

A Traveler-Guide to Carbohydrates in the Cyber-Space



Composition

Topology

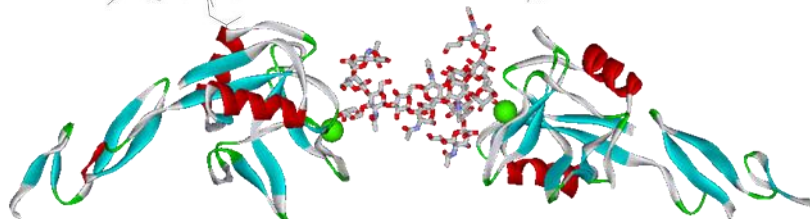
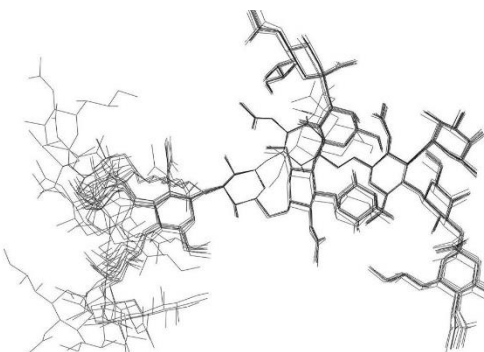
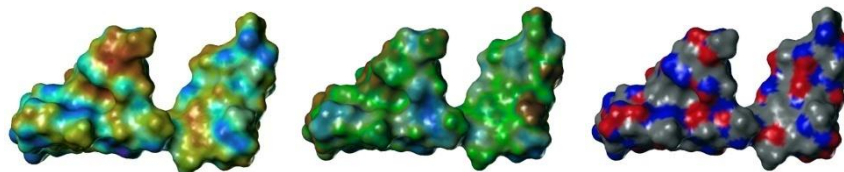
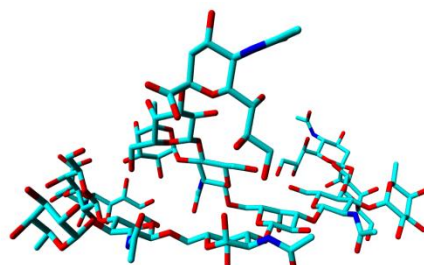
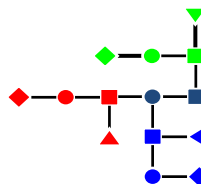
Conformation

Properties

Dynamics

Interactions

NeuAc)3 (Fuc)3 (GlcNac)3 (Gal)4 (GalNac)1 Ser



MS, HPLC, CE

MS, HPLC
CE, NMR

NMR
XRAY
MS

MM
CAMD

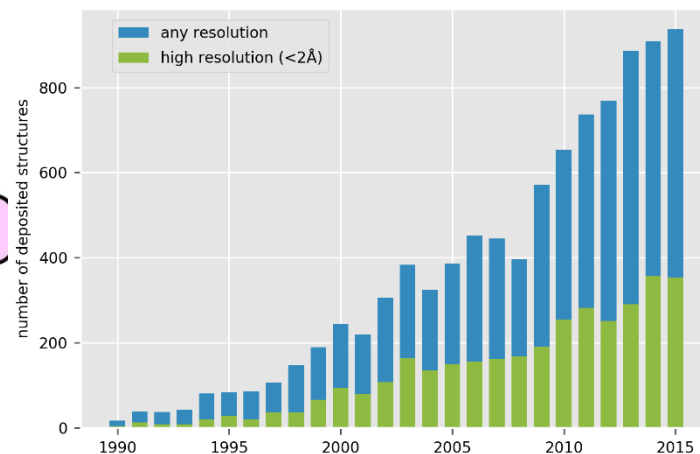
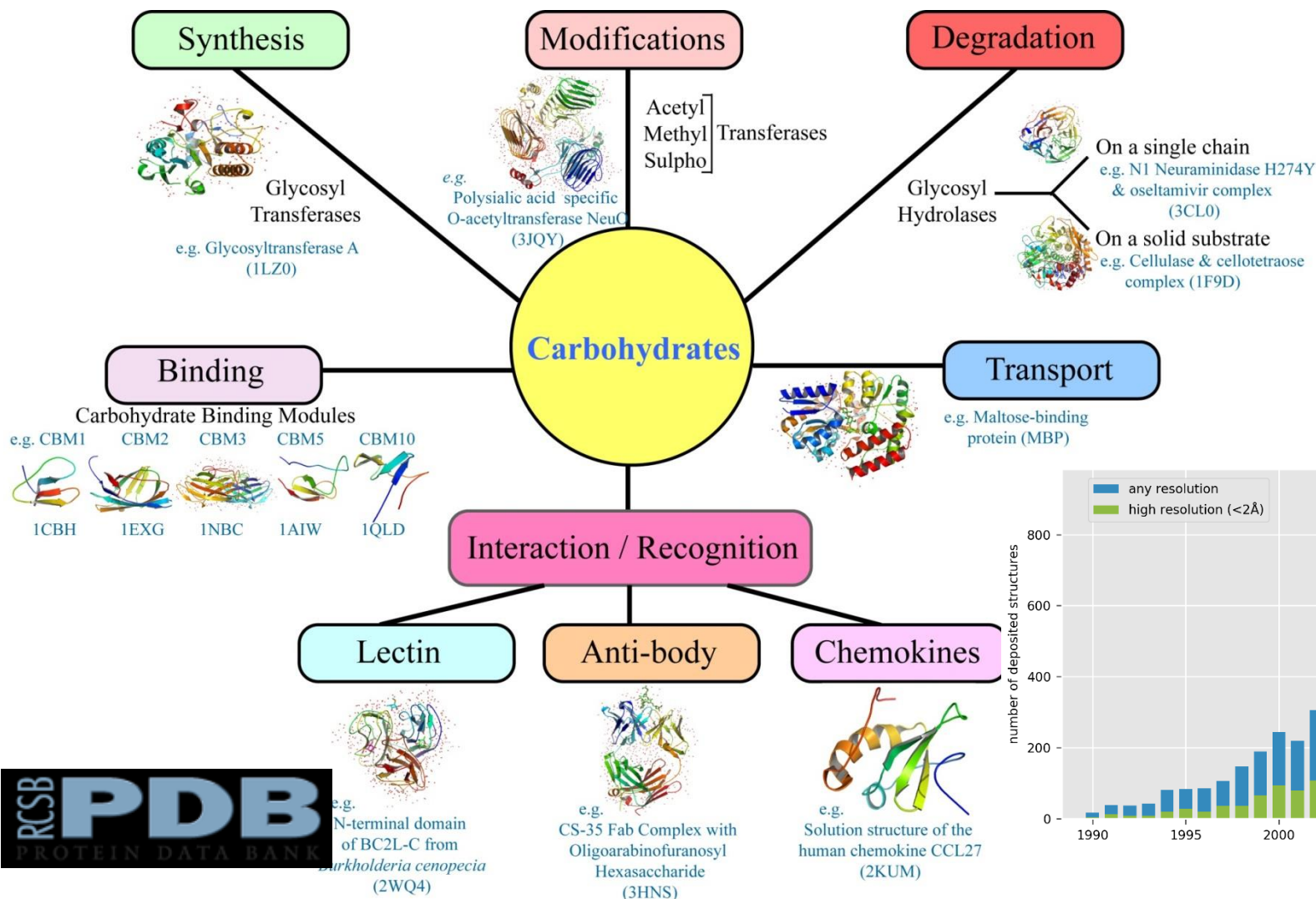
NMR
MM
MD

XRAY
MM

Methods

Crystalline Conformations of Oligosaccharides in Proteins

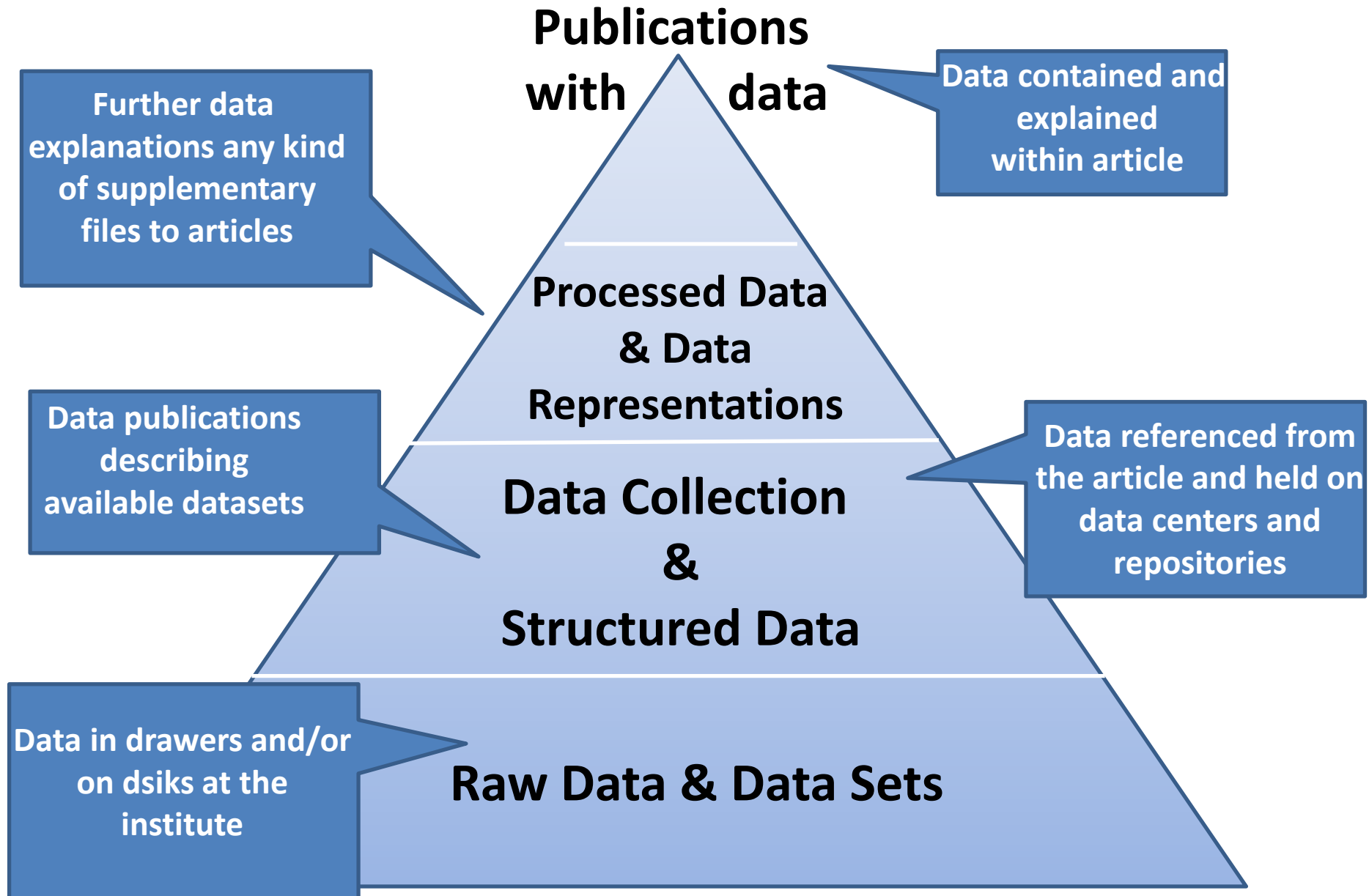
Protein-Carbohydrate Interactions



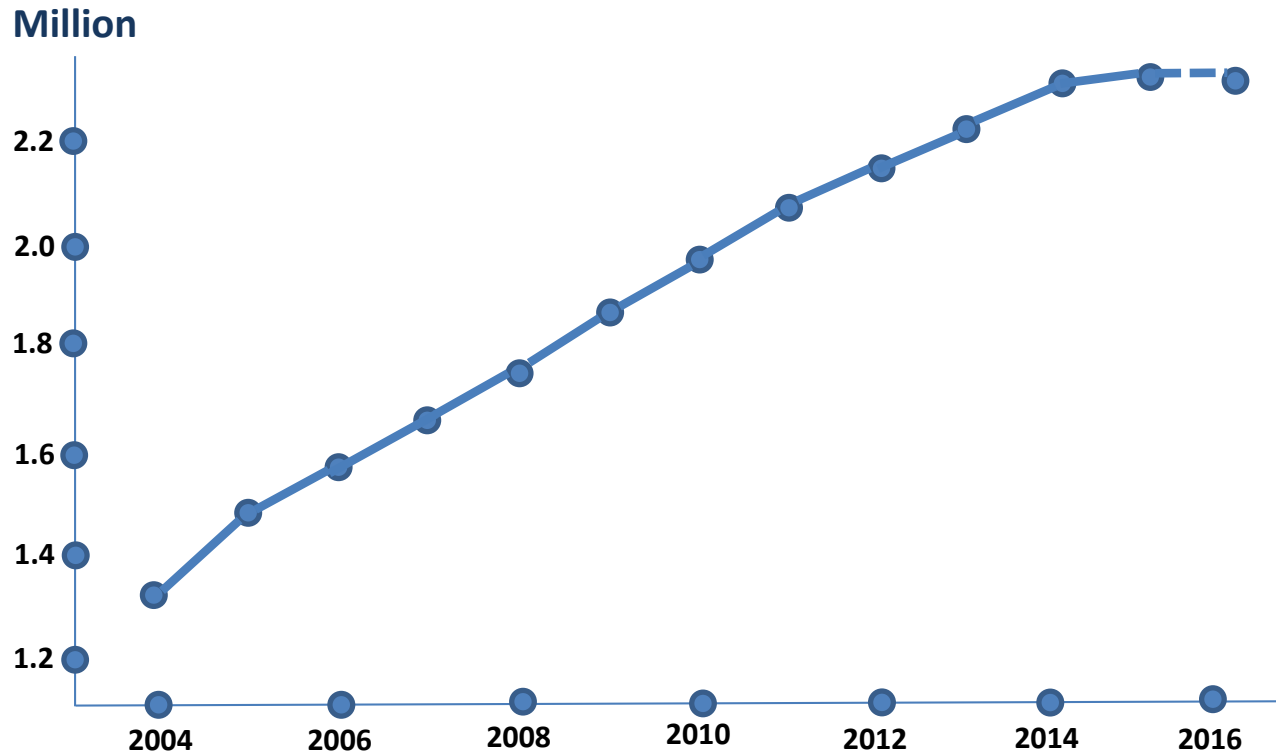
The background of the slide is a light blue color with a repeating pattern of various chemical structures, including aromatic rings, aliphatic chains, and functional groups, rendered in a darker blue color.

From Structures to 3D Databases

An avalanche of data...



An avalanche of data...

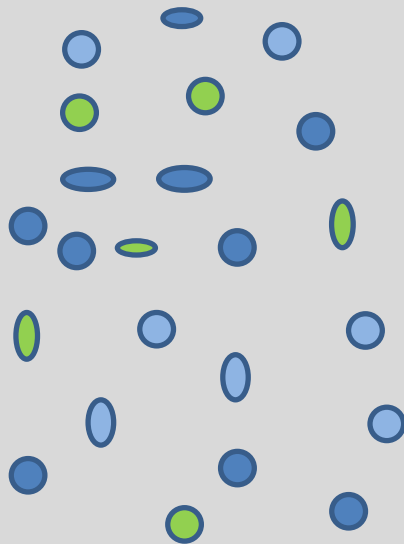


Global scientific output doubles every nine-years

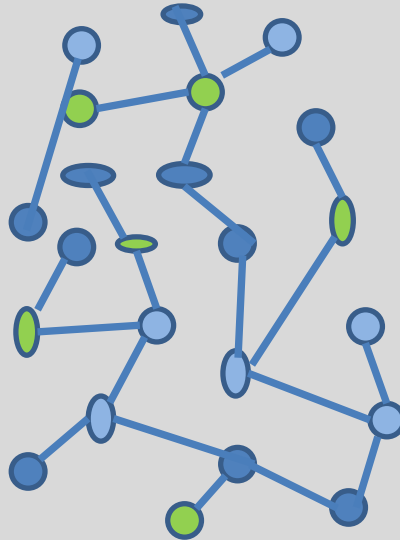
Number of active researchers world-wide 8 Millions

Knowledge, Experience, Creativity

Knowledge



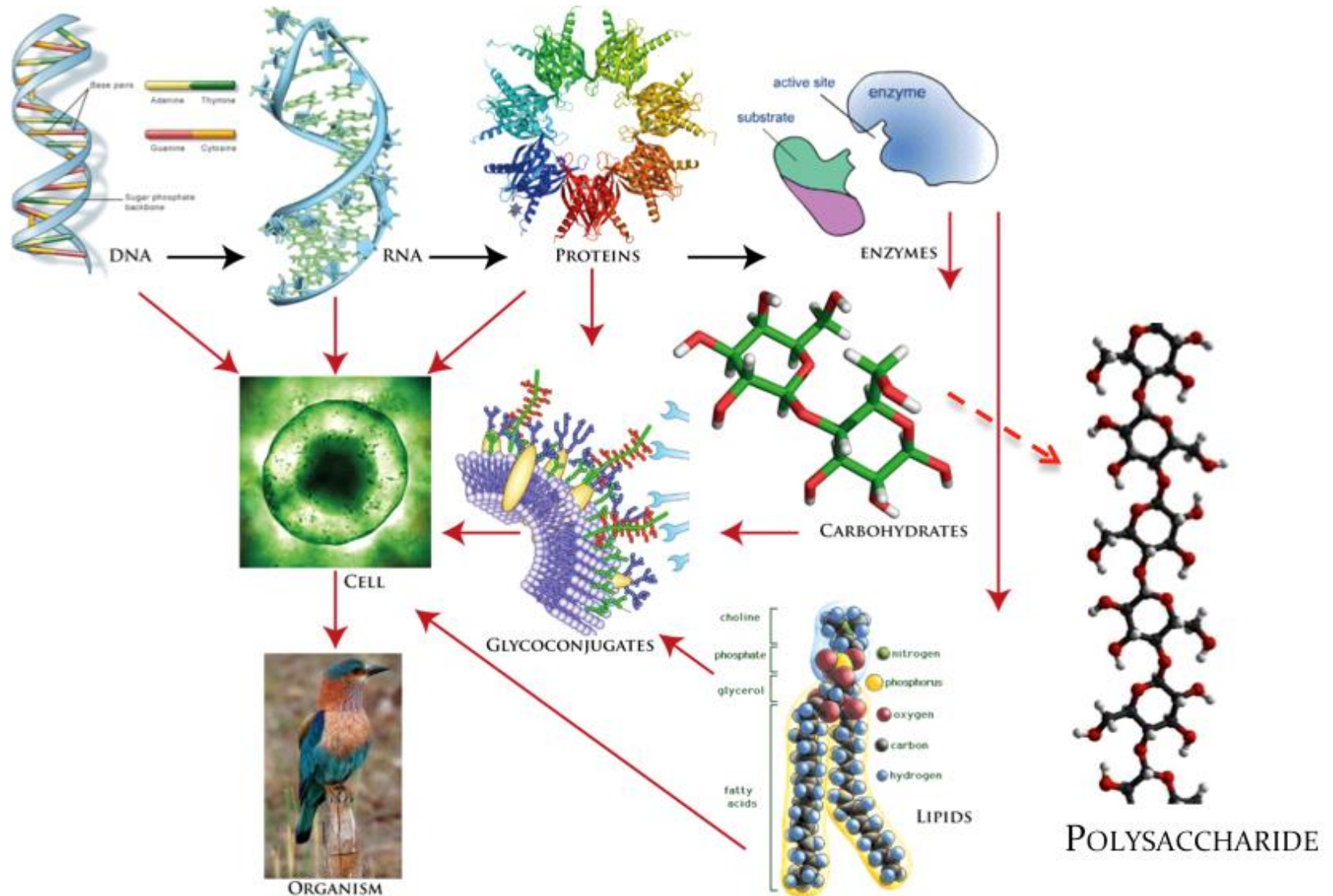
Experience



Creativity



Carbohydrates in the Scheme of the Central Dogma of Life



Glycoinformatics

Genomics

The screenshot shows the NCBI UniGene website. The top navigation bar includes links for NCBI, UniGene, and a search bar. The left sidebar contains links for UniGene, Home, News, FAQs, Query Tools, Download, and Related Databases. The main content area is titled "Blast" and provides information about the Basic Local Alignment Search Tool (BLAST). It includes a section for "General Blast Programs" with a table listing various tools and their descriptions, and a section for "Specialised Blast Programs" with a table listing more specific tools and their descriptions.

| Tool | Description |
|------------------------|------------------------|
| WU-Blast2 Protein | WU-Blast2 Protein |
| WU-Blast2 Nucleotide | WU-Blast2 Nucleotide |
| NCBI-Blast2 Protein | NCBI-Blast2 Protein |
| NCBI-Blast2 Nucleotide | NCBI-Blast2 Nucleotide |

| Tool | Description |
|---------------------|--|
| WU-Blast2 ASD | ASD blast server |
| WU-Blast2 Parasites | Parasite Genomes blast server |
| NCBI-Blast2 EVEC | European blast2 Vector Searches. Check your sequences for vector contamination. |
| PSI-Blast | Position specific Iterative Blast (PSI-Blast) refers to a feature of Blast 2.0 in which a profile is automatically constructed from the first set of Blast alignments. |
| PHI-Blast | Pattern Hit Initiated Blast (PHI-Blast) treats two occurrences of the same pattern within the query sequence as two independent sequences. |

Proteomics

The screenshot shows the Mascot search results page. The top navigation bar includes links for ExPASy Home page, Site Map, Search ExPASy, Contact us, PROSITE, and Proteomics tools. The main content area is titled "Mascot Search Results" and displays the search parameters and results. It includes a section for "Probability Based Mowse Score" with a bar chart showing the distribution of scores. The chart has a y-axis labeled "Number of hits" and an x-axis labeled "Probability Based Mowse Score". The results table shows the top hit for the query "PML_HUMAN".

| Rank | Accession | Score | Expect | Queryes matched | |
|------|-----------|-------------|------------|-----------------|---------------------|
| 1. | PML_HUMAN | Mass: 97455 | Score: 194 | Expect: 1e-14 | Queryes matched: 15 |

Glycomics

Challenges for Glycoinformatics

Structures as Primary Access Key

Bioinformatic

Galectin-1

```
source      organism="Homo sapiens"
```

gene gene="LGALS1"

Site /site_type="binding"

/note="Beta-galactoside (Potential)."

1 MACGLVASNL NLKPGECLRV RGEVAPDAKS

31 FVLNLGKDSN NLCLHFNPRF NAHGDANTIV

61 CNSKDGGAWG TEQREAVFPF QPGSVAEVC

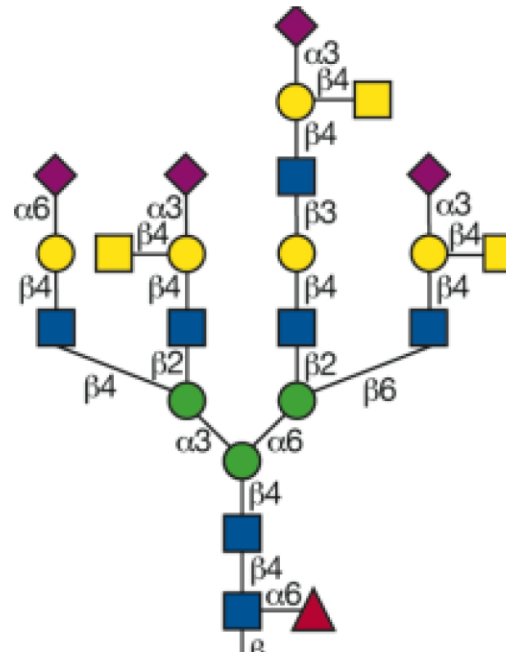
91 TFDQANLTVK LPDGYEFKFP NRLNLEAINY

121 MAADGDFKIK CVAFD

Sequences of residues

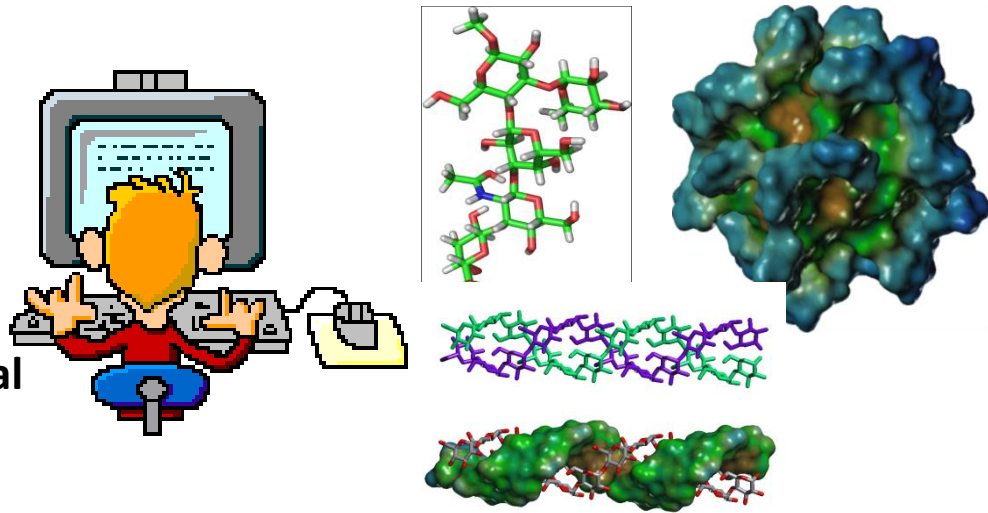
Glycoinformatic

Topology of Residues



e-Glycoscience

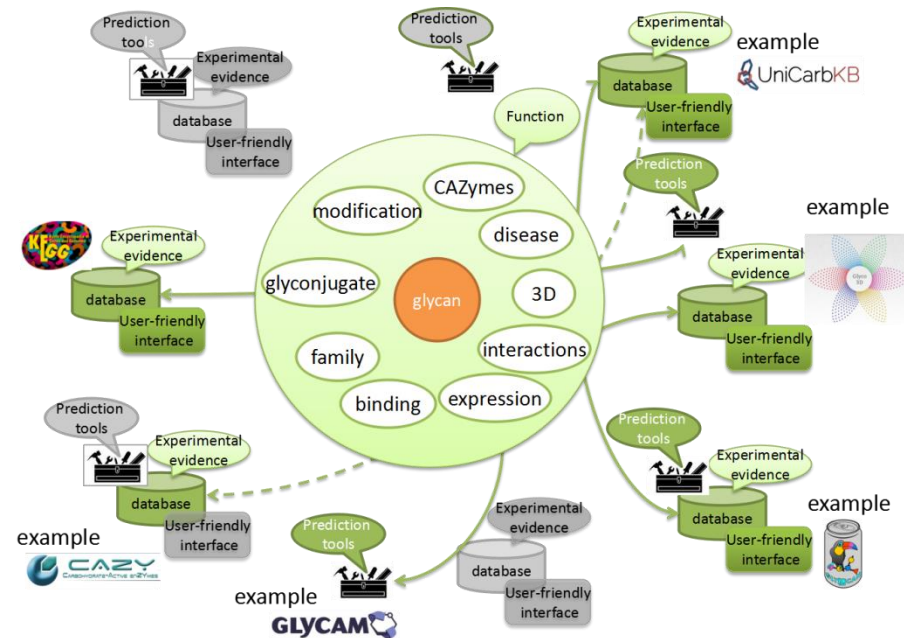
Continued advances in molecular modeling has generated insights for understanding glycan structures and properties. Robust, validated informatics tools are developed in to enable accurate and fast determination of complex **carbohydrate and glycoconjugate structural prediction, computational modeling, and data mining.**



Database have been developed and cover including mammalian, plant and microbial carbohydrates and glycoconjugates.

The carbohydrate **structural database needs to be fully cross-referenced with databases that provide complementary biological information.**

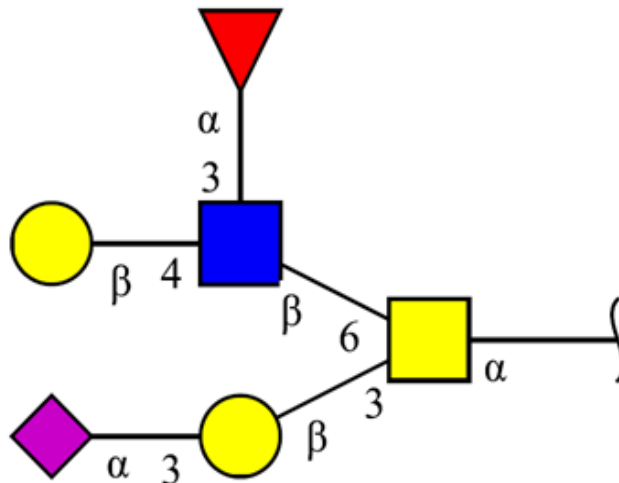
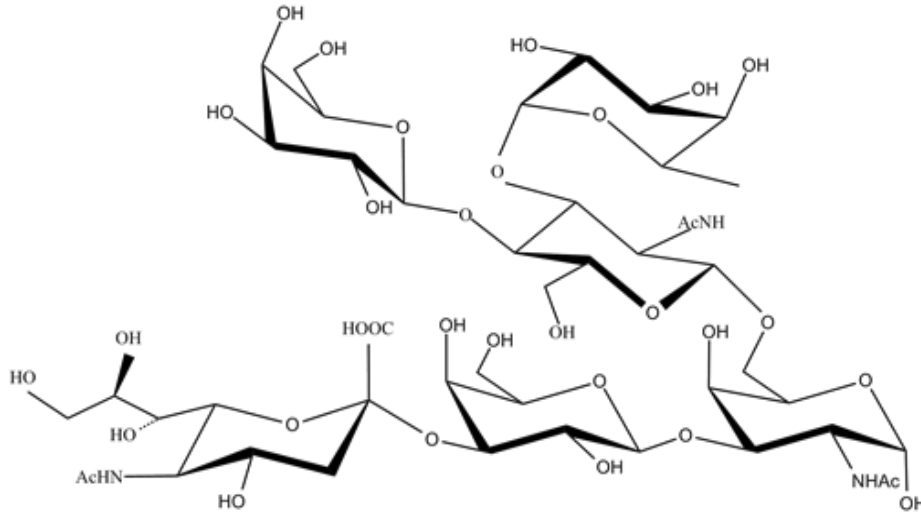
There should be a requirement for deposition of new structures into the database using a reporting standard for minimal information.



Encoding of Glycan Structures

Lewis X and Sialyl Acid on Core 2

Neu5Ac a2-3 Gal b1-3 (Gal b1-4 (Fuc a1-3) GlcNAc b1-6) GalNAc



RES

1b:a-dgal-HEX-1:5

2s:n-acetyl

3b:b-dgal-HEX-1:5

4b:a-dgro-dgal-NON-2:6 | 1:a | 2:keto | 3:d

5s:n-acetyl

6b:b-dglc-HEX-1:5

7s:n-acetyl

8b:a-lgal-HEX-1:5 | 6:d

9b:b-dgal-HEX-1:5

LIN

$$1:1d(2+1)2n$$

2:1o(3+3)3d

3:30(3+2)4d

$$4:4d(5+1)5n$$

5:1o(6+1)6d




































































$$6:6d(2+1)7n$$

7:6o(3+1)8d

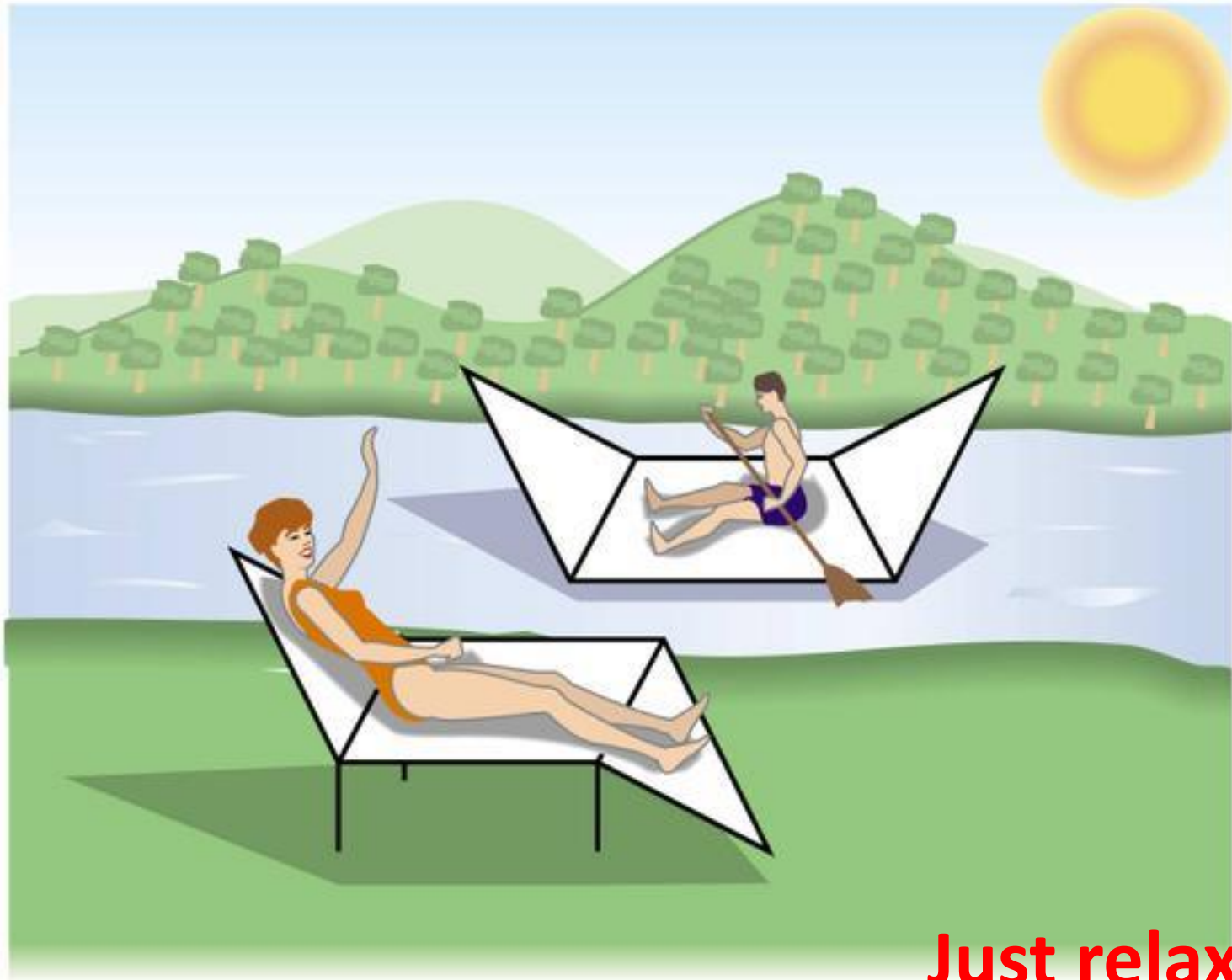
8:6o(4+1)9d

GlycoCT

Symbol Nomenclature for Graphical Representation of Glycans (2015), *Glycobiology*, 25, 1323-1324

| | | | | | | | | | |
|----------------|---|---|---|---|--|---|---|---|---|
| Hexose | Glc  | Man  | Gal  | Gul  | Alt  | All  | Tal  | Ido  | |
| HexNAc | GlcNAc  | ManNAc  | GalNAc  | GulNAc  | AltNAc  | AllNAc  | TalNAc  | IdoNAc  | |
| Hexosamine | GlcN  | ManN  | GalN  | GulN  | AltN  | AllN  | TalN  | IdoN  | |
| Hexuronate | GlcA  | ManA  | GalA  | GulA  | AltA  | AltA  | TalA  | IdoA  | |
| DeoxyHexose | Qui  | Rha  | | | 6dAltA  | | 6dTal  | | Fuc  |
| Deoxy HexNAc | QuiNAc  | RhaNAc  | | | | | | | FucNAc  |
| Dideoxy Hexose | Oli  | Tyv  | | Abe  | Par  | Dig  | Col  | | |
| Pentose | | Ara  | Lyx  | Xyl  | Rib  | | | | |
| Nonulosonate | | Kdn  | | | | Neu5Ac  | Neu5GC  | Neu  | |
| Assigned (i) | Bac  | ManHep  LD | Kdo  | Dha  | ManHep  DD | MurNAc  | MurNGc  | Mur  | |
| Assigned (ii) | Api  | Fru  | Tag  | Sor  | Psi  | | | | |

No Comments



Just relax¹⁴

Extending the Symbolic Representation of Monosaccharides



Residue Letter Name: Rib, Ara, Xyl, Lyx, All, Alt, Glc, Man, Gul, Ido, Gal, Tal,....

[O-ester and ethers]: (when present) are shown attached to the symbol with a number, e.g.

6Ac for 6-*O*-acetyl group, 3S for 3-*O*-sulfate group

6P for 6-*O*-phosphate group, 6Me for 6-*O*-Methyl group

36Anh for 3,6-anhydro, Pyr for pyruvate group

Absolute Configuration: D or L

The D-configuration for monosaccharide and the L configuration for Fucose and Idose are implicit and does not appear in the symbol. Otherwise the L configuration, is indicated in the symbol, as in the case of Arabinose or L-Galactose.

For those occurring in the furanose form, a letter *N* or *S* is inserted in the symbol, indicating the northern (*N*) or Southern (*S*) conformation of the five membered ring.

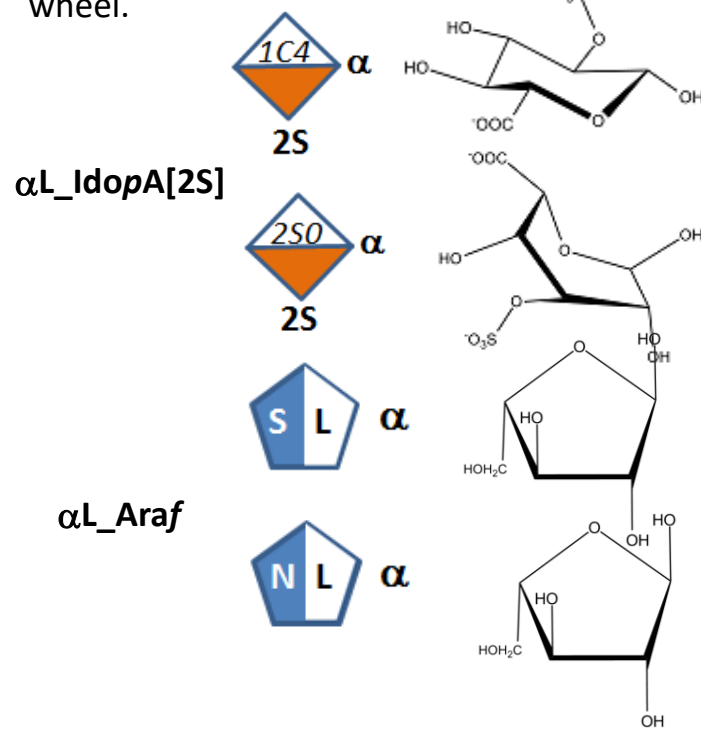
Anomeric Configuration.

The nature of the glycosidic configuration (α or β) is explicitly set within the symbol.

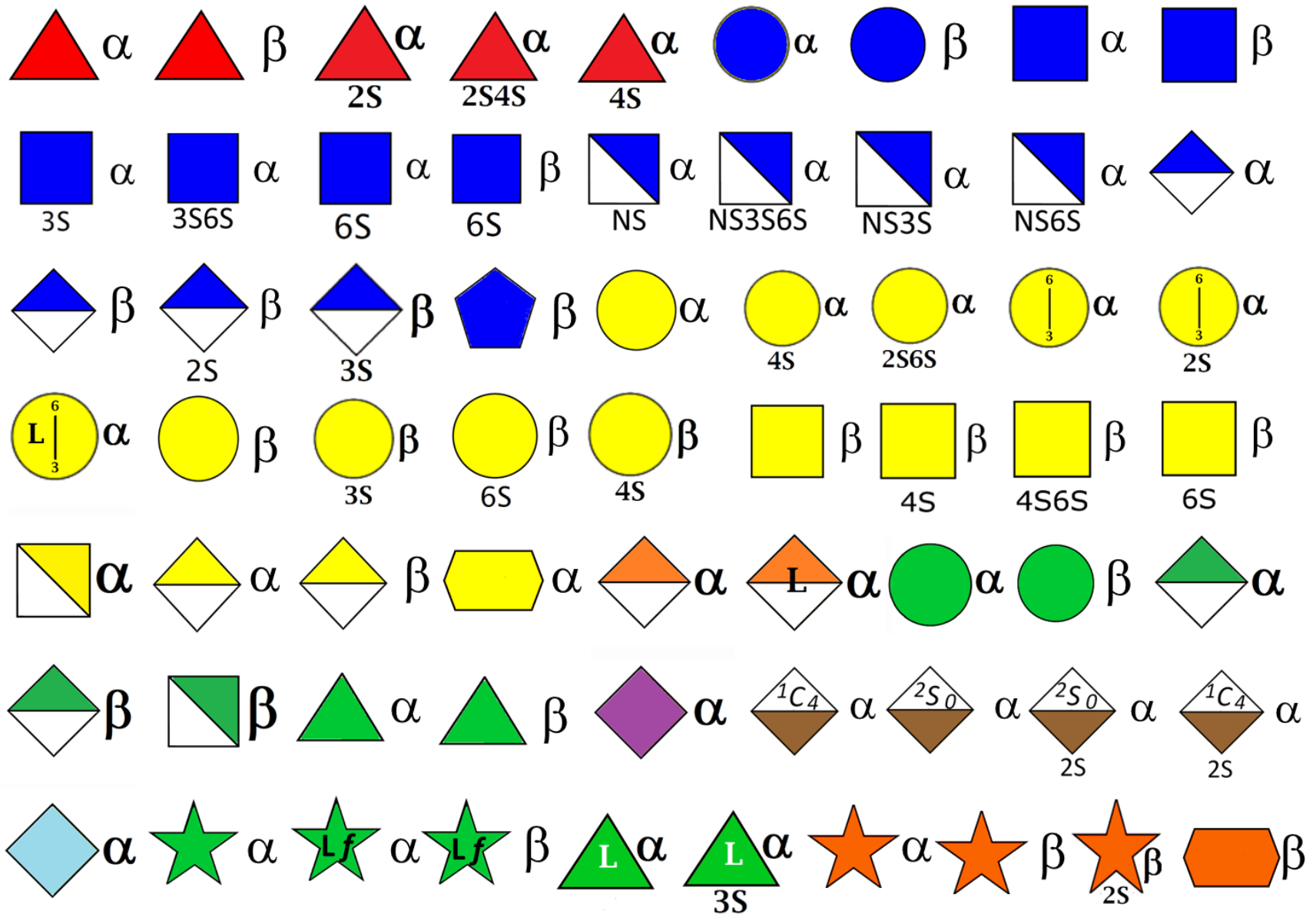
Ring Conformation.

All pyranoses in the D-configuration are assumed to have 4C_1 chair conformation; those in the L configuration are assumed to have 1C_4 chair conformation. Otherwise, the ring conformation is indicated in the symbol, as 2S_0 in the case of α -L-Idopyranose.

N or *S* indicates the conformation of the five membered rings on the conformational wheel.



More than 150 Monosaccharides



Tools and DataBases

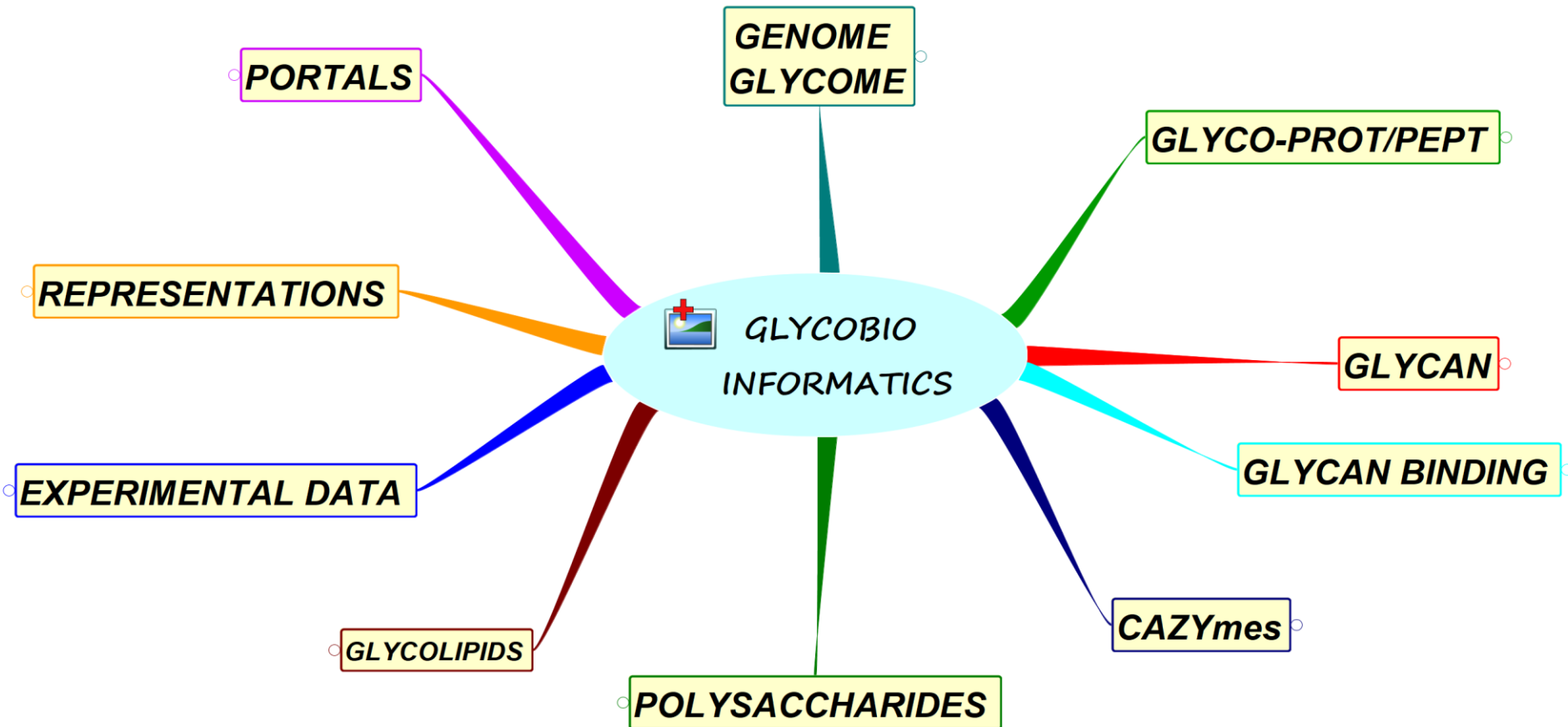
Protocole: Search on Internet Tools and DataBases
in Glycosciences

Sites should be up to date (checked) and
freely available.

Results: 94 Tools 32 DataBases

Analysis and Clustering

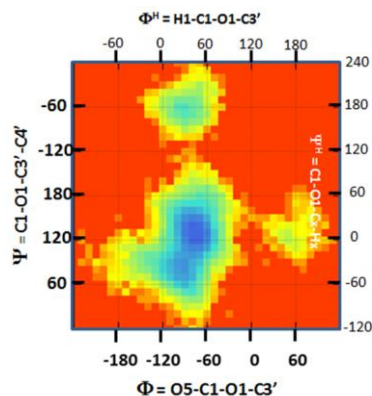
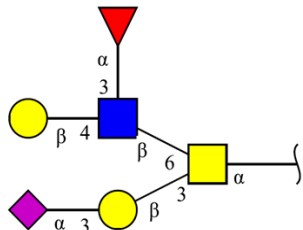
Tools and DataBases



Representations

Symbol Nomenclature for Glycans: SNFG

| Residue | Glc | Man | Gal | Gul | Alt | All | Tal | Ido | |
|-----------------------|-----|-----|-----|-----|-----|-----|-----|-----|--|
| Hexose | | | | | | | | | |
| HexNAc | | | | | | | | | |
| Hexosamine | | | | | | | | | |
| Hexosaminic acid | | | | | | | | | |
| Deoxyhexose | | | | | | | | | |
| Deoxyhexosamine | | | | | | | | | |
| Deoxyhexosaminic acid | | | | | | | | | |
| Deoxyhexosaminic acid | | | | | | | | | |
| Deoxyhexosamine | | | | | | | | | |
| Deoxyhexosaminic acid | | | | | | | | | |
| Deoxyhexosaminic acid | | | | | | | | | |
| Deoxyhexosaminic acid | | | | | | | | | |
| Deoxyhexosamine | | | | | | | | | |
| Deoxyhexosaminic acid | | | | | | | | | |
| Deoxyhexosaminic acid | | | | | | | | | |
| Deoxyhexosaminic acid | | | | | | | | | |
| Deoxyhexosamine | | | | | | | | | |
| Deoxyhexosaminic acid | | | | | | | | | |
| Deoxyhexosaminic acid | | | | | | | | | |
| Deoxyhexosaminic acid | | | | | | | | | |

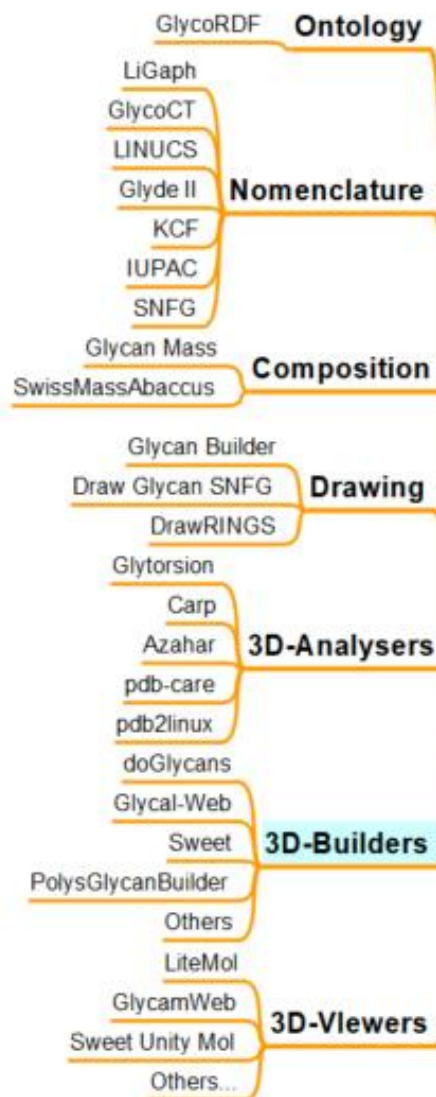


RES

1b:a-dgal-HEX-1:5
 2s:n-acetyl
 3b:b-dgal-HEX-1:5
 4b:a-dgro-dgal-NON-
 2:6|1:a|2:keto|3:d
 5s:n-acetyl
 6b:b-dglc-HEX-1:5
 7s:n-acetyl
 8b:a-lgal-HEX-1:5|6:d
 9b:b-dgal-HEX-1:5

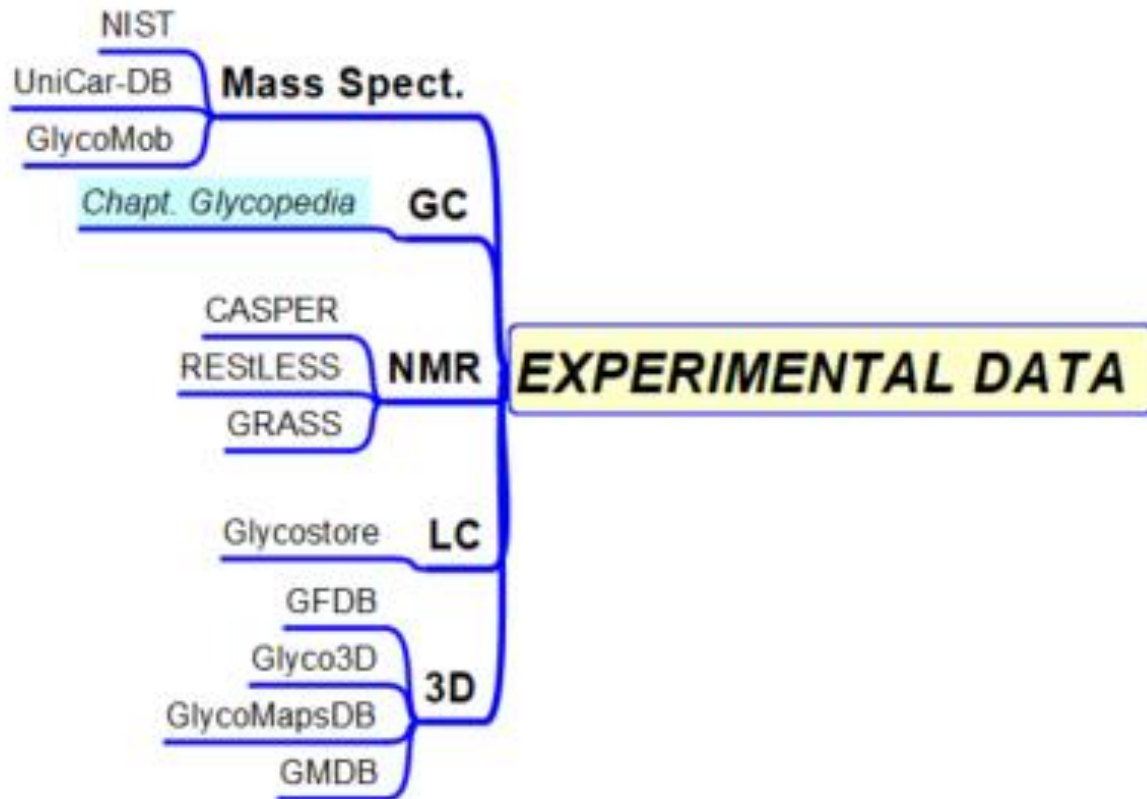
LIN

1:1d(2+1)2n
 2:1o(3+3)3d
 3:3o(3+2)4d
 4:4d(5+1)5n
 5:1o(6+1)6d
 6:6d(2+1)7n
 7:6o(3+1)8d
 8:6o(4+1)9d

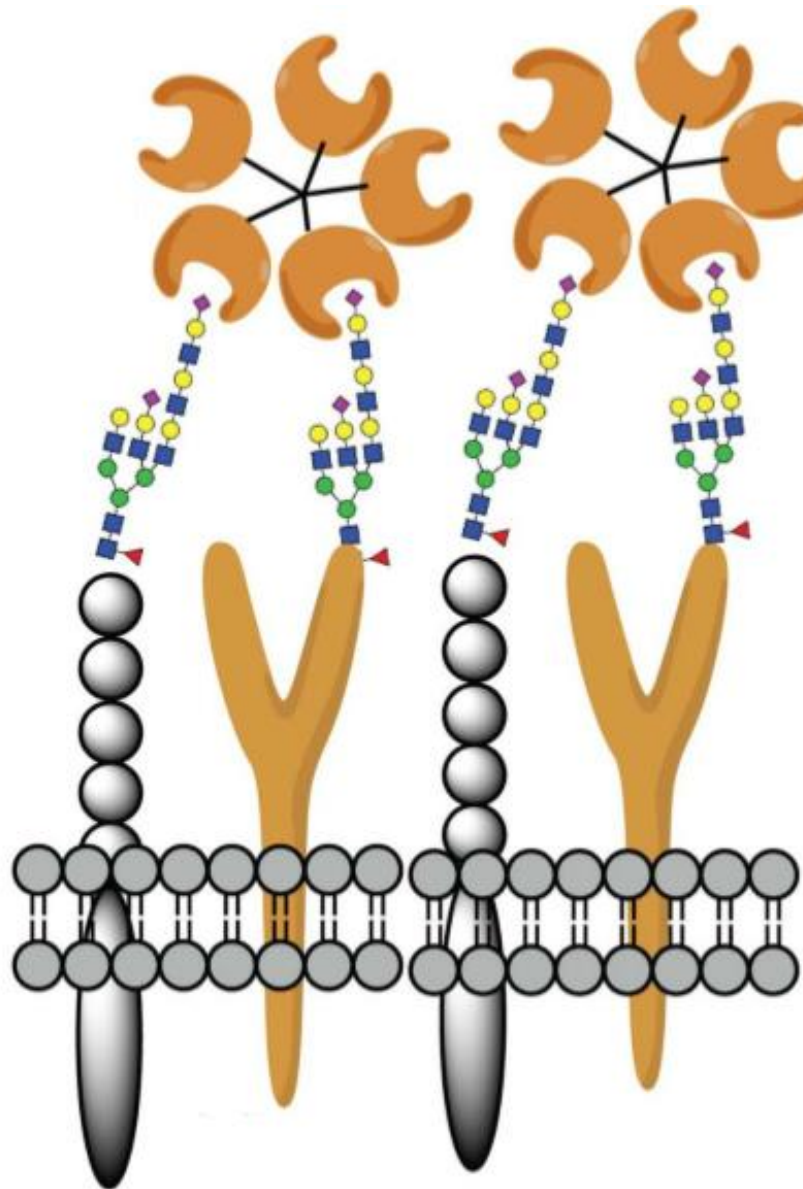


REPRESENTATIONS

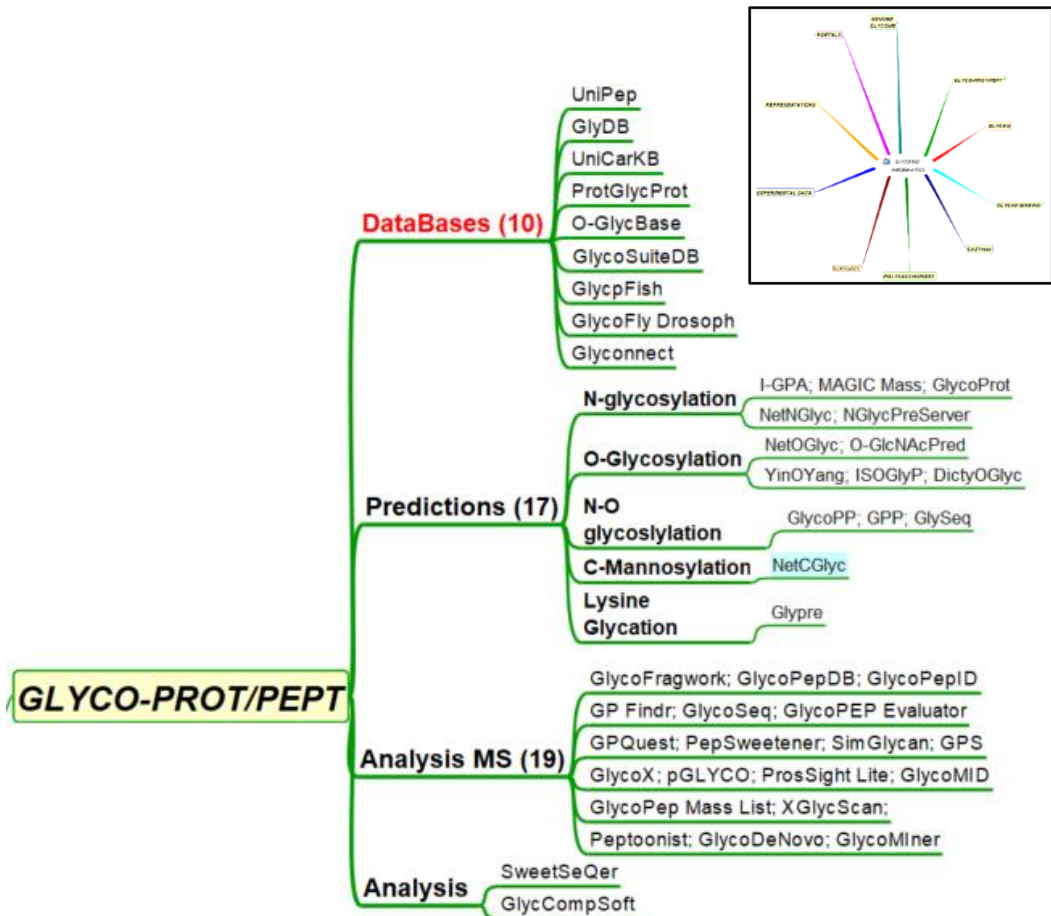
A Traveller-Guide in Glycoscience Cyber-Space



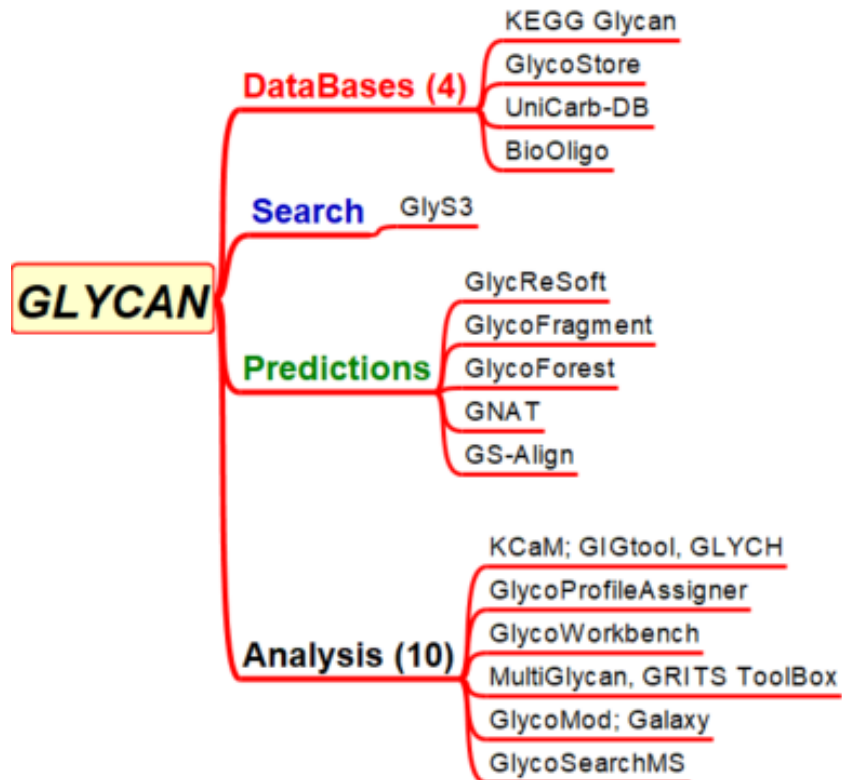
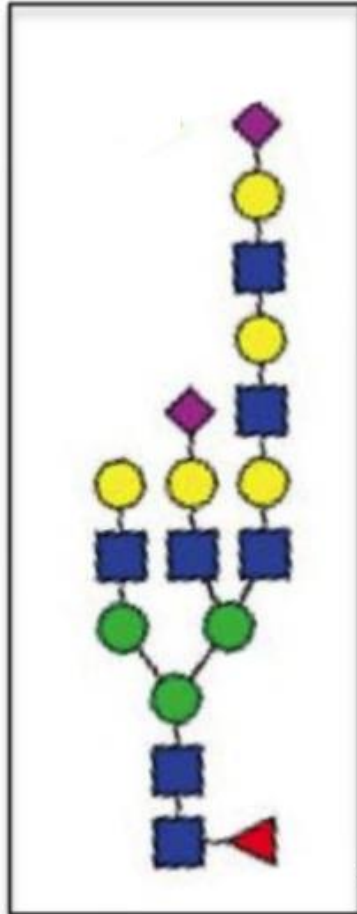
Glycomics



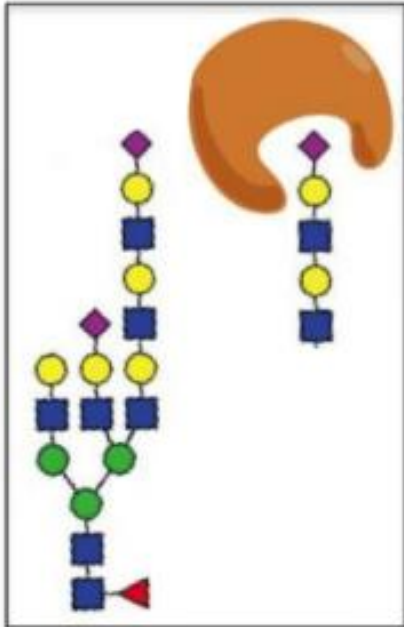
Glycoproteomics



Glycans

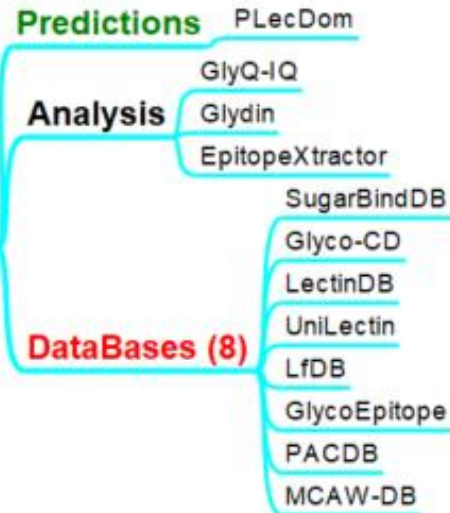


Functional Glycomics

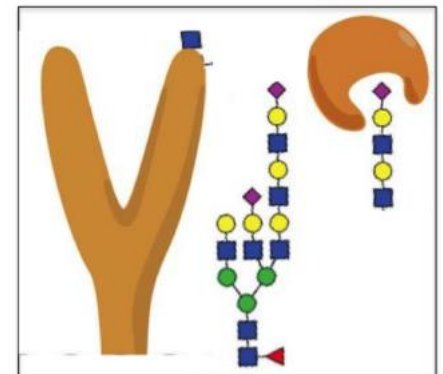


Functional
Glycomics

GLYCAN BINDING

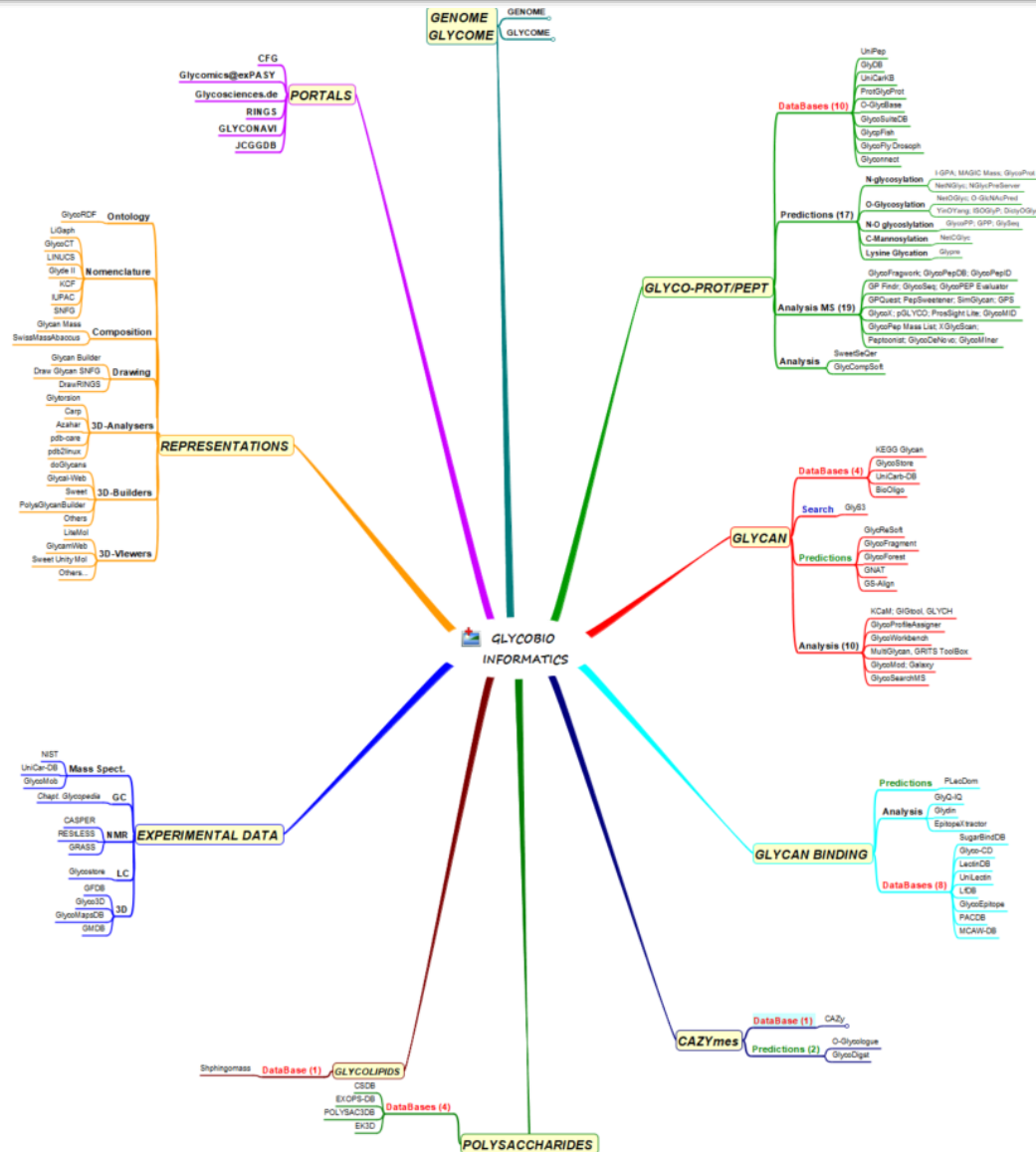


Glycoproteomics



Glyconnect

A Traveller-Guide in Glycoscience Cyber-Space



available soon at : <https://glycopedia.eu>

*Yes
we
Glycan !*

