# Symbol and Text Nomenclature for Representation of Glycan Structure Nomenclature Committee Consortium for Functional Glycomics

#### I. Symbol nomenclature

The Nomenclature Committee evaluated widely used symbol nomenclatures and consulted with a variety of interested parties. As a result, the committee selected a version originally put forth by Stuart Kornfeld and later adapted by the editors of the textbook 'Essentials of Glycobiology' (first edition, Cold Spring Harbor Laboratory Press). In consultation with the editors of the 'Essentials of Glycobiology' it was further modified based on the following criteria:

- The symbol nomenclature must be convenient for the annotation of mass spectra. To this end, it was decided that::
  - Each sugar type (i.e. sugars of the same mass: hexose, hexosamine and N-acetylhexosamine), should have the same symbol shape.
  - Isomers of each sugar type (e.g. mannose/galactose/glucose) should be differentiated by color or by black/white/shading.
  - Where possible, the same color or shading should be used for derivatives of hexose (e.g. the corresponding N-acetylhexosamine and hexosamine).
  - Representing different sugars using the same shape but different orientation should be avoided so that structures can be represented either horizontally or vertically.
- Colored symbols should still appear distinguishable when copied or printed in black and white.
- Considering 10% of the population is color blind, the use of both red and green for the same shaped symbols should be avoided.
- When desired, linkage information can be represented in text next to a line connecting the symbols (e.g. α4, β4).

#### Symbol nomenclature – color version printed in color:

Hexoses: Circles N-Acetylhexosamines: Squares Hexosamines: Squares divided diagonally	Prin	t in co	lor
·Galactose stereochemistry: Yellow (255,255,0) with Black outline	$\circ$		
•Glucose stereochemistry: BLUE (0,0,250) with Black outline	<u> </u>		
·Mannose stereochemistry: GREEN (0,200,50) with Black outline			
•Fucose: RED (250,0,0) with Black outline	<u> </u>		
·Xylose: (5-pointed star) ORANGE (250,234,213) with Black outline			
	X		
Acidic Sugars (Diamonds)			
NeuAc: PURPLE (200,0,200) with Black outline	<b></b>	•	
NeuGc: LIGHT BLUE (233,255,255) with Black outline	$\Diamond$	>	
•KDN: GREEN (0,200,50) with Pattern & Black outline	<b></b>	>	
<ul> <li>GlcA: BLUE (0,0,250)/Upper segment with Black outline</li> </ul>	♦	>	
<ul> <li>IdoA: TAN (150,100,50)/Lower segment with Black outline</li> </ul>	<del>Q</del>	•	
<ul> <li>GalA: Yellow (255,255,0) /Left segment with Black outline</li> </ul>	<b></b>	>	
<ul> <li>ManA: GREEN (0,200,50)/Right segment with Black outline</li> </ul>	<b>4</b>	•	

<sup>\*</sup> GalA symbol switched from red to yellow, to keep with the convention that sugars with the Gal configuration is yellow.

Symbol nomenclature – color version printed in black and white:

Hexoses: Circles  N-Acetylhexosamines: Squares  Hexosamines: Squares divided diagonally	Print in l	black &	white
<ul> <li>Galactose stereochemistry: Yellow (255,255,0) with Black outli</li> </ul>	ine 🔿		
<ul> <li>Glucose stereochemistry: BLUE (0,0,250) with Black outline</li> </ul>			
<ul> <li>Mannose stereochemistry: GREEN (0,200,50) with Black outling</li> </ul>	ie O	Ξ	
•Fucose: RED (250,0,0) with Black outline	Ă	_	
•Xylose: (5-pointed star) ORANGE (250,234,213) with Black out	line☆		
Acidic Sugars (Diamonds)		•	
<ul> <li>NeuAc: PURPLE (200,0,200) with Black outline</li> </ul>	•	•	
<ul> <li>NeuGc: LIGHT BLUE (233,255,255) with Black outline</li> </ul>	•	$\Diamond$	
<ul> <li>KDN: GREEN (0,200,50) with Pattern &amp; Black outline</li> </ul>	•	<b>♦</b>	
<ul> <li>GlcA: BLUE (0,0,250)/Upper segment with Black outline</li> </ul>	•	<b>♦</b> <b>♦</b> <b>♦</b>	
<ul> <li>IdoA: TAN (150,100,50)/Lower segment with Black outline</li> </ul>	•	<b>₩</b>	
<ul> <li>GalA: Yellow (255,255,0) /Left segment with Black outline</li> </ul>			
• ManA: GREEN (0,200,50)/Right segment with Black outline	•	<b>•</b>	
Symbol nomenclature – black and white version:			
Hexoses; Circles			
N-Acetylhexosamines: Squares			
Hexosamines: Squares divided diagonally	_		
•Galactose stereochemistry: White with Black outline	$\circ$		
•Glucose stereochemistry: Black with Black outline			
Mannose stereochemistry: Gray with Black outline			
•Fucose: Gray with Black outline			
·Xylose: (5-pointed star) White with Black outline	*		
Acidic Sugars (Diamonds)	, ,		
NeuAc: Black with Black outline		$\Diamond$	
NeuGc: White with Black outline		$\Diamond$	
<ul> <li>KDN: Gray with Pattern &amp; Black outline</li> </ul>		$\Diamond$ $\Diamond$ $\Diamond$ $\Diamond$	
GlcA: Black/Upper segment with Black outline		$\Diamond$	
<ul> <li>IdoA: Black/Lower segment with Black outline</li> </ul>		<b>\rightarrow</b>	
<ul> <li>GalA: White /Left segment with Black outline</li> </ul>		$\Phi$	
ManA: Gray/Right segment with Black outline		◆	

#### II. Text nomenclature

The committee recommends a "modified IUPAC condensed" text nomenclature which includes the anomeric carbon but not the parentheses, and which can be written in either a linear or 2D version. The Committee felt that:

- Including the anomeric carbon is important, and is likely to become increasingly more so in the future as more complicated structures are discovered.
- The presence of parentheses (which then necessitates the use of brackets to indicate branching structures) is unnecessarily cumbersome, particularly when representing the structure in 2D form.

## **Example of chosen text nomenclature:**

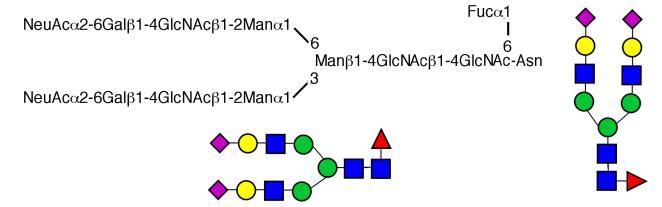
## Modified IUPAC condensed

**Linear:** NeuAcα2-3Galβ1-4(Fucα1-3)GlcNAcβ1-2Manα1-R

2D: NeuAcα2-3Galβ1 $_4$ GlcNAcβ1-2Manα1-R

III. Examples of symbol nomenclature used to illustrate N- and O-linked glycans written in the 2D version of the text nomenclature. Note that symbol structures will be used to annotate data where linkages have not been defined (e.g MALDI profiling), and if linkages between monosaccharides are known, they can be added above or to the side of the line connecting the symbols if desired (e.g.  $\alpha$ 6 or  $\beta$ 4).

# N-linked glycan:



#### O-linked Glycan:

