

# PROTEOMICS

## Supporting Information for Proteomics

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**Symbol nomenclature for glycan representation**

**“Essentials of Glycobiology”**

**Final Plan for**

**Usage of Sugar Symbols**

**for the Second Edition**

# General Principles

- **Modify monosaccharide symbol set from First Edition of “Essentials” to achieve common ground with as many other interested groups as possible (NCBI, Consortium for Functional Glycomics, KEGG pathways etc.)**
- **Avoid same shape/color but different orientation to represent different sugars since annotation of mass spectra are hard to show as horizontal cartoons.**
- **Choice of symbols should be logical and simple to remember.**
- **Each monosaccharide type (e.g. hexose) should have the same shape, and isomers are to be differentiated by color/black/white/shading.**
- **Use same shading/color for different monosaccharides of same stereochemical designation e.g., Gal, GalNAc, GalA should all be the same shading/color.**
- **To minimise variations, sialic acids and uronic acids are same shape. Only major uronic and sialic acid types are represented.**
- **While color is useful, the system should also function with black and white, and colored representations should survive black-and white printing or xeroxing.**
- **Positions of linkage origin are assumed to be common ones unless indicated. Anomeric notation and destination linkage indicated without spacing/dashes.**
- **Modifications of monosaccharides (e.g., sulfation, O-acetylation) indicated by attached small letters, with numbers indicating linkage positions, if known.**
- **Only common monosaccharides in vertebrate systems are assigned a specific symbol. All other monosaccharides are represented by an open Hexagon, and defined in the figure legend. If there is more than one type of undesignated monosaccharide in a figure, an letter designation internal to the Hexagon can be included to differentiate between them - again, specified in the figure legend.**
- **Note: To reproduce precise colors, use the color sliders. Click on the paint pot icon and select “more colors”. Then, click on sliders in the menu bar and fill in numbers. Or, you can copy an existing fill color by using the eye dropper and touching the color you want.**

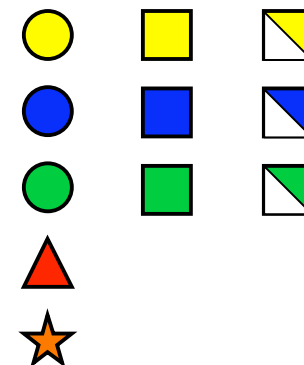
# Essentials Second Edition Symbols : RGB colors

Hexoses: Circles      N-Acetylhexosamines: Squares

Hexosamines: Squares divided diagonally

*Print in color*

- Galactose stereochemistry: **Yellow (255,255,0)** with Black outline
- Glucose stereochemistry: **BLUE (0,0,250)** with Black outline
- Mannose stereochemistry: **GREEN (0,200,50)** with Black outline
- Fucose: **RED (250,0,0)** with Black outline
- Xylose: (5-pointed star) **ORANGE (250,100,0)** with Black outline



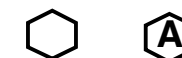
## Acidic Sugars (Diamonds)

- Neu5Ac: **PURPLE (125,0,125)** with Black outline
- Neu5Gc: **LIGHT BLUE (200,250,250)** with Black outline
- KDN: **GREEN (0,200,50)** with Pattern & Black outline
- GlcA: **BLUE (0,0,250)**/Upper segment with Black outline
- IdoA: **TAN (150,100,50)**/Lower segment with Black outline
- GalA: **RED (250,0,0)**/Left segment with Black outline
- ManA: **GREEN (0,200,50)**/Right segment with Black outline



## Other Monosaccharide

(use letter designation inside symbol to specify if needed)



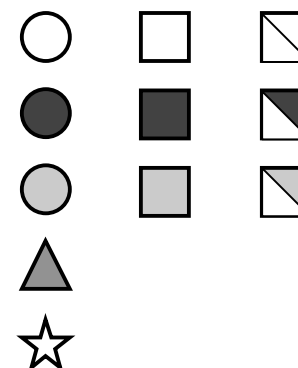
# Essentials Second Edition Symbols : Black & White

Hexoses: Circles      N-Acetylhexosamines: Squares

Hexosamines: Squares divided diagonally

*Print in black & white*

- Galactose stereochemistry: white with Black outline
- Glucose stereochemistry: Black with Black outline
- Mannose stereochemistry: Grey with Black outline
- Fucose: Dark Grey with Black outline
- Xylose: (5-pointed star) with Black outline



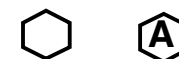
## Acidic Sugars (Diamonds)

- Neu5Ac: Dark Grey with Black outline
- Neu5Gc: White with Black outline
- KDN: Light Grey Pattern & Black outline
- GlcA: Grey upper segment with Black outline
- IdoA: Grey Lower segment with Black outline
- GalA: Grey Left segment with Black outline
- ManA: Grey Right segment with Black outline



## Other Monosaccharide

(use letter designation inside symbol to specify if needed)



# Linkages/Configuration/Modifications

## Unless otherwise indicated:

All monosaccharides are assumed to be in the D-configuration except for Fucose and Iduronic acid, which are in the L- configuration

All glycosidically-linked monosaccharides assumed to be in the pyranose form

All monosaccharide glycosidic linkages are assumed to originate from the 1-position except for the sialic acids, which are linked from the 2-position

O-esters and ethers are shown attached to the symbol with a number e.g.,

9Ac for 9-O-acetyl group

3S for 3-O-sulfate group

6P for a 6-O-phosphate group

8Me for 8-O-Methyl group

9Acy for 9-O-acyl group

9Lt for 9-O-Lactyl group

For N-substituted groups assume there is only one Amino group on the monosaccharide with an already known position e.g., use NS for N-sulfate group on Glucosamine, assumed to be at the 2-position



## Examples - Simplified Text and Symbolic Representation of Glycosaminoglycans (GAGs)

GlcNAc $\beta$ 4GlcA $\beta$ 3GlcNAc $\beta$ 4GlcA $\beta$ 3GlcNAc $\beta$ 4GlcA $\beta$ 3GlcNAc $\beta$ 4GlcA $\beta$ 3GlcNAc



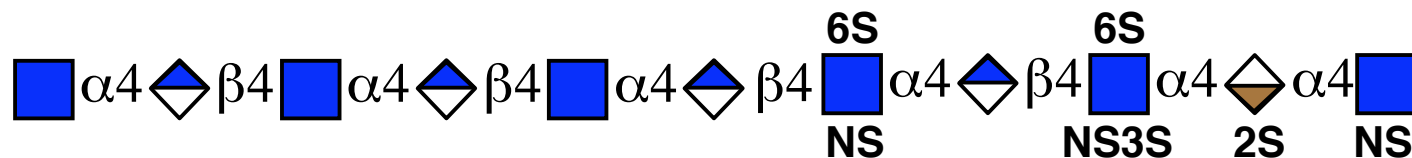
Hyaluronan

GalNAc $4S\beta$ 4GlcA $\beta$ 3GalNAc $4S\beta$ 4IdoA $\alpha$ 3GalNAc $4S\beta$ 4IdoA $2S\alpha$ 3GalNAc $4S\beta$ 4GlcA $\beta$ 3



Chondroitin/Dermatan Sulfate

GlcNAc $\alpha$ 4GlcA $\beta$ 4GlcNAc $\alpha$ 4GlcA $\beta$ 4GlcNAc $\alpha$ 4GlcA $\beta$ 4GlcNS $6S\alpha$ 4GlcA $\beta$ 4GlcNS $3S6S\alpha$ 4IdoA $2S\alpha$ 4GlcNS



Heparin/Heparan Sulfate