

Package: glycoTraitR (via r-universe)

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Type Package

Title Compute and analyze the glycan structural traits from GPSM data

Version 1.0.0

Description GlycoTraitR is an R package for analyzing glycoproteomics data, particularly glycopeptide-spectrum matches (GPSMs). It supports results generated by the pGlyco3 and Glyco-Decipher search engines. The package parses glycan structures, computes monosaccharide compositions and structural traits, and performs differential analysis of glycan heterogeneity. It constructs trait-by-PSM matrices stored in a SummarizedExperiment object, supports user-defined structural motifs, and provides visualization utilities for interpreting glycan trait changes.

URL <https://github.com/matsui-lab/glycoTraitR>

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analyze_trait_changes *Differential analysis of glycan traits between experimental groups*

Description

Perform group-wise statistical testing on glycan trait matrices stored in a SummarizedExperiment created by `build_trait_se`. For each glycan trait and each site/protein row, the function compares trait intensities across user-specified experimental groups using Welch's t-test and Levene's variance test.

Usage

```
analyze_trait_changes(trait_se, group_col, group_levels, min_psm = 20)
```

Arguments

trait_se	A SummarizedExperiment containing trait matrices (one assay per trait), typically returned by <code>build_trait_se</code> .
group_col	The column name in <code>colData(trait_se)</code> defining sample group membership.
group_levels	Character vector specifying which values of <code>group_col</code> to compare (e.g., <code>c("Control","Treatment")</code>).
min_psm	Minimum required PSM count per group for statistical testing. Default = 20.

Details

Each assay in `trait_se` represents a glycan trait matrix. The rows are glycopeptides (site-level) or proteins (protein-level). The columns are GPSM count found in samples. For each trait × feature combination, Extract PSM-level trait intensities for samples belonging to the specified `group_levels`. Exclude traits where either group has fewer than `min_psm` GPSMs. Exclude all-zero traits (boolean-like traits) Run Welch two-sample t-test (`t.test`) and Levene's variance test (`car::leveneTest`, median centered). A result is returned only if either test shows $p < 0.05$.

Value

A data frame of significant trait–site (or trait–protein) comparisons with:

- trait — glycan trait name
- level — site/protein identifier
- l_pval — Levene test p-value
- f_val — Levene test F statistic
- t_pval — Welch t-test p-value
- t_val — t-statistic

Rows correspond only to significant comparisons ($p < 0.05$) for ‘l_pval’ or ‘t_pval’.

Examples

```
# Load toy pGlyco3 GPSM data included with the package
path <- system.file("extdata", "pGlyco3_gpsm_toyexample.txt",
  package = "glycoTraitR"
)
gpsm_toyexample <- read_pGlyco3_gpsm(path)

# Load accompanying toy metadata
data("meta_toyexample")

# Build glycan trait SummarizedExperiment at the protein level
trait_se <- build_trait_se(
  gpsm = gpsm_toyexample,
  from = "pGlyco3",
  motifs = NULL,
  level = "protein",
  meta = meta_toyexample
)

# Identify glycan traits significantly changed between groups
changed_traits <- analyze_trait_changes(
  trait_se = trait_se,
  group_col = "Diagnosis",
  group_levels = c("Normal", "Symptomatic"),
  min_psm = 20
)
changed_traits
```

build_glycan_igraph *Construct an igraph representation of a glycan tree*

Description

Convert a parsed glycan tree into a directed ‘igraph’ object with parent–child relationships and residue-level metadata suitable for structural motif detection.

Usage

```
build_glycan_igraph(tree)
```

Arguments

tree A parsed glycan tree from [pGlyco3_to_tree](#) or [wurcs_to_tree](#).

Details

The resulting graph contains the following vertex attributes:

- name — synthetic node label ("a", "b", ...)
- residue — residue type (H, N, A, F, G)
- type — identical to residue (for convenience)
- color — color encoding of residue type
- is_root — TRUE if the vertex is the structural root

Value

A directed 'igraph' object representing the glycan structure.

Examples

```
# Example: parse a pGlyco3 monosaccharide expression into a glycan tree
pGlyco_expr <- "(N(N(H(H(H)))(H(H)(H)(H(H))))))"

# Convert expression into a parsed tree structure
tree <- pGlyco3_to_tree(pGlyco_expr)
g <- build_glycan_igraph(tree)
g
```

build_trait_se

Build a SummarizedExperiment of glycan trait matrices

Description

Convert a GPSM table into peptide- or protein-level glycan trait matrices and store them in a SummarizedExperiment object. Each trait becomes an assay matrix whose rows represent peptides or proteins, and whose columns represent individual GPSMs. This function provides a unified container for downstream analyses such as differential testing and visualization.

Usage

```
build_trait_se(gpsm, from, motifs = NULL, level, meta)
```

Arguments

gpsm	A GPSM table containing at least: 'Protein', 'Peptide', 'GlycanStructure', 'File', and 'Count'.
from	Character; glycan format used in the GPSM input. One of 'decipher' or 'pGlyco3'.
motifs	Optional named list of user-defined motif structures passed to compute_glycan_traits .
level	Summarization level. Either 'site (peptide)' or "protein".
meta	Data frame of sample metadata with a column 'file' matching 'gpsm\$File'.

Value

A 'SummarizedExperiment' where each assay is a glycan-trait matrix (trait × PSM), 'rowData' contains peptide/protein names, and 'colData' contains metadata aligned to PSMs.

Examples

```
# Load toy GPSM table exported by pGlyco3
path <- system.file("extdata", "pGlyco3_gpsm_toyexample.txt",
  package = "glycoTraitR"
)
gpsm_toyexample <- read_pGlyco3_gpsm(path)

# Load toy metadata for summarization
data("meta_toyexample")

# Build glycan trait SummarizedExperiment at protein level
trait_se <- build_trait_se(
  gpsm = gpsm_toyexample,
  from = "pGlyco3",
  motifs = NULL,
  level = "protein",
  meta = meta_toyexample
)

# Inspect assay names and dimensions
SummarizedExperiment::assayNames(trait_se)
dim(trait_se)
```

compute_glycan_traits *Compute glycan traits from a parsed glycan tree*

Description

Combine residue-level composition traits (see [count_residues](#)), structural traits (see [compute_structural_traits](#)), and user-defined motifs (see [compute_userdefined_traits](#)) into a unified trait vector.

Usage

```
compute_glycan_traits(tree, motifs)
```

Arguments

`tree` A parsed glycan tree from [pGlyco3_to_tree](#) or [wurcs_to_tree](#).
`motifs` Optional named list of user-defined glycan motifs.

Value

A named list of numeric trait values.

Examples

```
# Example: parse a pGlyco3-style glycan expression into a tree
pGlyco_expr <- "(N(N(H(H(H))) (H(H)(H)(H(H))))))"

# Convert to glycan tree structure
tree <- pGlyco3_to_tree(pGlyco_expr)

# Explore parsed nodes and edges
tree$node
tree$edge

# Build igraph representation
g <- build_glycan_igraph(tree)
plot_glycan_tree(g)

# Define user motifs for trait computation
user_motifs <- list(
  LinearH3 = list(
    node = c("H", "H", "H"),
    edge = c("a-b", "b-c")
  ),
  FucBranch = list(
    node = c("H", "N", "F"),
    edge = c("a-b", "b-c")
  )
)

# Compute glycan structural traits
compute_glycan_traits(tree, motifs = user_motifs)
```

Description

A curated reference table mapping glycan IDs to their structures, used internally by glycoTraitR and also available to users.

Usage

```
data(glycanDatabase)
```

Format

A data frame with N rows and M columns.

Examples

```
data(glycanDatabase)
head(glycanDatabase)
```

meta_toyexample

Toy metadata for glycoTraitR examples

Description

A toy example metadata table used in vignettes, examples, and tests.

Usage

```
data(meta_toyexample)
```

Format

A data frame with 34 rows and 2 variables:

Diagnosis Clinical diagnosis (factor)

Sample number Sample ID (numeric)

file File Name (character)

Examples

```
data(meta_toyexample)
head(meta_toyexample)
```

pGlyco3_to_tree *Convert a pGlyco3 glycan string into a glycan tree structure*

Description

Parse a pGlyco3-style glycan expression (e.g. "N(H(H))") and reconstruct the residue sequence and edge relationships as a tree suitable for downstream structural analysis. This parser assumes simple pGlyco3 monosaccharide symbols (e.g. "N", "H", "A", "F").

Usage

```
pGlyco3_to_tree(expr)
```

Arguments

expr A character string representing the pGlyco3 glycan structure.

Details

This function interprets parentheses as branch delimiters and assigns:

1. one residue per character (e.g. N, H, A)
2. parent-child edges based on bracket nesting

Each residue is assigned a synthetic node label (a, b, c, ...), ensuring compatibility with graph-based trait extraction.

Value

A list with:

- node: character vector of residue types
- edge: character vector of edges in "a-b" format

Examples

```
# Example: parse a pGlyco3-style glycan expression into a tree
pGlyco_expr <- "(N(N(H(H))(H(H)(H)(H(H))))))"
# Convert to glycan tree structure
tree <- pGlyco3_to_tree(pGlyco_expr)
tree
```

plot_glycan_tree *Plot a glycan structure represented as an igraph tree*

Description

Visualize a glycan structure encoded as an igraph object produced by [build_glycan_igraph](#). This plot is mainly intended for inspecting glycan topology (branching, residue types, connectivity).

Usage

```
plot_glycan_tree(g)
```

Arguments

`g` An igraph object representing a glycan tree from [build_glycan_igraph](#).

Value

A glycan topology plot is drawn as a side effect.

Examples

```
# Example: parse a pGlyco3-style glycan expression into a tree
pGlyco_expr <- "(N(N(H(H(H)))(H(H)(H)(H(H))))))"

# Convert to glycan tree structure
tree <- pGlyco3_to_tree(pGlyco_expr)

# Explore parsed nodes and edges
tree$node
tree$edge

# Build igraph representation
g <- build_glycan_igraph(tree)
plot_glycan_tree(g)
```

plot_trait_distribution *Plot the distribution of a glycan trait across experimental groups*

Description

Generate two diagnostic plots—a histogram and a boxplot—for a selected glycan trait at a specific site/protein feature. This function extracts GPSM-level values from a trait matrix stored in a ‘SummarizedExperiment’, subsets them by group, removes missing values, and visualizes the resulting distribution.

Usage

```
plot_trait_distribution(trait_se, group_col, group_levels, trait_name, feature)
```

Arguments

trait_se	A SummarizedExperiment object generated by <code>build_trait_se</code> , containing one assay matrix per glycan trait.
group_col	Column name in <code>'colData(trait_se)'</code> that defines sample group membership.
group_levels	Character vector specifying the group values to include in the plot. Typically two values (e.g. <code>'c("Control","Treatment")'</code>).
trait_name	Name of the glycan trait to plot. Must match an assay name in <code>'assays(trait_se)'</code> .
feature	Row identifier within the trait matrix (peptide, or protein). Must match a row name in <code>'assays(trait_se)[[trait_name]]'</code> .

Value

A named list of two 'ggplot2' objects: * 'p_hist' — histogram of trait intensities * 'p_box' — boxplot with jitter overlay

Examples

```
# Load the toy GPSM table exported by pGlyco3 (included in the package)
path <- system.file("extdata", "pGlyco3_gpsm_toyexample.txt",
  package = "glycoTraitR"
)
gpsm_toyexample <- read_pGlyco3_gpsm(path)

# Load the accompanying toy metadata
data("meta_toyexample")

# Build a protein-level glycan trait SummarizedExperiment object
trait_se <- build_trait_se(
  gpsm = gpsm_toyexample,
  from = "pGlyco3",
  motifs = NULL,
  level = "protein",
  meta = meta_toyexample
)

# Identify glycan traits significantly changed between two groups
changed_traits <- analyze_trait_changes(
  trait_se = trait_se,
  group_col = "Diagnosis",
  group_levels = c("Normal", "Symptomatic"),
  min_psm = 20
)

# Extract one trait name and one protein/site feature to visualize
trait_name <- changed_traits$trait[1]
feature <- changed_traits$level[1]
```

```
# Plot the distribution of this selected trait
p <- plot_trait_distribution(
  trait_se      = trait_se,
  group_col     = "Diagnosis",
  group_levels = c("Normal", "Symptomatic"),
  trait_name    = trait_name,
  feature       = feature
)

# Show histogram and boxplot
p$p_hist
p$p_box
```

read_decipher_gpsm	<i>Combine Glyco-Decipher GPSM results into a long-format table</i>
--------------------	---

Description

Read multiple Glyco-Decipher GPSM files from a folder, merge them into a unified protein–peptide–glycan table, and attach glycan structures (WURCS 2.0).

Usage

```
read_decipher_gpsm(gpsm_folder_dir)
```

Arguments

gpsm_folder_dir

The path to a folder containing Glyco-Decipher GPSM files (e.g. files ending with "_GPSM_DatabaseGlycan.txt").

Details

This function assumes that the input folder contains one or more Glyco-Decipher GPSM files, typically named with the suffix "_GPSM_DatabaseGlycan.txt". For each file, GPSM records are read and collapsed by Protein, Peptide, GlycanID, File, and Count. All files are then combined into a single table, and glycan IDs are mapped to WURCS structures via the global glycanDatabase object. The final table uses a standardized glycan column name GlycanStructure for compatibility with downstream functions.

Value

A data frame in long format with one row per Protein–Peptide–GlycanStructure–File combination and the following columns:

- Protein — protein identifier(s)
- Peptide — peptide sequence

- GlycanStructure — glycan structural annotation (WURCS 2.0)
- File — raw file name
- Count — spectral count (number of GPSMs) for this combination

The returned table is designed to be passed to [build_trait_se](#) for glycan trait computation.

See Also

[read_pGlyco3_gpsm](#), [build_trait_se](#)

Examples

```
folder <- system.file("extdata", "decipher_toyexample", package = "glycoTraitR")
gpsm <- read_decipher_gpsm(folder)
head(gpsm)
```

read_pGlyco3_gpsm *Import pGlyco3 GPSM results as a long-format table*

Description

Read a pGlyco3 GPSM result file and convert it into a long-format protein–peptide–glycan table with spectral counts per raw file. Each row corresponds to a unique combination of protein, peptide, glycan structure, and file.

Usage

```
read_pGlyco3_gpsm(gpsm_dir)
```

Arguments

`gpsm_dir` The path to the pGlyco3 GPSM output file (for example, "pGlycoDB-GP-FDR-Pro-Quant-Site.txt").

Details

This function takes a pGlyco3 GPSM file as input (typically named pGlycoDB-GP-FDR-Pro-Quant-Site.txt). The following steps are performed:

- Select relevant columns (RawName, Proteins, Peptide, PlausibleStruct).
- Rename them to a standardized schema: File, Protein, Peptide, GlycanStructure.
- Collapse multiple protein IDs per PSM into a single pipe-separated string (e.g. "P00123|P00456").
- Aggregate rows by Protein, Peptide, GlycanStructure, and File as GPSM counts in each group.

The output of this function is typically used as the input for [build_trait_se](#).

Value

A data frame with one row per Protein–Peptide–GlycanStructure–File combination and the following columns:

- Protein — protein identifier(s)
- Peptide — peptide sequence
- GlycanStructure — glycan structural annotation from pGlyco3
- File — raw file name
- Count — spectral count (number of GPSMs) for this combination

See Also

[read_decipher_gpsm](#), [build_trait_se](#)

Examples

```
# Load toy example data included in glycoTraitR
path <- system.file("extdata", "pGlyco3_gpsm_toyexample.txt",
  package = "glycoTraitR"
)
gpsm <- read_pGlyco3_gpsm(path)
head(gpsm)
```

wurcs_to_tree

Convert a WURCS string into a glycan tree structure

Description

Parse a WURCS (WURCS 2.0) glycan annotation and extract:

- residue sequence (as a character vector)
- edge list (parent–child relationships)

Usage

```
wurcs_to_tree(w)
```

Arguments

w A character string containing a WURCS 2.0 glycan annotation.

Details

This function is used internally to convert WURCS strings into a tree representation that can support structural trait computation and graph construction.

The function performs several parsing steps:

1. Remove the WURCS prefix and split the string into components.
2. Extract *UniqueRES* entries and map them to residue symbols using the internal WURCS_RES_MAP table.
3. Follow the *RES sequence* index to reconstruct the residue vector.
4. Parse *LIN* entries and normalize them into simple "X-Y" edges.

Value

A list with two elements:

- node: character vector of residue types in order
- edge: character vector of edges in "A-B" format

Examples

```
# Example WURCS glycan string
w <- paste0(
  "WURCS=2.0/4,9,8/",
  "[u2122h_2*NCC/3=0]",
  "[a2122h-1b_1-5_2*NCC/3=0]",
  "[a1122h-1b_1-5]",
  "[a1122h-1a_1-5]",
  "/1-2-3-4-4-4-4-4-4/",
  "a4-b1_b4-c1_c3-d1_c6-f1_d2-e1_f3-g1_f6-h1_h2-i1"
)
tree <- wurcs_to_tree(w)
tree
```

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