

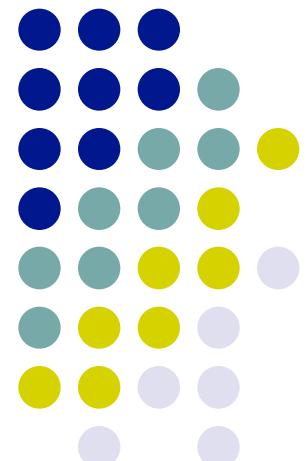
GNOme – A glycan naming and subsumption ontology

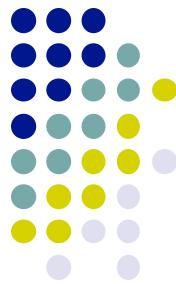


Nathan Edwards

Department of Biochemistry and
Molecular & Cellular Biology

Georgetown University Medical Center

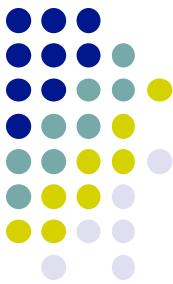




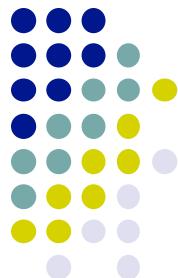
About me...

- Celera Genomics + Applied Biosystems
 - Proteomics pipelines, peptide identification software, informatics of new MS technologies
- NCI Clinical Proteomics Tumor Analysis Consortium (CPTAC Phases I,II,III):
 - Novel peptides using genomic/transcripts data
 - Data Coordinating Center (DCC/Portal)
 - Common Data Analysis Pipeline (AWS/Galaxy)
- Intact glycopeptide MS/MS / SWATH tools
 - w/ Rado Goldman (also Georgetown)

Glycans are complex molecules



- Difficult to completely characterize
 - Mass spectrometry, etc.
- Partial characterization is common
 - Prior (biological) knowledge can fill in some gaps
 - Sample manipulation (glycosidases, etc.), too...
- Difficult to describe extent of characterization
 - Complex “sequence” formats precisely describe known and missing details
- Accessions provide a stable identifier
 - Link to explicit sequence formats



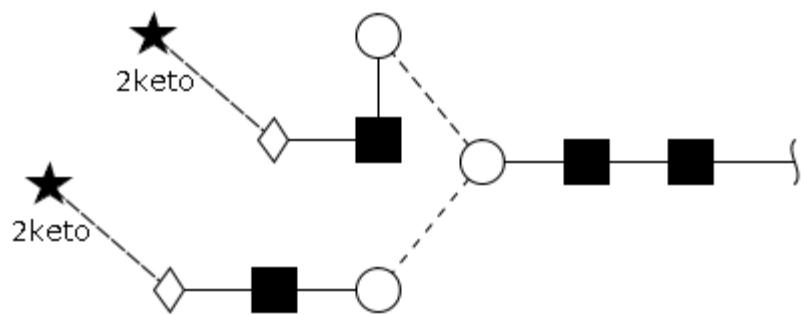
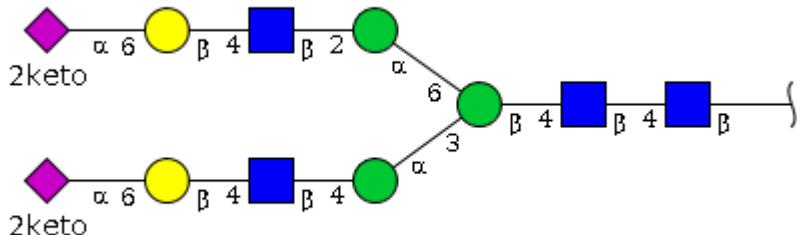
Glycan Structure Descriptions

GlyTouCan: G39764AC
 PubChem: SID252281000
 GlycomeDb: 9088

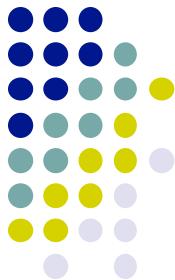
Neu5Ac(a2-6)Gal(b1-4)GlcNAc(b1-4)Man(a1-3)[Neu5Ac(a2-6)Gal(b1-4)GlcNAc(b1-2)Man(a1-6)]Man(b1-4)GlcNAc(b1-4)GlcNAc(b1-

WURCS=2.0/5,11,10/[a2122h-1b_1-5_2*NCC/3=O][a1122h-1b_1-5][a1122h-1a_1-5][a2112h-1b_1-5][Aad21122h-2a_2-6_5*NCC/3=O]/
1-1-2-3-1-4-5-3-1-4-5/a4-b1_b4-c1_c3-d1_c6-h1_d4-e1_e4-f1_f6-g2_h2-i1_i4-j1_j6-k2

RES	LIN
1b:b-dglc-HEX-1:5	1:1d(2+1)2n
2s:n-acetyl	2:1o(4+1)3d
3b:b-dglc-HEX-1:5	3:3d(2+1)4n
4s:n-acetyl	4:3o(4+1)5d
5b:b-dman-HEX-1:5	5:5o(3+1)6d
6b:a-dman-HEX-1:5	6:6o(4+1)7d
7b:b-dglc-HEX-1:5	7:7d(2+1)8n
8s:n-acetyl	8:7o(4+1)9d
9b:b-dgal-HEX-1:5	9:9o(6+2)10d
10b:a-dgro-dgal-NON-2:6 1:a 2:keto 3:d	10:10d(5+1)11n
11s:n-acetyl	11:5o(6+1)12d
12b:a-dman-HEX-1:5	12:12o(2+1)13d
13b:b-dglc-HEX-1:5	13:13d(2+1)14n
14s:n-acetyl	14:13o(4+1)15d
15b:b-dgal-HEX-1:5	15:15o(6+2)16d
16b:a-dgro-dgal-NON-2:6 1:a 2:keto 3:d	16:16d(5+1)17n
17s:n-acetyl	



Glycan (Partial) Structure Descriptions

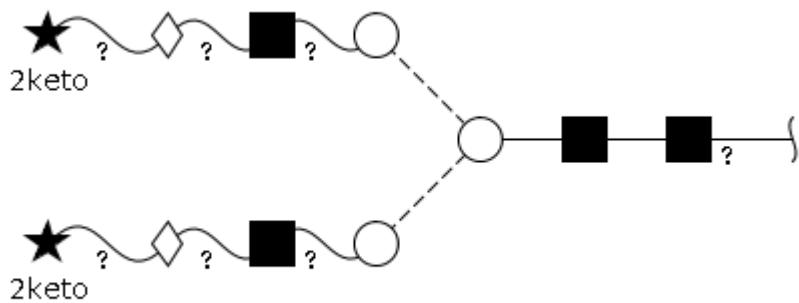
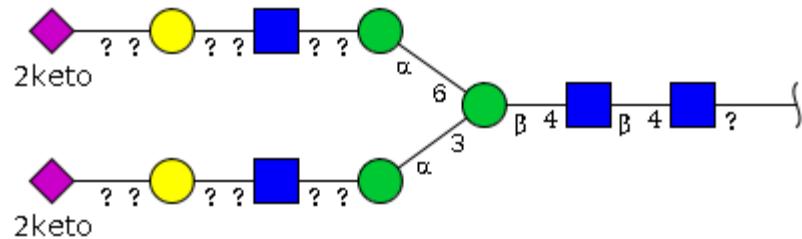


GlyTouCan: G27817LK
UniCarbKB: 4923
GlycomeDb: 39722

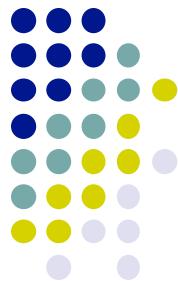
Neu5Ac(?2-?)Gal(?1-?)GlcNAc(?1-?)Man(a1-3)[Neu5Ac(?2-?)Gal(?1-?)GlcNAc(?1-?)Man(a1-6)]Man(b1-4)GlcNAc(b1-4)GlcNAc(?1-

WURCS=2.0/6,11,10/[a2122h-1x_1-5_2*NCC/3=O][a2122h-1b_1-5_2*NCC/3=O][a1122h-1b_1-5][a1122h-1a_1-5][a2112h-1x_1-5]
[Aad21122h-2x_2-6_5*NCC/3=O]/1-2-3-4-1-5-6-4-1-5-6/a4-b1_b4-c1_c3-d1_c6-h1_d?-e1_e?-f1_f?-g2_h?-i1_i?-j1_j?-k2

RES	LIN
1b:x-dglc-HEX-1:5	1:1d(2+1)2n
2s:n-acetyl	2:1o(4+1)3d
3b:b-dglc-HEX-1:5	3:3d(2+1)4n
4s:n-acetyl	4:3o(4+1)5d
5b:b-dman-HEX-1:5	5:5o(3+1)6d
6b:a-dman-HEX-1:5	6:6o(-1+1)7d
7b:x-dglc-HEX-1:5	7:7o(-1+1)8d
8b:x-dgal-HEX-1:5	8:8o(-1+2)9d
9b:x-dgro-dgal-NON-2:6 1:a 2:keto 3:d	9:9d(5+1)10n
10s:n-acetyl	10:7d(2+1)11n
11s:n-acetyl	11:5o(6+1)12d
12b:a-dman-HEX-1:5	12:12o(-1+1)13d
13b:x-dglc-HEX-1:5	13:13o(-1+1)14d
14b:x-dgal-HEX-1:5	14:14o(-1+2)15d
15b:x-dgro-dgal-NON-2:6 1:a 2:keto 3:d	15:15d(5+1)16n
16s:n-acetyl	16:13d(2+1)17n
17s:n-acetyl	



Glycan (Partial) Structure Descriptions

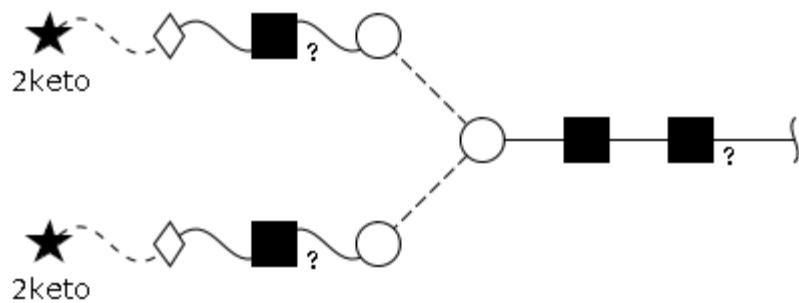
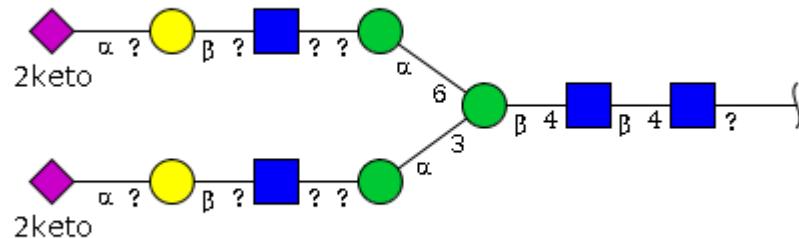


GlyTouCan: G97545TB
UniCarbKB: 4227
GlycomeDb: 39610

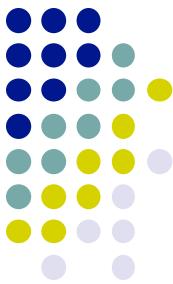
Neu5Ac(a2-?)Gal(b1-?)GlcNAc(?1-?)Man(a1-3)[Neu5Ac(a2-?)Gal(b1-?)GlcNAc(?1-?)Man(a1-6)]Man(b1-4)GlcNAc(b1-4)GlcNAc(?1-

WURCS=2.0/6,11,10/[a2122h-1x_1-5_2*NCC/3=O][a2122h-1b_1-5_2*NCC/3=O][a1122h-1b_1-5][a1122h-1a_1-5][a2112h-1b_1-5]
[Aad2112h-2a_2-6_5*NCC/3=O]/1-2-3-4-1-5-6-4-1-5-6/a4-b1_b4-c1_c3-d1_c6-h1_d?-e1_e?-f1_f?-g2_h?-i1_i?-j1_j?-k2

RES	LIN
1b:x-dglc-HEX-1:5	1:1d(2+1)2n
2s:n-acetyl	2:1o(4+1)3d
3b:b-dglc-HEX-1:5	3:3d(2+1)4n
4s:n-acetyl	4:3o(4+1)5d
5b:b-dman-HEX-1:5	5:5o(3+1)6d
6b:a-dman-HEX-1:5	6:6o(-1+1)7d
7b:x-dglc-HEX-1:5	7:7o(-1+1)8d
8b:b-dgal-HEX-1:5	8:8o(-1+2)9d
9b:a-dgro-dgal-NON-2:6 1:a 2:keto 3:d	9:9d(5+1)10n
10s:n-acetyl	10:7d(2+1)11n
11s:n-acetyl	11:5o(6+1)12d
12b:a-dman-HEX-1:5	12:12o(-1+1)13d
13b:x-dglc-HEX-1:5	13:13o(-1+1)14d
14b:b-dgal-HEX-1:5	14:14o(-1+2)15d
15b:a-dgro-dgal-NON-2:6 1:a 2:keto 3:d	15:15d(5+1)16n
16s:n-acetyl	16:13d(2+1)17n
17s:n-acetyl	

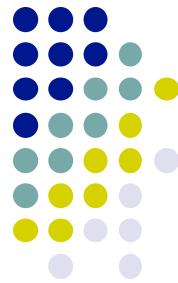


Glycans are complex molecules



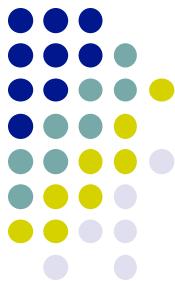
- Manuscripts and tools often use a short-hand
 - Monosaccharide composition
 - 4 GlcNAc, 3 Man, 2 Gal, 2 Neu5Ac (4-3-2-2-0)
 - 4 HexNAc, 5 Hex, 2 Neu5Ac (4-5-2-0)
 - Words (!)
 - Bi-antennary di-sialated complex N-glycan
 - Abbreviations
 - A2G2S2, 2A2SA,
 - Pictures
- Linking with accessions is difficult...

Finding GlyTouCan Structure Descriptions



- 49 GlyTouCan glycans by composition
- 68 GlyTouCan glycans by mol. weight
- 95 GlyTouCan glycans by int. mol wt

Finding GlyTouCan Structure Descriptions



Glycan Repository [Secure | https://glytoucan.org/Structures](https://glytoucan.org/Structures)

Registration Search View All Preferences Sign in Accession Number

Number of Glycans: 133 [Reset all conditions](#)

Current status

- Motif
- Monosaccharide
- Mass range 2222~2223
- Linked DB

List WURCS GlycoCT Sort Date Entered Down 1 2 ... 7 >

Accession Number G80123ZU

Calculated Monoisotopic Mass 2222.783

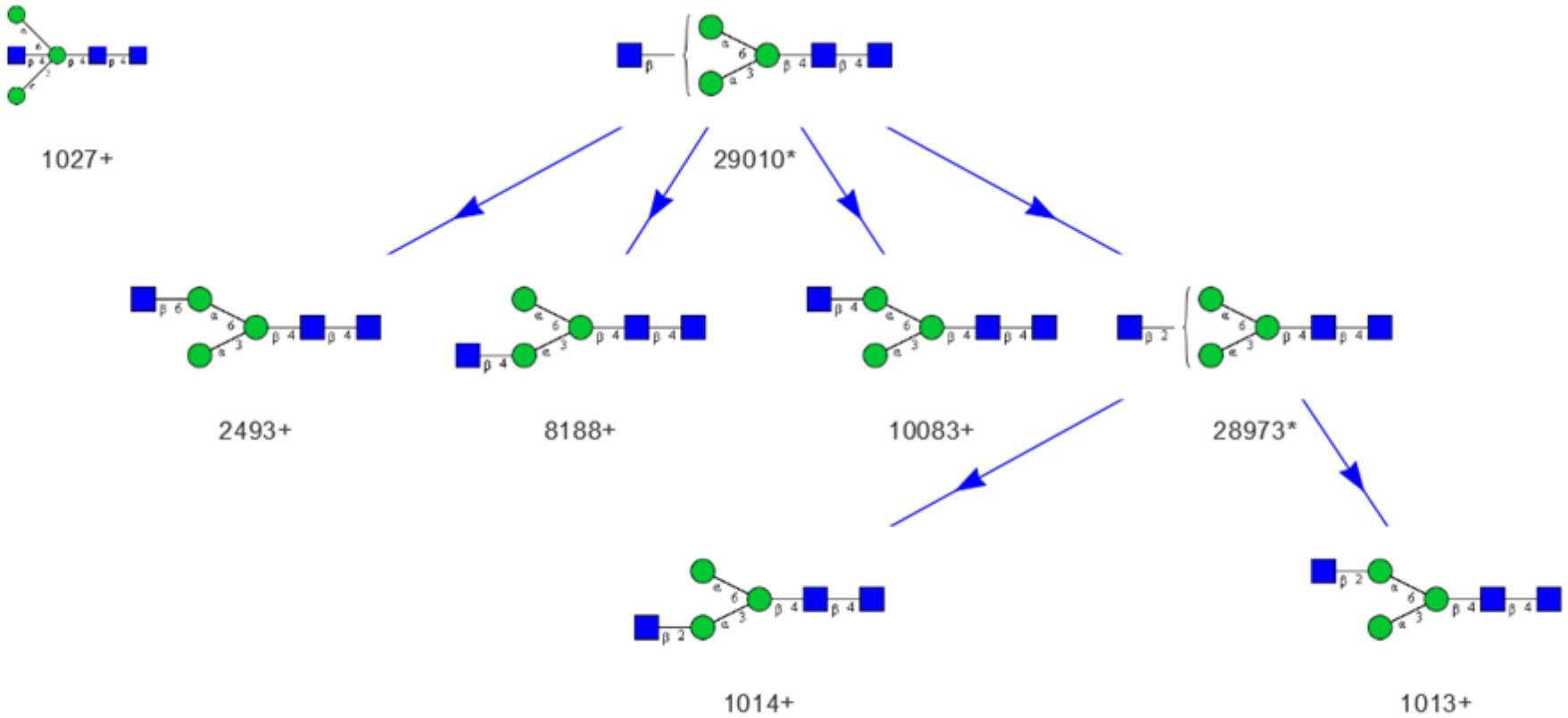
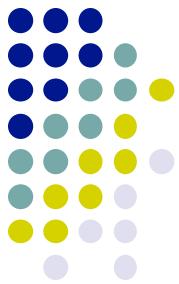
Contribution time Tue, 31 Oct 2017 22:21:52 GMT

Accession Number G34449FW

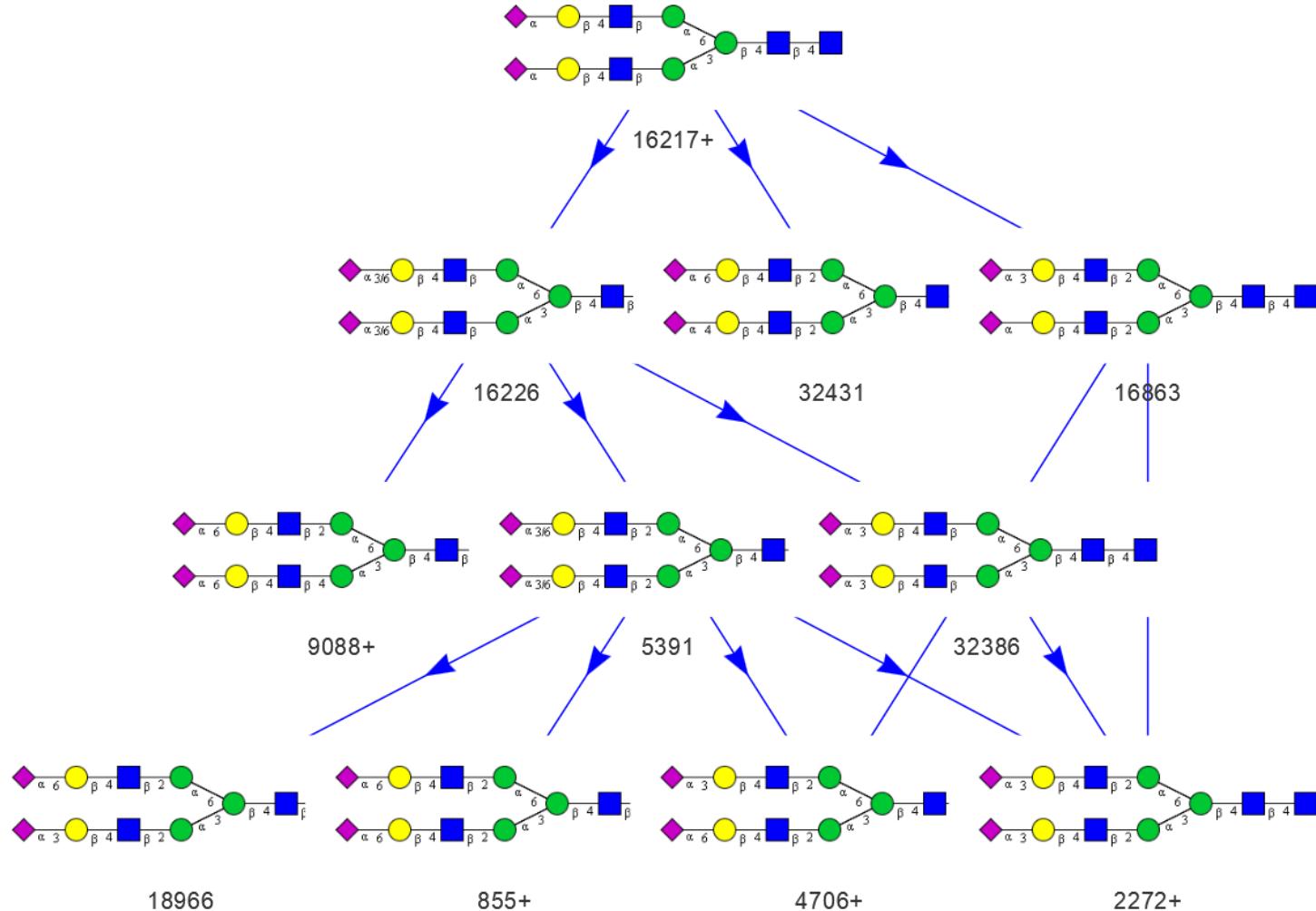
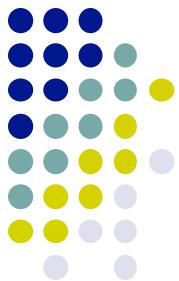
Calculated Monoisotopic Mass 2222.783

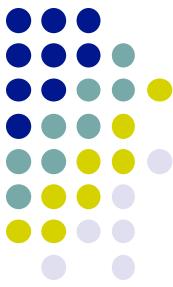
Contribution time Tue, 31 Oct 2017 22:20:29 GMT

Glycan (Partial) Structure Subsumption



Glycan (Partial) Structure Subsumption





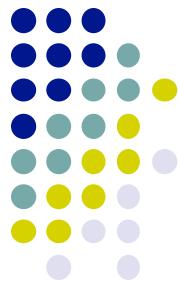
GlyGen Glycans

- Glycans from GlyTouCan
 - Primary accessions
 - Complete WURCS coverage - GlycoCT partial
 - Species/Motif annotations
- Glycans from UniCarbKB
 - Connection to UniProt proteins (vital!)
 - Species / Protein-based species annotations
 - Accessions linked from GlyTouCan



GlyGen Glycans (Year 1)

- Require human and mouse glycans, but...
 - Species annotations are sparse
- Data-resources do not annotate consistent (partial) structure descriptions
 - Human curators extract structure descriptions from manuscripts inconsistently,
 - Different resources see different manuscripts
- Human Glycans:
 - GlyTouCan: 2261; UniCarbKB: 1854 (1471);
 - In common: 486



GlyGen Glycans

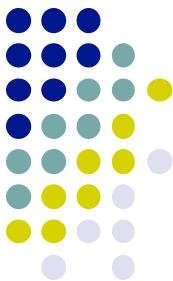
- Which compositions, topologies are human?
 - Use subsumption relationships to propagate annotation
 - Semantics: ...at least one glycan structure...
- Merged human annotation:
 - (Partial?) Structures: 3455 (+621)
 - Topologies: 1720 (+1707)
 - Compositions: 0 (+1062)



GlyGen Glycoenzymes

- Glycosylation enzyme annotations
 - ID mapping: GlycO → GlycomeDb → GlyTouCan
- GlycO “tree” of potential structures
 - w/ species specific glycotransferase annotations
 - Glycan monosaccharide indexing
- Will York, Alison Nairn, Kelley Moremen (CCRC)

GlyGen Glycan Data Integration



SMW x + - ×

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Main Page

Summary

BaseCompositions	834
Compositions	1132
Topologies	2915
Saccharides	8585
All	13466

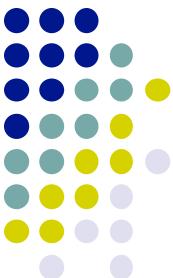
Annotation

Saccharides	GlyTouCan	UniCarbKB	UniCarb-DB	GlycO	Subsumption	Any
Human	2224	1364	31		802	3455
Mouse	345	238	3		346	817
N-Linked	2905				1237	3058
O-Linked	944				390	1032
Human Enzyme				0		0
Mouse Enzyme				583		583
Human Substrate		838				838
Mouse Substrate		85				85

Topologies	GlyTouCan	UniCarbKB	UniCarb-DB	GlycO	Subsumption	Any
Human	3	11	0		1717	1720
Mouse	2	2	0		391	393

Contents [hide]

- 1 Summary
- 2 Annotation
- 3 Human N-Linked Glycans
- 4 Mouse N-Linked Glycans
- 5 Other N-Linked Glycans
- 6 Human O-Linked Glycans
- 7 Mouse O-Linked Glycans
- 8 Other O-Linked Glycans
- 9 Human Misc. Glycans
- 10 Mouse Misc. Glycans
- 11 Other Misc. Glycans



GlyGen Glycan Data Integration

G35370OW - SMW x + - □ ×

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G35370OW

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Identifiers

GlyTouCan	G35370OW
UniCarbKB	7102
GlycomeDB	40175

Type

Type Saccharide

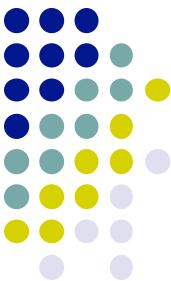
Motif

N-Linked Subsumption

Organism

Contents [hide]

- 1 Identifiers
- 2 Type
- 3 Motif
- 4 Organism
- 5 Enzyme
- 6 Substrate
- 7 Groups
- 8 Relationships
- 9 Sequence



GlyGen Glycan Data Integration

G35370OW - SMW x +

edwardslab.bmcb.georgetown.edu/smw/G35370OW

Identifiers

GlyTouCan	G35370OW
UniCarbKB	7102
GlycomeDB	40175

Type

Type Saccharide

Motif

N-Linked Subsumption

Organism

Human Subsumption, UniCarbKB, UniCarbKB-Protein

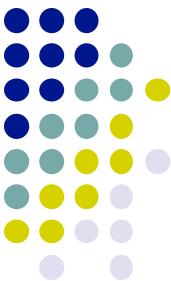
Enzyme

Substrate

Human P04114 (UniCarbKB)

Groups

Molecular Weight	1599.5656228 (17 Saccharides)
Base Composition	G28541PG (17 Saccharides)
Composition	G55719HL (7 Saccharides)
Topology	G95951LZ (6 Saccharides)



GlyGen Glycan Data Integration

G35370OW - SMW + - X

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Groups

Molecular Weight	1599.5656228 (17 Saccharides)
Base Composition	G28541PG (17 Saccharides)
Composition	G55719HL (7 Saccharides)
Topology	G95951LZ (6 Saccharides)

Relationships

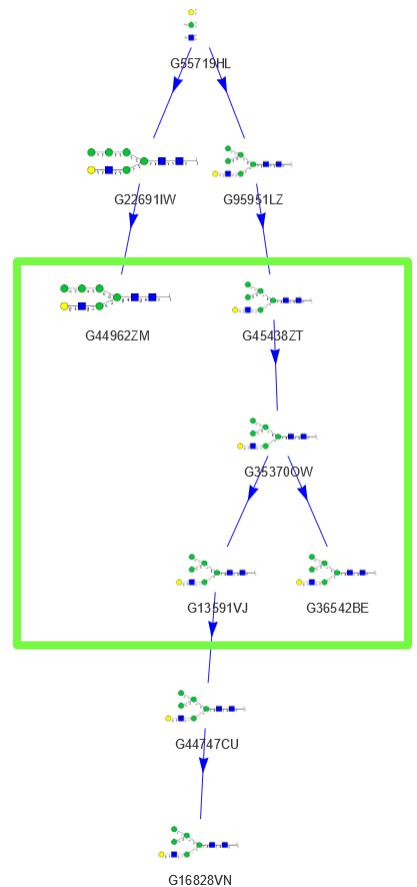
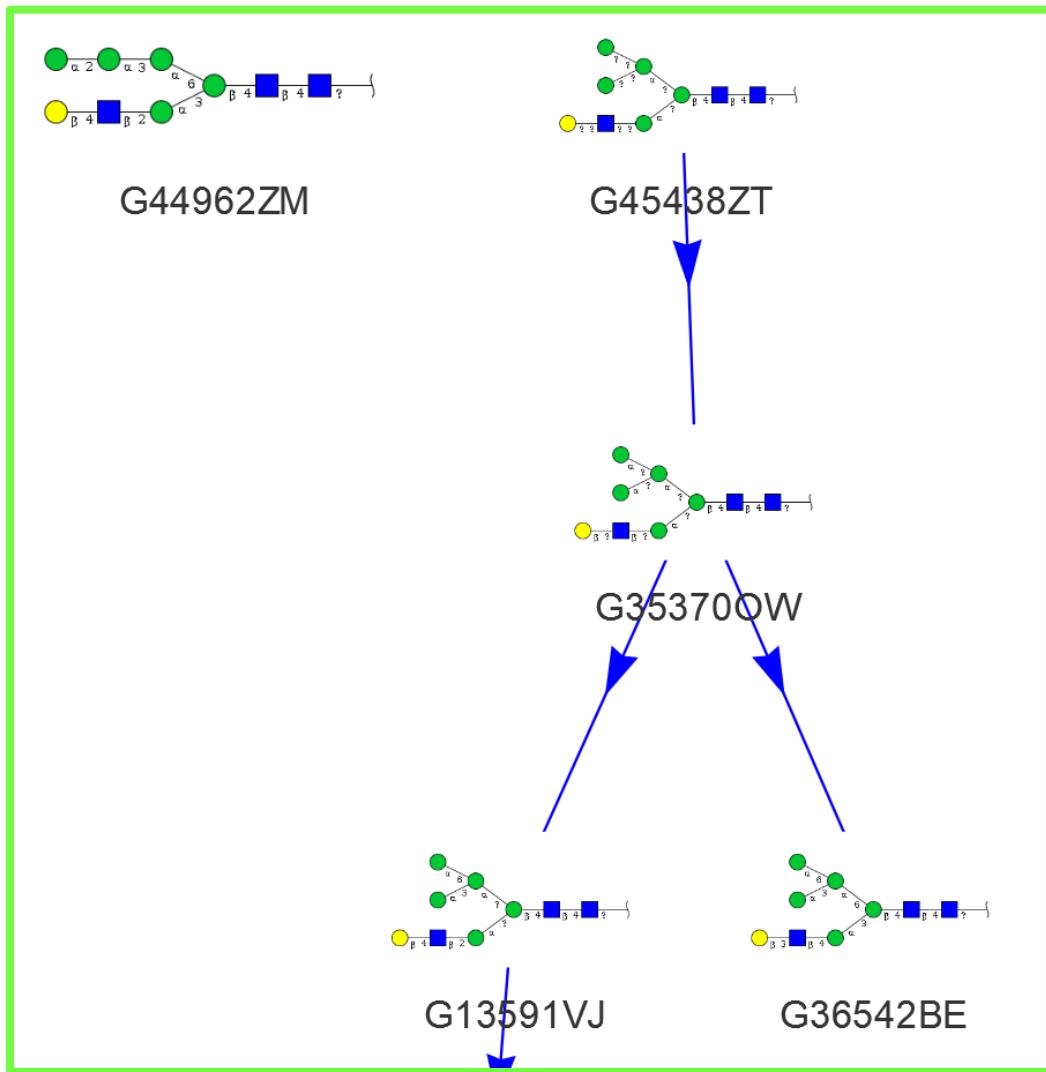
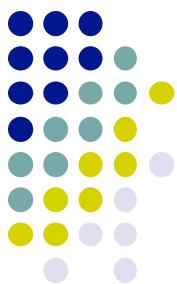
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Subsumes	G13591VJ , G36542BE

[Explore](#)

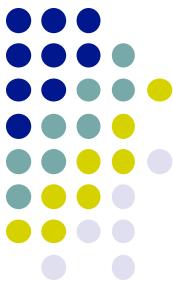
Sequence

IUPAC Condensed	Gal(b1-?)GlcNAc(b1-?)Man(a1-?) [Man(a1-?) [Man(a1-?)]Man(a1-?)]Man(b1-4)GlcNAc(b1-4)GlcNAc(?1-
IUPAC	[beta-L-Galp-(1->?)-beta-D-GlcpNAc-(1->?)-alpha-L-Manp-(1->?)-[alpha-L-Manp-(1->?)-alpha-L-Manp-(1->?)-alpha-L-Manp-(1->?)]-beta-L-Manp-(1->4)]-beta-D-GlcpNAc-(1->4)-?-D-GlcpNAc(1->
WURCS	WURCS=2.0/5,9,8/[a2122h-1x_1-5_2*NCC/3=O][a2122h-1b_1-5_2*NCC/3=O][a1122h-1b_1-5][a1122h-1a_1-5][a2112h-1b_1-5]/1-2-3-4-2-5-4-4/a4-b1_b4-c1_c?-d1_c?-g1_d?-e1_e?-f1_g?-h1_g?-i1
	RES 1b:x-dglc-HEX-1:5 2s:n-acetyl

Explore subsumption relationships



GlyGen Glycan Data Integration



G82312JY - SMW X SVG glycan X edwardslab.bmcb.georgetown.edu +

edwardslab.bmcb.georgetown.edu/smw/G82312JY

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G82312JY

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Identifiers

GlyTouCan	G82312JY
PubChem	SID252282805
GlycomeDB	13652
GlycoO	GOG357

Contents [hide]

- 1 Identifiers
- 2 Type
- 3 Motif
- 4 Organism
- 5 Enzyme
- 6 Substrate
- 7 Groups
- 8 Relationships
- 9 Sequence

Type

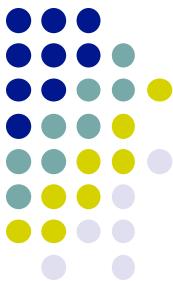
Type Saccharide

Motif

N-Linked GlyTouCan

Organism

GlyGen Glycan Data Integration



G82312JY - SMW X SVG glycan X edwardslab.bmcb.georgetown.edu +

edwardslab.bmcb.georgetown.edu/G82312JY

- X +

Organism

Enzyme

Mouse [Alg1 \(208211, GlycO\)](#), [Alg13 \(67574, GlycO\)](#), [Alg14 \(66789, GlycO\)](#), [Alg2 \(56737, GlycO\)](#), [Fut8 \(53618, GlycO\)](#), [Glt28d2 \(320302, GlycO\)](#), [Mgat1 \(17308, GlycO\)](#), [Mgat2 \(217664, GlycO\)](#)

[Explore...](#)

Substrate

Groups

Molecular Weight	1665.6238064 (25 Saccharides)
Base Composition	G88725PI (25 Saccharides)
Composition	G29913WR (8 Saccharides)
Topology	G63253XC (6 Saccharides)

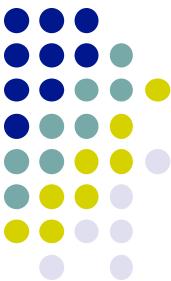
Relationships

Subsumed By [G98855LF](#)

[Explore...](#)

Sequence

IUPAC Condensed	GlcNAc (b1-2) Man (a1-3) [GalNAc (b1-4) GlcNAc (b1-2) Man (a1-6)] Man (b1-4) GlcNAc (b1-4) [Fuc (a1-6)] GlcNAc (b1-
IUPAC	[alpha-D-Fucp-(1->6)-[beta-L-GalpNAc-(1->4)-beta-D-GlcpNAc-(1->2)-alpha-L-Manp-(1->6)-beta-D-GlcpNAc-(1->2)-alpha-L-Manp-(1->3)-beta-L-Manp-(1->4)]-beta-D-GlcpNAc-(1->4)-beta-D-GlcpNAc(1-)-



Explore Glycoenzymes

G82312JY - SMW X SVG glycan X edwardslab.bmcb.georgetown.edu +

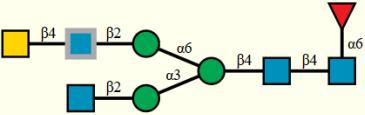
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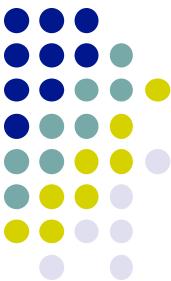
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Absolute Configuration: D
GlycO ID: N5
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[PubChem Record](#)
Enzyme: [NM_146035](#)

GOG357

Enter URL for JSON file describing the glycan:



The diagram shows a branched glycan structure. It consists of a terminal chain of three glucose residues (blue squares) linked by beta(1-4) bonds. The first residue has a beta(1-2) branch to a glucose residue (green circle). The second residue has a beta(1-3) branch to another glucose residue (green circle). The third residue has a beta(1-6) branch to a sialic acid residue (red triangle). The linkages are labeled with their respective anomeric configurations: beta(1-4), beta(1-2), alpha(1-3), and alpha(1-6).



Semantic Media-Wiki

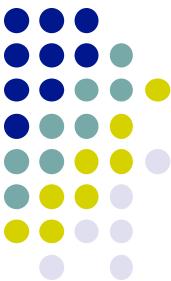
G82312JY

edwardslab.bmcb.georgetown.edu/smw/Special:Browse/:G82312JY

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G82312JY

Accession	G82312JY + edit
Has BaseComposition	G88725PI + edit
Has Composition	G29913WR + edit
Has GlyTouCan Accession	G82312JY + edit
Has GlyTouCan Type	Saccharide + edit
Has Glyco ID	GOG357 + edit
Has GlycoCT	true + edit
Has GlycomeDB ID	13652 + edit
Has Image	true + edit
Has Molecular Weight	1,665.624 + edit
Has Pubchem SID	SID252282805 + edit
Has Topology	G63253XC + edit
Human	false + edit
ImageCRC	1484706336 + edit
ImageHeight	160 + edit
ImageRedundancy	1 + edit
ImageWidth	394 + edit
IsFullySpecified	true + edit
IsLeaf	true + edit
Mouse	false + edit
MouseEnzyme	Alg1 (208211, GlycO) + edit , Alg13 (67574 , GlycO) + edit , Alg14 (66789 , GlycO) + edit , Alg2 (56737 , GlycO) + edit , Fut8 (53618 , GlycO) + edit , Glt28d2 (320302 , GlycO) + edit , Mgtat1 (17308 , GlycO) + edit , Mgtat2 (217664 , GlycO) + edit
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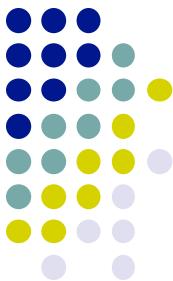


Semantic Media-Wiki

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GlyGen Glycan Data Integration



SMW x + - ×

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Main Page

Summary

BaseCompositions	834
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Topologies	2915
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All	13466

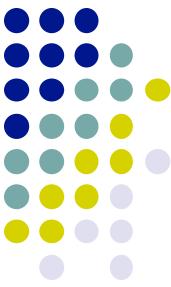
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Human	2224	1364	31		802	3455
Mouse	345	238	3		346	817
N-Linked	2905				1237	3058
O-Linked	944				390	1032
Human Enzyme				0		0
Mouse Enzyme				583		583
Human Substrate		838				838
Mouse Substrate		85				85

Topologies	GlyTouCan	UniCarbKB	UniCarb-DB	GlycO	Subsumption	Any
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Mouse	2	2	0		391	393

Contents [hide]

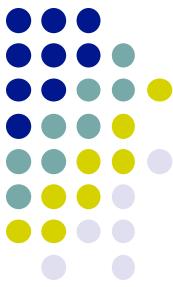
- 1 Summary
- 2 Annotation
- 3 Human N-Linked Glycans
- 4 Mouse N-Linked Glycans
- 5 Other N-Linked Glycans
- 6 Human O-Linked Glycans
- 7 Mouse O-Linked Glycans
- 8 Other O-Linked Glycans
- 9 Human Misc. Glycans
- 10 Mouse Misc. Glycans
- 11 Other Misc. Glycans



GNOME

- Glycan Naming (and Subsumption) Ontology
- Pre-compute GlyTouCan subsumption relationships
 - Publish as OBO Foundry Ontology
- Ontologies good for structured terms
- Name/identifier resolution
 - Human terminology, synonyms, ID mapping

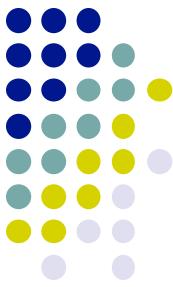




GNOME

- Provide browsing tools for interactive glycan (partial) structure description discovery
 - Help humans navigate glycan descriptions
- Well defined (partial) structure levels
- Glycan annotation propagation and inference





Acknowledgments

- GlyGen Glycoscience Portal Team
 - Will York (CCRC), Rene Ranzinger (CCRC, Glycome-DB), Raja Mazumder (GWU)
 - Kiyoko F Aoki-Kinoshita (GlyTouCan)
 - Matthew Campbell (UniCarbKB)
- NIH Common Fund: U01 - GlyGen