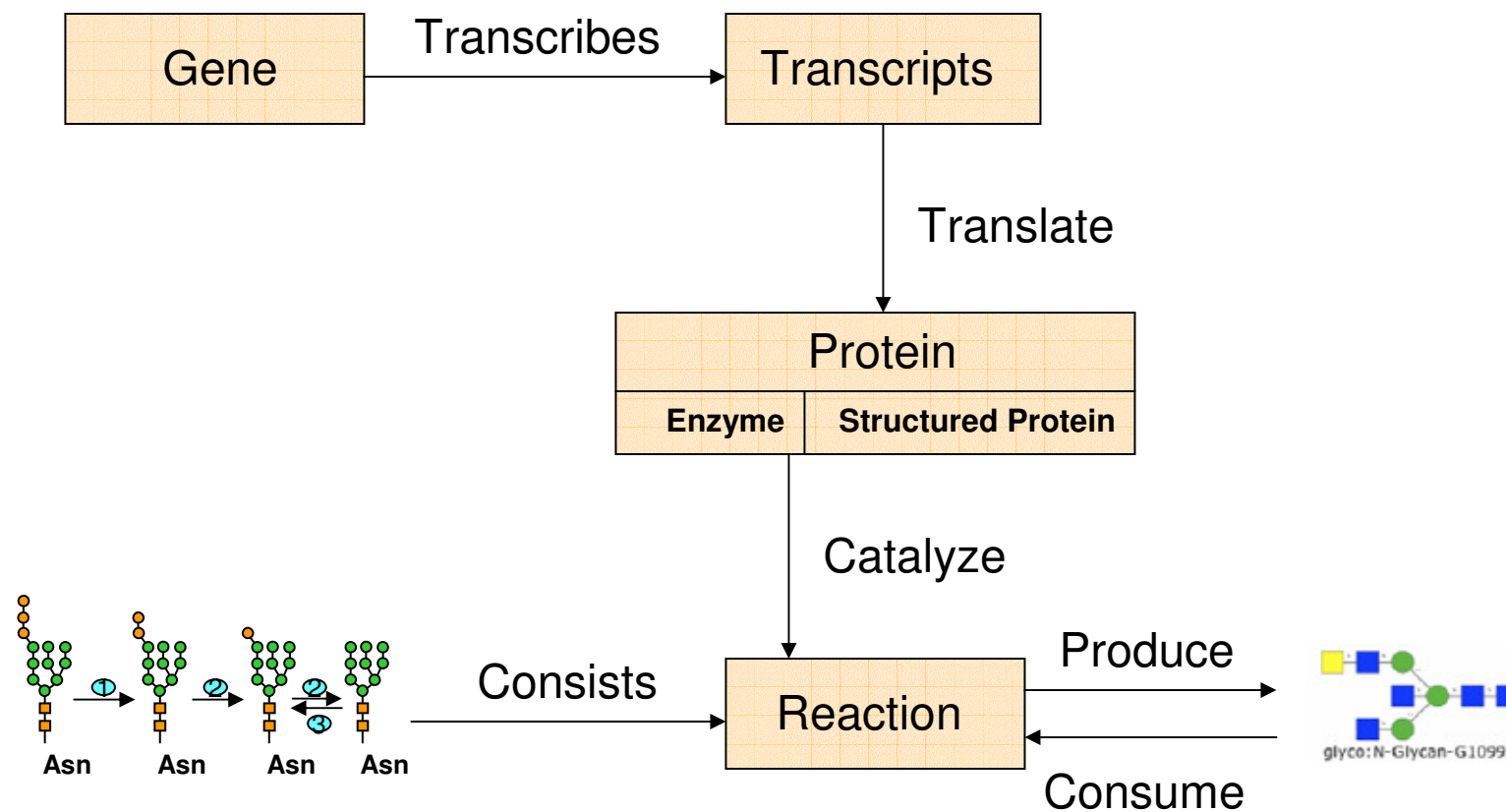
- GlycoVault supports data retrieval in different formats that can be used by other applications instantly
- Some of the applications supported include:
 - GlycoBrowser
 - Ontology based visualization tool that supports glycan pathway analysis
 - GlyMpse
 - Ontology driven simulation tool for biochemical pathways

System Architecture





Example for Contents in GlycoVault





How It Is Populated?

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

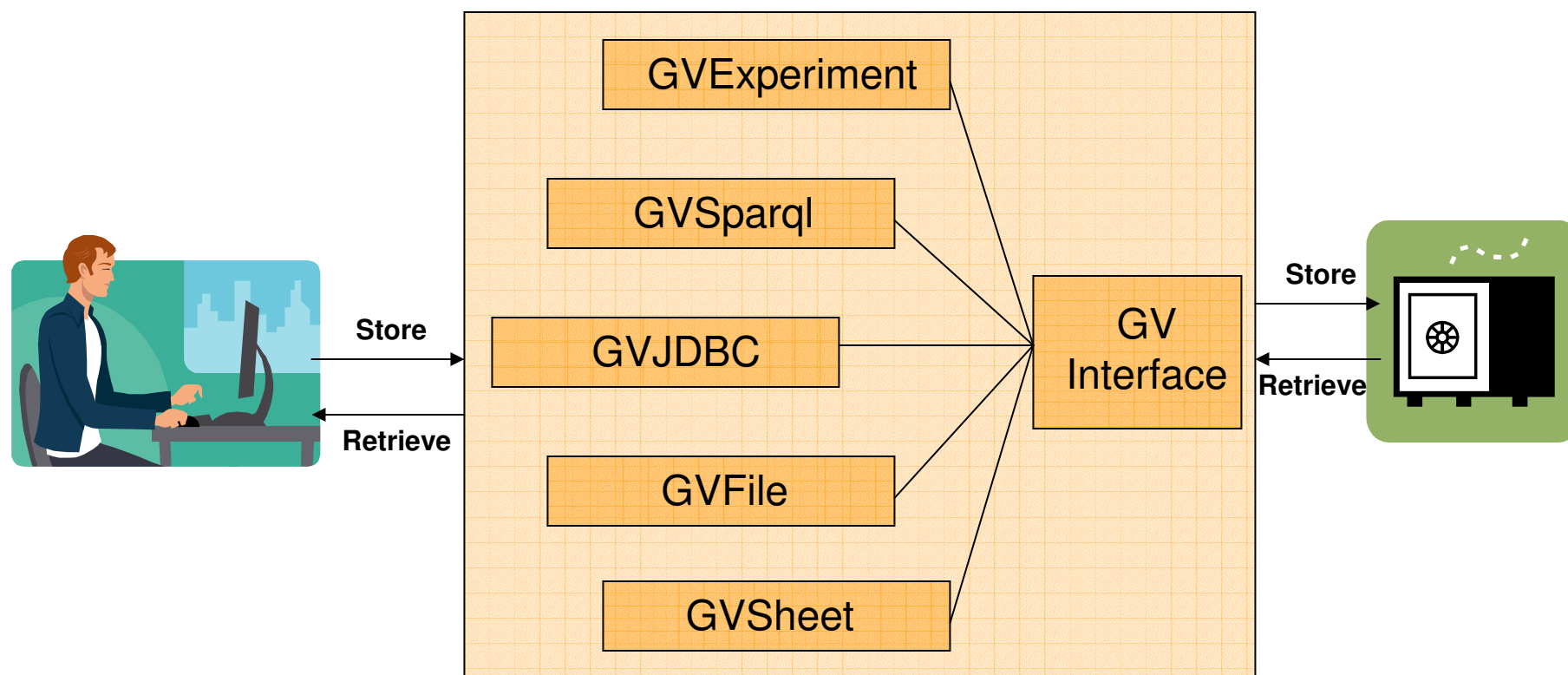
- Ontology Population
 - Glyco Qrator

- Administrators would be able to upload files using the GlycoVault API



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GlycoVault API (Local Access)



GlycoVault API



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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

New Page 1 - Windows Internet Explorer

C:\Documents and Settings\Rajesh\Desktop\glycanbrowser.html

Google

Home LSDIS Glycomics About Us

GlycoVault Gateway

GlycoVault provides a means of storing and retrieving data to support glycomics research at the Complex Carbohydrates Research Center (CCRC) at the University of Georgia. These data include quantitative Real-Time Polymerase Chain Reaction (qRT-PCR) data as well as basic glycomics data. Biologically relevant parameters (such as flow cytometry profiles) and various types of data collected by the analytical services component of the Center, along with the explicit and implicit knowledge required to analyze and interpret these data. GlycoVault consists of databases, ontologies, and variously formatted data files that are integrated by a sophisticated organizational structure and accessed by a comprehensive. GlycoVault Browser provides access to data and knowledge stored as XML, RDF, OWL, Relational Tables, Object Model and Spreadsheets.

	Structures/Sequences	Abundance Data
Glycans		
N-linked	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
O-linked	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Gene	<input checked="" type="checkbox"/>	
Protein		
Enzyme	<input checked="" type="checkbox"/>	
Structural Protein	<input checked="" type="checkbox"/>	
Transcript		

Services				Applications
Service Name	Description	Sample Client	Input Form	
Query Glycans	Service to retrieve glycan.....more	Glycan Client	Query	GlycoBrowser
Glyde2SVG	Convert Glydell structure to ...more	SVGClient	SVG	
File Download	Download Experiment...more	FileClient	File	GlyMpse
Glydell to Linucs	Convert Glydell format...more	Glydell Client	Gly2Li	
Linucs to IUPAC	Convert form Linucs format...more	Lin2IUP Client	Lin2IUP	

..more services

Done

start

New Page 1 - Windo...

My Computer 100%

6:17 PM



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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



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