Package ‘gglycan’

January 18, 2026

Title Plot Glycans using 'ggplot2'

Version 0.0.3

Description Plot glycans following the Symbol Nomenclature for Glycans (SNFG) using 'ggplot2'. SNFG provides a standardized visual representation of glycan structures.

License Artistic-2.0

Encoding UTF-8

Depends R (>= 4.1.0)

Imports dplyr, ggplot2, ggtangle (>= 0.1.0), ggstar, ggrepel, igraph, rlang, yulab.utils

Suggests quarto

VignetteBuilder quarto

RoxygenNote 7.3.3

NeedsCompilation no

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Repository CRAN

Date/Publication 2026-01-18 11:00:08 UTC

Contents

`format_linkage_label` *Format Linkage Labels*

Description

Converts ’a’/’b’ to Greek letters alpha/beta.

Usage

```
format_linkage_label(labels)
```

Arguments

`labels`	A character vector of linkage labels.

Value

A character vector with Greek letters.

Examples

```
labels <- c("a1-3", "b1-4")
format_linkage_label(labels)
```

`geom_glycan` *Glycan Geometry Layer*

Description

A convenient wrapper to add edges, edge labels, and SNFG nodes to a glycan plot.

Usage

```
geom_glycan(
  edge_color = "black",
  edge_width = 0.5,
  arrow_length = unit(2, "mm"),
  node_size = 5,
  node_label = FALSE,
  label_size = 3.88,
  edge_label_size = 3.88,
  ...
)
```

Arguments

`edge_color`	Color of the edges.
`edge_width`	Width of the edges.
`arrow_length`	Length of the edge arrows.
`node_size`	Size of the node symbols.
`node_label`	Logical. Whether to show node labels (monosaccharide names). Default is FALSE.
`label_size`	Size of the node labels.
`edge_label_size`	Size of the edge labels (linkage).
`...`	Additional arguments (currently unused).

Value

A list of ‘ggplot2‘ layers.

Examples

```
s <- "Neu5Ac(a2-3)Gal(b1-4)GlcNAc(b1-2)Man(a1-3)Man(b1-4)GlcNAc(b1-4)GlcNAc"
## Not run:
gglycan(s) + geom_glycan()

## End(Not run)
```

`get_hl_alpha` *Get Highlight Alpha*

Description

Gets the current alpha value for motif highlighting.

Usage

```
get_hl_alpha(default = 0.4)
```

Arguments

`default`	Default value if not set (0.4).

Value

A numeric value representing the alpha level.

Examples

```
get_hl_alpha()
```

`gglycan` *Plot Glycan Structure*

Description

Visualizes a glycan structure using ggplot2 and ggtangle.

Usage

```
gglycan(
  data,
  mapping = aes(),
  layout = ggtangle::layout_fishbone,
  direction = "left",
  length = 1,
  angle_sep = 30,
  motif = NULL,
  ...
)
```

Arguments

`data`	A glycan graph object (from ‘read_glycan‘) or an IUPAC string.
`mapping`	Default list of aesthetic mappings to use for plot.
`layout`	The layout algorithm to use. Default is ‘ggtangle::layout_fishbone‘. Can be a string ("tree", "nicely") or a function.
`direction`	The direction of the main chain growth ("left", "right", "up", "down"). Default is "left".
`length`	The distance between nodes. Default is 1.
`angle_sep`	The angle separation for branches in degrees. Default is 30.
`motif`	A motif string (IUPAC format) to highlight in the structure. Default is NULL.
`...`	Additional arguments passed to ‘ggplot‘.

Value

A ‘ggplot‘ object.

Examples

```
s <- "Neu5Ac(a2-3)Gal(b1-4)GlcNAc(b1-2)Man(a1-3)Man(b1-4)GlcNAc(b1-4)GlcNAc"
## Not run:
gglycan(s) + geom_glycan()

## End(Not run)
```

`highlight_motif` *Identify Motif in Glycan Graph*

Description

Finds occurrences of a motif subsequence in the main glycan graph and marks them.

Usage

```
highlight_motif(graph, motif_str)
```

Arguments

`graph`	The main glycan graph (an ‘igraph‘ object).
`motif_str`	The motif string (IUPAC format).

Value

An ‘igraph‘ object with an added ‘alpha‘ vertex attribute (1 for motif, 0.4 for others).

Examples

```
s <- "Neu5Ac(a2-3)Gal(b1-4)GlcNAc(b1-2)Man(a1-3)Man(b1-4)GlcNAc(b1-4)GlcNAc"
g <- read_glycan(s)
g <- highlight_motif(g, "Neu5Ac(a2-3)Gal(b1-4)GlcNAc")
```

`match_snfg_style` *Match SNFG Style to Graph Nodes*

Description

Maps glycan node labels to SNFG shapes and colors.

Usage

```
match_snfg_style(graph)
```

Arguments

`graph`	An ‘igraph‘ object.

Value

An ‘igraph‘ object with additional vertex attributes: ‘snfg_shape‘ (numeric starshape) and ‘snfg_fill‘ (color).

Examples

```
s <- "Neu5Ac(a2-3)Gal(b1-4)GlcNAc(b1-2)Man(a1-3)Man(b1-4)GlcNAc(b1-4)GlcNAc"
g <- read_glycan(s)
g <- match_snfg_style(g)
```

`read_glycan` *Read Glycan Data*

Description

Parses a glycan string (IUPAC condensed format) and returns a graph object.

Usage

```
read_glycan(x, format = "iupac")
```

Arguments

`x`	A character string representing the glycan structure.
`format`	The format of the string. Currently only "iupac" is supported.

Value

An ‘igraph‘ object representing the glycan structure.

Examples

```
s <- "Neu5Ac(a2-3)Gal(b1-4)GlcNAc(b1-2)Man(a1-3)Man(b1-4)GlcNAc(b1-4)GlcNAc"
g <- read_glycan(s)
```

`set_hl_alpha` *Set Highlight Alpha*

Description

Sets the alpha value for motif highlighting.

Usage

```
set_hl_alpha(value = 0.4)
```

Arguments

`value`	Numeric value for alpha (default 0.4).

Value

No return value, called for side effects.

Examples

```
set_hl_alpha(0.5)
```

`snfg_map` *SNFG Symbol Mapping*

Description

A dataset containing the shapes and colors for SNFG symbols.

Usage

```
snfg_map
```

Format

A data frame with columns:

monosaccharide The name of the monosaccharide (e.g., Glc, Gal, Man)

shape The shape of the symbol (e.g., circle, square)

color The fill color of the symbol (hex code)

starshape The ggstar shape ID

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