

# Package ‘glycoTraitR’

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**Type** Package

**Title** Compute and analyze the glycan structural traits from GPSM data

**Version** 1.1.0

**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>

**License** MIT + file LICENSE

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glycoTraitR-package	<i>glycoTraitR: Compute and analyze the glycan structural traits from GPSM data</i>
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## 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.

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## See Also

Useful links:

- <https://github.com/matsui-lab/glycoTraitR>
- Report bugs at <https://github.com/matsui-lab/glycoTraitR/issues>

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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

<code>trait_se</code>	A SummarizedExperiment containing trait matrices (one assay per trait), typically returned by <code>build_trait_se</code> .
<code>group_col</code>	The column name in <code>colData(trait_se)</code> defining sample group membership.
<code>group_levels</code>	Character vector specifying which values of <code>group_col</code> to compare (e.g., <code>c("Control", "Treatment")</code> ).
<code>min_psm</code>	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  $\times$  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	<i>Build a SummarizedExperiment of glycan trait matrices</i>
----------------	--------------------------------------------------------------

---

**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 <a href="#">compute_glycan_traits</a> .
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 <a href="#">pGlyco3_to_tree</a> or <a href="#">wurcs_to_tree</a> .
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)
```

---

glycanDatabase

*Glycan annotation reference database*

---

### 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	<i>Convert a pGlyco3 glycan string into a glycan tree structure</i>
-----------------	---------------------------------------------------------------------

---

**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	<i>Import pGlyco3 GPSM results as a long-format table</i>
-------------------	-----------------------------------------------------------

---

## 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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