GlycoRDF version 0.15

# Namespaces

The following RDF namespaces and prefixes will be used in the documentation.

|  |  |
| --- | --- |
| **Prefix** | **URI** |
| rdf | http://www.w3.org/1999/02/22-rdf-syntax-ns# |
| bibo | http://purl.org/ontology/bibo/ |
| foaf | http://xmlns.com/foaf/0.1/ |
| owl | http://www.w3.org/2002/07/owl# |
| glycan | http://purl.jp/bio/12/glyco/glycan# |
| dcterms | http://purl.org/dc/terms/ |
| dc | http://purl.org/dc/elements/1.1/ |
| xsd | http://www.w3.org/2001/XMLSchema# |
| rdfs | http://www.w3.org/2000/01/rdf-schema# |

# Buffer

A buffer is an aqueous solution consisting of a mixture of a weak acid and its conjugate base or a weak base and its conjugate acid.

**URI:** http://purl.jp/bio/12/glyco/glycan#buffer

**Superclass:** glycan:role

# Carbohydrate Format

Instances of this class are the carbohydrate sequence formats.

**URI:** http://purl.jp/bio/12/glyco/glycan#carbohydrate\_format

**Superclass:** owl:Thing

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:carbohydrate\_format\_wurcs | wurcs |  |
| glycan:carbohydrate\_format\_glycoct | glycoct |  |
| glycan:carbohydrate\_format\_iupac\_short | iupac short |  |
| glycan:carbohydrate\_format\_iupac\_condensed | iupac condensed |  |
| glycan:carbohydrate\_format\_csdb | csdb |  |
| glycan:carbohydrate\_format\_linearcode | linearcode |  |
| glycan:carbohydrate\_format\_glyde2 | glyde2 |  |
| glycan:carbohydrate\_format\_iupac\_extended | iupac extended |  |
| glycan:carbohydrate\_format\_kcf | kcf |  |
| glycan:carbohydrate\_format\_carbbank | carbbank |  |
| glycan:carbohydrate\_format\_linucs | linucs |  |

# Citation

References are publications related to the glycan structures or features. This can be journal papers, book chapters, conference articles and so on.

**URI:** http://purl.jp/bio/12/glyco/glycan#citation

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| bibo:authorList | rdfs:Literal |  |  |
| bibo:pageEnd | xsd:string | yes |  |
| bibo:pageStart | xsd:string | yes |  |
| bibo:shortTitle | xsd:string |  |  |
| bibo:volume | xsd:string | yes |  |
| dc:publisher | xsd:string | yes |  |
| dc:title | xsd:string |  |  |
| dcterms:issued | xsd:integer |  | Publication year |
| glycan:has\_keyword | xsd:anyURI |  | Keyword for the publication. Object is a URI in MeSH. |
| glycan:has\_method | xsd:anyURI |  | experimental procedures described in the article |
| glycan:has\_pmid | xsd:integer |  |  |
| glycan:has\_reference | glycan:referenced\_compound |  | Reference between :compound, :citation, :evidence, :source and :referenced\_compound. |

# Component

Components are used to specify the composition of glycans. A component has a reference to the molecule (monosaccharide, substituent) and a number of occurrences for this molecule in the glycan.

**URI:** http://purl.jp/bio/12/glyco/glycan#component

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_cardinality | xsd:integer | yes | Number of occurrences of an element (e.g. a monosaccharide) in the subject. This information can be missing in case the cardinality cannot be defined (e.g. repeat units with unknown or under-defined repeats). Missing for non-stoichiometrical residues. |
| glycan:has\_cardinality\_per\_repeat | xsd:integer | yes | Number of occurrences of an element (e.g. a monosaccharide) in the repeat unit. Applicable to :repeatUnits only. Missing for non-stoichiometrical residues. |
| glycan:has\_monosaccharide | glycan:monosaccharide | yes | URI to a RDF resource describing the monosaccharide (usually MonosaccharideDB). |

# Compound

Superclass of types of glycan related molecules and fragments.

**URI:** http://purl.jp/bio/12/glyco/glycan#compound

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| foaf:name | xsd:string |  | Name of the compound. |
| glycan:has\_reference | glycan:referenced\_compound |  | Reference between :compound, :citation, :evidence, :source and :referenced\_compound. |
| glycan:has\_resource\_entry | glycan:resource\_entry |  | Assigns a resource entry to a compound. |

## Aglycon

Instances of this class represent the aglyca which are covalently attached to the glycans. It contains information about the aglycon, the linkage position in aglycon and glycan.

**URI:** http://purl.jp/bio/12/glyco/glycan#aglycon

**Superclass:** glycan:compound

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| foaf:name | xsd:string |  | trivial name |

### Lipid

**URI:** http://purl.jp/bio/12/glyco/glycan#lipid

**Superclass:** glycan:aglycon

### Peptide

Part of a protein amino acid sequence generated by digestion for analysis.

**URI:** http://purl.jp/bio/12/glyco/glycan#peptide

**Superclass:** glycan:aglycon

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_AA\_sequence | xsd:string | yes | Amino acid sequence is represented in the standard IUPAC-IUB amino acid code. Even if any modification were known, any modified amino acid residues are represented with a single letter of a nascent residue. |

### Protein

Proteinous part of glycoprotein. equivalent to nascent peptide or protein entities found in Uniprot or other protein databases.

**URI:** http://purl.jp/bio/12/glyco/glycan#protein

**Superclass:** glycan:aglycon

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_AA\_sequence | xsd:string | yes | Amino acid sequence is represented in the standard IUPAC-IUB amino acid code. Even if any modification were known, any modified amino acid residues are represented with a single letter of a nascent residue. |
| glycan:has\_uniprot\_accession | http://www.uniprot.org/core/Protein | yes | When the subject of this predicate is :glycoprotein, the range instance is equivalent to proteineous part of the subject glycoprotein. |

## Amino Acid

**URI:** http://purl.jp/bio/12/glyco/glycan#amino\_acid

**Superclass:** glycan:compound

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:glutamine | glutamine |  |
| glycan:aspartic\_acid | aspartic acid |  |
| glycan:lysine | lysine |  |
| glycan:phenylalanine | phenylalanine |  |
| glycan:histidine | histidine |  |
| glycan:proline | proline |  |
| glycan:cysteine | cysteine |  |
| glycan:selenocysteine | selenocysteine |  |
| glycan:leucine | leucine |  |
| glycan:asparagine | asparagine |  |
| glycan:isoleucine | isoleucine |  |
| glycan:glutamic\_acid | glutamic acid |  |
| glycan:methionine | methionine |  |
| glycan:glycine | glycine |  |
| glycan:arginine | arginine |  |
| glycan:threonine | threonine |  |
| glycan:tyrosine | tyrosine |  |
| glycan:serine | serine |  |
| glycan:tryptophan | tryptophan |  |
| glycan:valine | valine |  |
| glycan:alanine | Alanine |  |

## Glycoconjugate

Superclass of biomolecules consisting of a glycan part and an aglycon part, that are covalently attached to each other.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycoconjugate

**Superclass:** glycan:compound

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:catalyzed\_by | glycan:reaction |  | Object is a reaction process. |
| glycan:degraded\_by | glycan:glycosyl\_hydrolase\_reaction |  | Object is a reaction process, which degrades the subject. |
| glycan:has\_aglycon | glycan:aglycon |  | This property is used to specify the aglycon portion of a glycoconjugate compound. |
| glycan:has\_attached\_glycan | glycan:saccharide |  | This property is used to specify a glycan portion of a glycoconjugate compound. |
| glycan:synthesized\_by | glycan:glycosyltransferase\_reaction |  | Object is a reaction process, which synthesizes the subject. |

### Glycolipid

Lipid with saccharide(s) attached wit glycosidic bond(s).

**URI:** http://purl.jp/bio/12/glyco/glycan#glycolipid

**Superclass:** glycan:glycoconjugate

### Glycopeptide

A class involves artificial degradation products of glycoproteins with protease digestion, typically results from proteomics experiment analyses. There are any reason or trace for the glycosylation modification, that at least one amino acid residue of the peptide is glycosylated.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycopeptide

**Superclass:** glycan:glycoconjugate

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_AA\_sequence | xsd:string | yes | Amino acid sequence is represented in the standard IUPAC-IUB amino acid code. Even if any modification were known, any modified amino acid residues are represented with a single letter of a nascent residue. |
| glycan:has\_glycosylated\_AA | glycan:glycosylated\_AA |  | This property is used to specify a glycosylated amino acid residue in an object glycoprotein or glycopeptide. |
| glycan:has\_uniprot\_accession | http://www.uniprot.org/core/Protein | yes | When the subject of this predicate is :glycoprotein, the range instance is equivalent to proteineous part of the subject glycoprotein. |

### Glycoprotein

A compound that consists of protein and glycan parts; they are covalently attached to each other by a glycosidic bond. There are any reason or trace for the glycosylation modification, that at least one amino acid residue of the protein is glycosylated.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycoprotein

**Superclass:** glycan:glycoconjugate

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_AA\_sequence | xsd:string | yes | Amino acid sequence is represented in the standard IUPAC-IUB amino acid code. Even if any modification were known, any modified amino acid residues are represented with a single letter of a nascent residue. |
| glycan:has\_glycosylated\_AA | glycan:glycosylated\_AA |  | This property is used to specify a glycosylated amino acid residue in an object glycoprotein or glycopeptide. |
| glycan:has\_uniprot\_accession | http://www.uniprot.org/core/Protein | yes | When the subject of this predicate is :glycoprotein, the range instance is equivalent to proteineous part of the subject glycoprotein. |

### Glycoside

**URI:** http://purl.jp/bio/12/glyco/glycan#glycoside

**Superclass:** glycan:glycoconjugate

### Glycosylated AA

Amino acid residue(s), to which a glycan covalently attached, in a glycopeptide or glycoprotein. To specify glycosylation type or bond of glycoprotein.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycosylated\_AA

**Superclass:** glycan:glycoconjugate

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_amino\_acid\_type | glycan:amino\_acid | yes |  |
| glycan:modification\_type | http://www.uniprot.org/core/Glycosylation\_Annotation | yes | Modification type is represented due to biological process, typically N-linked or O-linked. |

## Saccharide

Instances of this class represent the molecule information of the glycans. That includes chemical composition, molecular weight but also related information such as images of the glycans.

**URI:** http://purl.jp/bio/12/glyco/glycan#saccharide

**Superclass:** glycan:compound

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:catalyzed\_by | glycan:reaction |  | Object is a reaction process. |
| glycan:degraded\_by | glycan:glycosyl\_hydrolase\_reaction |  | Object is a reaction process, which degrades the subject. |
| glycan:has\_affinity\_to | glycan:glycan\_binder |  | Subject is a glycan or glycoconjugate, which non-covalently binds to the object, usually :glycan\_binder. |
| glycan:has\_epitope | glycan:glycan\_epitope |  | The object is a structural motif with biological relevance; subproperty of has\_motif. |
| glycan:has\_glycoconjugate\_sequence | glycan:glycoconjugate\_sequence |  | Sequence information to object of rdf:type :glycoconjugate\_sequence if the subject is part of a glycoconjugate. |
| glycan:has\_glycosequence | glycan:glycosequence |  | glycan sequence information to object of rdf:type :glycosequence representing the subject in a text format. |
| glycan:has\_image | glycan:image |  | Object is a URI to an image instance describing a graphical representation of the glycan. |
| glycan:has\_motif | glycan:glycan\_motif |  | The object is a structurally defined motif E.g. for Neo-lacto motif http://jcggdb.jp/idb/motif?id=JCGG-MOTIF3009.rdf inverse of ”contained\_in”. should have sequence, composition, image ... |
| glycan:is\_ambiguous | xsd:boolean | yes | Boolean indicating whether the subject is a fully defined structure including all linkage information, or not. |
| glycan:synthesized\_by | glycan:glycosyltransferase\_reaction |  | Object is a reaction process, which synthesizes the subject. |

### N-glycan

A subclass of saccharide primarily found on eurokaryotic glycoproteins. This class of glycan typically contains a specific glycan substructure motif (http://jcggdb.jp/idb/motif?id=JCGG-MOTIF1001), and the reducing terminal GlcNAc of the glycan is attached to the N-atom of an asparagine residue of the protein in a beta configuration. A class of glycoconjugate including dolichyl-diphospho esters also involves the same glycan motif, but they are attached in an alpha configuration. The dolichyl-diphosphooligosaccharides are precursors or intermediates in the protein N-glycosylation process, by which the specific dolichyl-diphosphooligosaccharide (http://jcggdb.jp/idb/jcggdb/JCGG-STR015745) is transferred from the dolichyl phospohate ester to an asparagine residue of the protein by an oligosacchayl transferase (GO:0004579).

**URI:** http://purl.jp/bio/12/glyco/glycan#N-glycan

**Superclass:** glycan:saccharide

### O-glycan

A subclass of saccharide primarily found in glycoproteins This class is subdivided into a variety of subclasses due to its expression in a variety of biological sources. In terms of structure, O-glycans consist depending on the type of O-Glycan of a GalNAc, Man, Fuc, Glc residue at the reducing end and are typical in animal proteins, which are attached to a serine, threonine, hydroxylysine or hydroxyproline residue of a protein in an alpha configuration.

**URI:** http://purl.jp/bio/12/glyco/glycan#O-glycan

**Superclass:** glycan:saccharide

### Cyclic Glycan

Cyclic glycans are a special form of glycans which are rarely found in nature. As implied by the name, they form cyclic structures, in contrast to the branched tree structures of commonly known glycans.

**URI:** http://purl.jp/bio/12/glyco/glycan#cyclic\_glycan

**Superclass:** glycan:saccharide

### Monosaccharide

Instances of this class represent monosaccharides and their information. These monosaccharides are used to specify the composition of glycans, referenced by glycan:component. Sample URI:
http://www.monosaccharidedb.org/rdf/monosaccharide.action?name=o-dall-HEX-0:0

**URI:** http://purl.jp/bio/12/glyco/glycan#monosaccharide

**Superclass:** glycan:saccharide

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_alias | glycan:monosaccharide\_alias |  | reference to aliases for the monosaccharide |
| glycan:has\_average\_molecular\_weight | xsd:double | yes | literal numeric with decimal, calculated from monosaccharide composition with average atomic weight |
| glycan:has\_basetype | glycan:basetype | yes | Object is the basetype of the monosaccharide (subject). |
| glycan:has\_linkage\_position | xsd:integer |  | Monosaccharide can be linked to other residues via standard glycosidic linkage at the given backbone position. |
| glycan:has\_monoisotopic\_molecular\_weight | xsd:double | yes | Literal numeric with decimal, calculated from monosaccharide composition with atomic weight of monoisotope. |
| glycan:has\_msdb\_id | xsd:integer | yes | Id of the monosaccharide in MonosaccharideDB. |
| glycan:has\_substitution | glycan:substituent |  | The substituent is linked to the basetype in this monosaccharide. |

### Polysaccharide

Polysaccharides are a special form of glycans that consist of large repetitive oligosaccharide parts. Often the exact number of repetitions cannot be specified because the experimental technique does not allow this or because the number of repetition in nature varies.

**URI:** http://purl.jp/bio/12/glyco/glycan#polysaccharide

**Superclass:** glycan:saccharide

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_polymerization\_degree | glycan:polymerization\_degree |  | Used only if the specified glycan structure (subject) itself is the oligomeric part forming a repeating unit. Repeating unit information to object of rdf:type :repeat\_count. |

#### Biological Repeat Unit

A biological repeat unit contains the monosaccharides of the repetitive oligosaccharide unit in the arrangement as they are synthesized.

**URI:** http://purl.jp/bio/12/glyco/glycan#biological\_repeat\_unit

**Superclass:** glycan:motif

#### Chemical Repeat Unit

A chemical repeat unit is generated when a polysaccharide is chopped down for the analysis. The sequence of the oligomer is based on the reaction chopping down the glycan and may not represent the biological repeat unit.

**URI:** http://purl.jp/bio/12/glyco/glycan#chemical\_repeat\_unit

**Superclass:** glycan:motif

# Enzyme

Enzyme that take part in synthesis anddegradation of glycan.

**URI:** http://purl.jp/bio/12/glyco/glycan#enzyme

**Superclass:** glycan:role

# Evidence

Evidences are any kind of experimental data that can be linked to glycans. These are mainly experiments to elucidate the carbohydrate structure or feature but can also be experiments for creating carbohydrates for example by synthesis.

**URI:** http://purl.jp/bio/12/glyco/glycan#evidence

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_manufacturer | xsd:string | yes | Manufacturer of the device used in the experiment. |
| glycan:has\_model | xsd:string | yes | Model of the device used in the experiment. |
| glycan:has\_reference | glycan:referenced\_compound |  | Reference between :compound, :citation, :evidence, :source and :referenced\_compound. |
| glycan:published\_in | glycan:citation | yes | Reference information for the subject. |

## Evidence Binding

Entities of this class represent molecular interactions between instancese of glycan:saccharide and glycan:glycan\_binder, elucidated by experimental results.

**URI:** http://purl.jp/bio/12/glyco/glycan#evidence\_binding

**Superclass:** glycan:evidence

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:captured\_by | glycan:glycan\_binder | yes | Object is compounds that have affinity to glycan or glycoconjugate. |
| glycan:has\_affinity\_value | xsd:double | yes | Binding affinity value for the lectin or antibody. |

### Evidence Binding Antibody

Entities of this class represent molecular interactions between instances of epitope and antibody, elucidated by experimental results.

**URI:** http://purl.jp/bio/12/glyco/glycan#evidence\_binding\_antibody

**Superclass:** glycan:evidence\_binding

### Evidence Binding Lectin

Entities of this class represent molecular interactions between instances of glycan and lectin, elucidated by experimental results.

**URI:** http://purl.jp/bio/12/glyco/glycan#evidence\_binding\_lectin

**Superclass:** glycan:evidence\_binding

## Evidence Ce

Experiments using capillary electrophoresis to identify carbohydrate structures.

**URI:** http://purl.jp/bio/12/glyco/glycan#evidence\_ce

**Superclass:** glycan:evidence

## Evidence Lc

Experiments using LC techniques to identify carbohydrates or using them for the separation of glycans.

**URI:** http://purl.jp/bio/12/glyco/glycan#evidence\_lc

**Superclass:** glycan:evidence

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:injection\_volume | xsd:double | yes |  |
| glycan:used\_lc\_flow\_rate | xsd:string | yes | Flow rate refers to the flow of mobile phase through the column and is measured in ml/min. |
| glycan:used\_lc\_gradient | glycan:gradient |  | Used gradient for the experiment. |
| glycan:used\_molecule | glycan:compound |  |  |
| glycan:used\_solvent | glycan:solvent |  | Link to solvent information, such as https://www.ebi.ac.uk/chebi/searchId.do?chebiId=41981. brutto-formula |

## Evidence Ms

Experiments using mass spectrometry to identify the carbohydrate structures.

**URI:** http://purl.jp/bio/12/glyco/glycan#evidence\_ms

**Superclass:** glycan:evidence

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_mass\_spectrum | glycan:mass\_spectrum |  |  |
| glycan:has\_precursor\_peak | glycan:ms\_peak |  | URI of the precursor peak of a MS^n spectra. |
| glycan:used\_ms | glycan:mass\_spectrometry\_device | yes |  |
| rdfs:seeAlso | xsd:anyURI |  | a link to a spectrum in some other database |

### Evidence Lc Ms

**URI:** http://purl.jp/bio/12/glyco/glycan#evidence\_lc\_ms

**Superclass:** glycan:evidence\_ms

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:injection\_volume | xsd:double | yes |  |
| glycan:used\_column | glycan:lc\_column | yes |  |
| glycan:used\_lc\_flow\_rate | xsd:string | yes | Flow rate refers to the flow of mobile phase through the column and is measured in ml/min. |
| glycan:used\_lc\_gradient | glycan:gradient |  | Used gradient for the experiment. |
| glycan:used\_molecule | glycan:compound |  |  |
| glycan:used\_solvent | glycan:solvent |  | Link to solvent information, such as https://www.ebi.ac.uk/chebi/searchId.do?chebiId=41981. brutto-formula |

#### Evidence IGOT

Is an IGOT experiment, subclass of glycan:evidence\_lc\_ms. IGOT experiment is a procedure for the large-scale identification of N-glycosylated proteins, with isotope-coded glycosylation-site-specific tagging. (PMID: 12754521)

**URI:** http://purl.jp/bio/12/glyco/glycan#evidence\_IGOT

**Superclass:** glycan:evidence\_lc\_ms

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_peptide | glycan:glycopeptide | yes |  |

## Evidence NMR

Experiments using NMR to identify the carbohydrate structure.

**URI:** http://purl.jp/bio/12/glyco/glycan#evidence\_nmr

**Superclass:** glycan:evidence

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_missing\_signals\_max | xsd:integer |  |  |
| glycan:has\_missing\_signals\_min | xsd:integer |  |  |
| glycan:has\_nucleus | xsd:string |  | Nucleus |
| glycan:has\_subspectrum | glycan:subspectrum |  |  |
| glycan:has\_unassigned\_signal | glycan:signal |  | Link to an unassigned signal which is just a chemical shift. |
| glycan:used\_amount\_mg | xsd:double |  | sample weight. |
| glycan:used\_buffer | glycan:buffer |  | Link to buffer information, such as http://en.wikipedia.org/wiki/Phosphate\_buffered\_saline. |
| glycan:used\_concentration | rdfs:Literal |  | sample concentration. |
| glycan:used\_frequency | xsd:double |  | frequency of NMR spectrometer. |
| glycan:used\_ph | xsd:double | yes | pH of solution |
| glycan:used\_reference\_standard | glycan:compound |  | reference\_standard is the accepted internal/external standard for calibrating chemical shift for NMR spectroscopy. |
| glycan:used\_solvent | glycan:solvent |  | Link to solvent information, such as https://www.ebi.ac.uk/chebi/searchId.do?chebiId=41981. brutto-formula |
| glycan:used\_temperature | xsd:string | yes | value or range in K (literal) |
| rdfs:seeAlso | xsd:anyURI |  | refer to raw/processed data file location if available |

# Evidence Type

List of evidence types.

**URI:** http://purl.jp/bio/12/glyco/glycan#evidence\_type

**Superclass:** owl:Thing

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:evidence\_type\_nmr | nmr |  |
| glycan:evidence\_type\_msms | msms |  |
| glycan:evidence\_type\_ms | ms |  |
| glycan:evidence\_type\_lc\_msms | lc msms |  |
| glycan:evidence\_type\_lc\_ms | lc ms |  |
| glycan:evidence\_type\_lc | lc |  |
| glycan:evidence\_type\_hplc | hplc |  |
| glycan:evidence\_type\_ce | ce |  |

# Glycan Binder

A class of compound that has affinity to a glycan or glycoconjugate. Usually a reference to a lectin, virus, bacteria, etc.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycan\_binder

**Superclass:** glycan:role

## Antibody

A subclass of glycan\_binder which binds to an epitope; in this namespace, this is a glycoepitope, which may be a (part of a) glycan or a part of a glycoconjugate.

**URI:** http://purl.jp/bio/12/glyco/glycan#antibody

**Superclass:** glycan:glycan\_binder

## Lectin

A class of protein that binds to glycans but is neither an antibody nor an enzyme.

**URI:** http://purl.jp/bio/12/glyco/glycan#lectin

**Superclass:** glycan:glycan\_binder

# Glycan Database

A class representing databases that store glycans and related information. If possible, owl:sameAs should be used referencing the biosharing entry for this database.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycan\_database

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_abbreviation | xsd:string | yes | Abbreviation of the database |
| glycan:has\_category | glycan:glycan\_database\_category |  | category of a glycan database |
| glycan:has\_url\_template | xsd:string | yes | xsd:string such as http://foo.bar.com/someglycan?id=%s |

# Glycan Database Category

Instances of this class are the categories for the classification of glycan databases.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycan\_database\_category

**Superclass:** owl:Thing

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:database\_category\_taxonomy | taxonomy | Taxonomical information regarding glycans are available. |
| glycan:database\_category\_monosaccharide | monosaccharide | Database containing monosaccharide information. |
| glycan:database\_category\_experimental | experimental | Database of glycomics experiments such as NMR, MS, array data, etc- |
| glycan:database\_category\_chemical\_compound | chemical compound | Database of carbohydrates at the atomic level. |
| glycan:database\_category\_cabohydrate\_structure | structure | Database containing glycan structure information. |
| glycan:database\_category\_bibliography | bibliography |  |

# Glycan Motif

A glycan motif is a sub-structure of glycans that has been named because of its frequent appearance or because of the biological meaning.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycan\_motif

**Superclass:** glycan:motif

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:contained\_in | glycan:saccharide |  | The subject is a structurally defined motif, and the object is a glycan structure or motif. |

## Glycan Epitope

A glycan epitope is a special motif which has a known biological function.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycan\_epitope

**Superclass:** glycan:glycan\_motif

# Lc Property

Class that contains Liquid Chromatography properties such as gradient, Lc column.

**URI:** http://purl.jp/bio/12/glyco/glycan#lc\_property

**Superclass:** owl:Thing

## Gradient

**URI:** http://purl.jp/bio/12/glyco/glycan#gradient

**Superclass:** glycan:lc\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:used\_lc\_run\_time | xsd:string | yes | Runtime of the LC |
| glycan:used\_percent\_max | xsd:double | yes |  |
| glycan:used\_percent\_min | xsd:double | yes |  |

## Lc Column

**URI:** http://purl.jp/bio/12/glyco/glycan#lc\_column

**Superclass:** glycan:lc\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_diameter | xsd:double | yes | diameter of the column in micro meter |
| glycan:has\_length | xsd:double | yes | Length of the column in milli meter |
| glycan:has\_material | xsd:string | yes |  |
| glycan:has\_particle\_size | xsd:double | yes | Size of the particle in micro meter. |

# Monosaccharide Property

Class that contains all monosaccharides properties such as anomer, basetype etc.

**URI:** http://purl.jp/bio/12/glyco/glycan#monosaccharide\_property

**Superclass:** owl:Thing

## Absolute Configuration

Absolute configuration of a monosaccharide basetype. Possible values are D, L or Unknown.

**URI:** http://purl.jp/bio/12/glyco/glycan#absolute\_configuration

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:absolute\_configuration\_unknown | unknown |  |
| glycan:absolute\_configuration\_laevus | laevus |  |
| glycan:absolute\_configuration\_dexter | dexter |  |

## Anomer

Anomer of a monosaccharide. Possible values are alpha, beta, unknown or none.

**URI:** http://purl.jp/bio/12/glyco/glycan#anomer

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:anomer\_unknown | unknown |  |
| glycan:anomer\_none | none |  |
| glycan:anomer\_beta | beta |  |
| glycan:anomer\_alpha | alpha |  |

## Basetype

Basetype of the monosaccharide in accordance to GlycoCT and MonosaccharideDB definitions.

**URI:** http://purl.jp/bio/12/glyco/glycan#basetype

**Superclass:** glycan:monosaccharide\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_anomer | glycan:anomer | yes | Anomeric state of the basetype. |
| glycan:has\_basetype\_id | xsd:integer | yes | Id of the basetype in MonosaccharideDB. |
| glycan:has\_configuration | glycan:configuration |  | Instance of class is configuration. |
| glycan:has\_core\_modification | glycan:core\_modification |  | reference to another RDF describing a core modification that is present in this basetype |
| glycan:has\_extended\_stereocode | xsd:string | yes | Extended stereocode of the basetype |
| glycan:has\_first\_configuration | glycan:configuration | yes | Reference to another RDF resource with URI describing the first monosaccharide configuration |
| glycan:has\_ring\_end | xsd:integer | yes | position of last carbon involved in ring closure |
| glycan:has\_ring\_start | xsd:integer | yes | position of first carbon involved in ring closure |
| glycan:has\_ring\_type | glycan:ring\_type | yes | Assigns the ring type to a basetype. |
| glycan:has\_second\_configuration | glycan:configuration | yes | Reference to another RDF resource with URI describing the second monosaccharide configuration in case there are more than four stereocenters |
| glycan:has\_size | xsd:integer | yes | number of backbone carbon atoms |
| glycan:has\_stereocode | xsd:string | yes | Stereocode describing the backbone stereochemistry |
| glycan:has\_third\_configuration | glycan:configuration | yes | Reference to another RDF resource with URI describing the third monosaccharide configuration in case there are more than eight stereocenters |

## Configuration

Configuration of a monosaccharide. Each monosaccharide can have several configurations (e.g. dgro-dgal). Each configuration consist of a absolute configuration and a relative configuration.

**URI:** http://purl.jp/bio/12/glyco/glycan#configuration

**Superclass:** glycan:monosaccharide\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_absolute\_configuration | glycan:absolute\_configuration | yes | Subject is a monosaccharide basetype. The object values for the predicate can be D, L or unknown. |
| glycan:has\_relative\_configuration | glycan:relative\_configuration | yes | IUPAC monosaccharide basetype information. Without absolute configuration D or L |

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:configuration\_x | x |  |

## Core Modification

Core modification of a monosaccharide. A core modification consists of a modification type and the position(s) at which this modification happened.

**URI:** http://purl.jp/bio/12/glyco/glycan#core\_modification

**Superclass:** glycan:monosaccharide\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_core\_modification\_type | glycan:core\_modification\_type | yes | Type of the core modification. Instances of class are core modification types. |
| glycan:has\_modification\_position | xsd:integer | yes | Position of the modification at the monosaccharide. |
| glycan:has\_modification\_position2 | xsd:integer | yes | Second position of the modification at the monosaccharide (eg. for double bounds) |

## Core Modification Type

List of core modifications that can appear on a monosaccharide.

**URI:** http://purl.jp/bio/12/glyco/glycan#core\_modification\_type

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:core\_modification\_type\_enx | enx | Double bond in the basetype backbone with unknown deoxygenation pattern. |
| glycan:core\_modification\_type\_deoxy | deoxy | Deoxygenation of a position: The OH group is removed and replaced by a hydrogen atom. |
| glycan:core\_modification\_type\_en | en | Double bond in the basetype backbone. This modification implies that - unless explicitly stated with a deoxy modification - hydroxyl groups are preserved. |
| glycan:core\_modification\_type\_yn | yn | Triple bond in the basetype backbone. |
| glycan:core\_modification\_type\_keto | keto | A carbonyl group in the open chain version of a monosaccharide. This modification is omitted if it is only present at position 1 (standard aldose). |
| glycan:core\_modification\_type\_acid | acid | Carboxyl (COOH) group. |
| glycan:core\_modification\_type\_sp | sp | Triple bond to a substituent. |
| glycan:core\_modification\_type\_geminal | geminal | Loss of stereochemistry due to identical substituents with DEOXY and H\_LOSE linkage types at a single position. |
| glycan:core\_modification\_type\_sp2 | sp2 | Double bond to a substituent. |
| glycan:core\_modification\_type\_aldi | aldi | Alditol: Reduction of the aldehyde group to CH2OH. |
| glycan:core\_modification\_type\_anhydro | anhydro | Intramolecular anhydride. |

## Linkage Type

List of linkage types that can appear on the monosaccharide side of monosaccharide to substituent linkages.

**URI:** http://purl.jp/bio/12/glyco/glycan#linkage\_type

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:linkage\_type\_s\_config | s config | Same as R\_CONFIG, but resulting in an S-Configuration of the carbon. |
| glycan:linkage\_type\_r\_config | r config | The substituent is linked directly to the basetype backbone by replacing a hydrogen atom at a terminal position, which would be non-chiral without the substituent, resulting in an R-configuration of the carbon. |
| glycan:linkage\_type\_h\_loss | h loss | The substituent is linked directly to the basetype backbone by replacing the hydrogen atom. |
| glycan:linkage\_type\_h\_at\_oh | h at oh | A standard O-linked substituent, i.e. the substituent replaces the hydrogen of an OH group. |
| glycan:linkage\_type\_deoxy | deoxy | The substituent is linked directly to the basetype backbone by replacing the OH group. |

## Monosaccharide Alias

Alternative names for the monosaccharide in different databases or resources. The aliases consist of the name and the monosaccharide notation scheme.

**URI:** http://purl.jp/bio/12/glyco/glycan#monosaccharide\_alias

**Superclass:** glycan:monosaccharide\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| foaf:name | xsd:string |  | Alternative name of the monosaccharide. |
| glycan:has\_alias\_name | xsd:string |  | Alias name of a monosaccharide. |
| glycan:has\_external\_substituent | glycan:substituent |  | Reference to a :substituent. |
| glycan:has\_monosaccharide\_notation\_scheme | glycan:monosaccharide\_notation\_scheme | yes | One of GLYCOSCIENCES, GLYCOCT, IUPAC, CARBBANK, CFG, BCSDB, PDB, or GLYCAM, see http://www.monosaccharidedb.org/notation.action?topic=schemes |
| glycan:is\_primary\_name | xsd:boolean | yes | indicates whether this is the name that should be used to uniquely identify this monosaccharide in the given :notation\_scheme, or whether this is a secondary alias name (e.g. to indicate whether a trivial name or a systematic name is to be used preferentially in case a trivial name exists for this monosaccharide) |
| glycan:is\_trivial\_name | xsd:boolean | yes | Indicates whether this is a trivial name that implies modifications, or a systematic name (e.g. KDO vs. D-3-deoxy-manOct2ulo-onic) |

## Monosaccharide Notation Scheme

List of monosaccharide notation scheme. One monosaccharide can have several different names depending on the notation scheme.

**URI:** http://purl.jp/bio/12/glyco/glycan#monosaccharide\_notation\_scheme

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:monosaccharide\_notation\_scheme\_pdb | pdb | The 3-letter residue names as used by the Protein Data Bank (PDB). Unlike most of the other notations, these names cannot be generated automatically by conversion routines but have to be assigned manually by the database administrators. Some PDB residue names that encode carbohydrate residues define disaccharides or oligosaccharides. These are not implemented in MonosaccharideDB, as the scope of this database is on monosaccharide residues. |
| glycan:monosaccharide\_notation\_scheme\_monosaccharidedb | monosaccharidedb | MonosaccharideDB's internal notation format. Basetype and substituent names are the same as in GlycoCT, with the exception that 'anhydro' and 'lactone' modifications are included in the basetype here, while they are defined as substituents in GlycoCT. As most glycobiologist and also most carbohydrate databases consider a monosaccharide that contains substituents as one residue, they are defined in this way in MonosaccharideDB as well. |
| glycan:monosaccharide\_notation\_scheme\_glycosciences\_de | glycosciences de | The Notation used in the Glycosciences.de web portal. It is based on the CarbBank notation. |
| glycan:monosaccharide\_notation\_scheme\_glycoct | glycoct | The nomenclature that is used by EUROCarbDB. For more information see www.eurocarbdb.org/recommendations/encoding/. |
| glycan:monosaccharide\_notation\_scheme\_cfg | cfg | The LinearCode notation used by the US Consortium for Functional Glycomics (CFG). |
| glycan:monosaccharide\_notation\_scheme\_carbbank | carbbank | The CarbBank notation is based on the IUPAC extended notation. It is used by the Complex Carbohydrate Structure Database (CCSD), which is better known by the name of its query software "carbbank". CarbBank style notation forms the basis of several other notations, such as the Glycosciences.de scheme. |
| glycan:monosaccharide\_notation\_scheme\_bcsdb | bcsdb | The notation used by the Russian BCSDB. For more information on this notation, see the description on the BCSDB homepage. |
| glycan:monosaccharide\_notation\_scheme\_amber\_glycam | amber glycam | Two-letter residue names used within the AMBER GLYCAM forcefield. For more information, see Carbohydrate Naming Convention in Glycam. Note (1): Monosaccharide alias names in GLYCAM notation also encode linkage positions (in the first character of a three-letter-code residue name). These depend on the context of a residue within an oligosaccharide and thus are no monosaccharide properties. GLYCAM names stored in MonosaccharideDB refer to a terminal residue. The first character might have to be adjusted according to the specific context of a residue, i.e. in case other residues linked are to the given one. Note (2): The GLYCAM notation is not yet supported by the notation parsing routines, i.e. GLYCAM alias names can be created, but not be read yet. |

## Relative Configuration

List of relative monosaccharide configurations according to IUPAC.

**URI:** http://purl.jp/bio/12/glyco/glycan#relative\_configuration

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:manno | manno |  |
| glycan:allo | allo |  |
| glycan:talo | talo |  |
| glycan:xylo | xylo |  |
| glycan:lyxo | lyxo |  |
| glycan:erythro | erythro |  |
| glycan:gluco | gluco |  |
| glycan:arabino | arabino |  |
| glycan:altro | altro |  |
| glycan:ribo | ribo |  |
| glycan:ido | ido |  |
| glycan:threo | threo |  |
| glycan:galacto | galacto |  |
| glycan:gulo | gulo |  |
| glycan:glycero | glycero |  |

## Ring Type

Ringtype of a basetype.

**URI:** http://purl.jp/bio/12/glyco/glycan#ring\_type

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:ring\_type\_unknown | unknown | A monosaccharide whose ring type is unknown. |
| glycan:pyranose | pyranose | A Pyranose is any cyclic isomer that has a five carbons and one oxygen in a ring of six atoms. |
| glycan:open | open | Open chain sugar that does not form a ring. |
| glycan:furanose | furanose | A furanose is a five member ring structure containing four carbon atoms and one oxygen atom. |

## Substituent

Substition of a monosaccharide by another molecule. The substituent consists of the substituent type and the linkage between monosaccharide and substituent. For example: http://www.monosaccharidedb.org/rdf/substituent/ethyl.rdf

**URI:** http://purl.jp/bio/12/glyco/glycan#substituent

**Superclass:** glycan:monosaccharide\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| foaf:name | xsd:string |  | Name of the substituent. |
| glycan:has\_substituent\_linkage | glycan:substituent\_linkage |  | linkage of the substituent |
| glycan:has\_substituent\_type | glycan:substituent\_type | yes | linkage type of the substituent |
| glycan:has\_substitution\_name | xsd:string |  | Name of substitution. |
| glycan:has\_valence | xsd:integer |  | Object is a valence of substituent. |
| glycan:is\_fuzzy | xsd:boolean |  | If a substituent is fuzzy. |
| glycan:is\_linkable | xsd:boolean |  | If a substituent is linkable. |

## Substituent Linkage

Linkage between a monosaccharide basetype and a substituent. It consist of the linkage position on the basetype side and the substituent side, and of the linkage type.

**URI:** http://purl.jp/bio/12/glyco/glycan#substituent\_linkage

**Superclass:** glycan:monosaccharide\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_basetype\_linkage\_position | xsd:integer | yes | Linkage position at the basetype. |
| glycan:has\_linkage\_type | glycan:linkage\_type | yes | GlycoCT linkage type of the monosaccharide to the substituent |
| glycan:has\_substituent\_linkage\_position | xsd:integer | yes | Linkage position at the substituent. |
| glycan:has\_substituent\_linkage\_position2 | xsd:integer | yes | Second linkage position at the substituent. |

## Substituent Type

List of substituent types possible on monosaccharides.

**URI:** http://purl.jp/bio/12/glyco/glycan#substituent\_type

**Superclass:** glycan:monosaccharide\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_default\_linkage\_bondorder | xsd:float |  | Object is bond order that is number of linkage in default. |
| glycan:has\_default\_linkage\_bondorder2 | xsd:float |  | Object is second bond order that is number of linkage in default. |
| glycan:has\_default\_linkage\_type | glycan:linkage\_type |  | Instances of this class are linkage type . |
| glycan:has\_default\_linkage\_type2 | glycan:linkage\_type |  | Instances of this class are second linkage type. |
| glycan:has\_default\_linking\_position | xsd:integer |  | A position that is number of linkage in default. |
| glycan:has\_default\_linking\_position2 | xsd:integer |  | A position that is number of second linkage in default. |

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:substituent\_type\_fluoro | fluoro | F |
| glycan:substituent\_type\_thio | thio | SH |
| glycan:substituent\_type\_s\_methyl | s methyl | SCH3 |
| glycan:substituent\_type\_glycolyl | glycolyl | COCH2OH |
| glycan:substituent\_type\_trifluoroacetyl | trifluoroacetyl | COCF3 |
| glycan:substituent\_type\_n\_trimethyl | n trimethyl | N(CH3)3 |
| glycan:substituent\_type\_n\_dimethyl | n dimethyl | N(CH3)2 |
| glycan:substituent\_type\_n\_alanine | n alanine | NHCOCHNH2CH3 |
| glycan:substituent\_type\_iodo | iodo | I |
| glycan:substituent\_type\_chloro | chloro | Cl |
| glycan:substituent\_type\_s\_pyruvate | s pyruvate | CH2CCOOH |
| glycan:substituent\_type\_imino | imino | NH |
| glycan:substituent\_type\_n\_trifluoroacetyl | n trifluoroacetyl | NHCOCF3 |
| glycan:substituent\_type\_r\_lactate | r lactate | CH3CHCOOH |
| glycan:substituent\_type\_sulfate | sulfate | SO3H |
| glycan:substituent\_type\_n\_formyl | n formyl | NHCHO |
| glycan:substituent\_type\_n\_sulfate | n sulfate | NHSO3H |
| glycan:substituent\_type\_ethanolamine | ethanolamine | NHCH2CH2OH |
| glycan:substituent\_type\_x\_lactate | x lactate | CH3CHCOOH |
| glycan:substituent\_type\_n\_succinate | n succinate | NCOCH2CH2COOH |
| glycan:substituent\_type\_ethyl | ethyl | CH2CH3 |
| glycan:substituent\_type\_n\_methyl | n methyl | NHCH3 |
| glycan:substituent\_type\_telluro | telluro | TeH |
| glycan:substituent\_type\_nitrat | nitrat | NO2 |
| glycan:substituent\_type\_amino | amino | NH2 |
| glycan:substituent\_type\_s\_lactate | s lactate | CH3CHCOOH |
| glycan:substituent\_type\_n\_glycolyl | n glycolyl | NCOCH2OH |
| glycan:substituent\_type\_acetyl | acetyl | COCH3 |
| glycan:substituent\_type\_hydroxymethyl | hydroxymethyl | CH2OH |
| glycan:substituent\_type\_seleno | seleno | SeH |
| glycan:substituent\_type\_formyl | formyl | CHO |
| glycan:substituent\_type\_x\_pyruvate | x pyruvate | CH2CCOOH |
| glycan:substituent\_type\_n\_ethyl | n ethyl | NHCH2CH3 |
| glycan:substituent\_type\_n\_acetyl | n acetyl | NHCOCH3 |
| glycan:substituent\_type\_r\_pyruvate | r pyruvate | CH2CCOOH |
| glycan:substituent\_type\_methyl | methyl | CH3 |
| glycan:substituent\_type\_bromo | bromo | Br |
| glycan:substituent\_type\_phosphate | phosphate | PO3H2 |

# Ms Property

Class that contains Mass Spectorometry properties such as adduct, adduct ion etc.

**URI:** http://purl.jp/bio/12/glyco/glycan#ms\_property

**Superclass:** owl:Thing

## Adduct

**URI:** http://purl.jp/bio/12/glyco/glycan#adduct

**Superclass:** glycan:ms\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_count | xsd:integer | yes |  |
| glycan:has\_ion | glycan:adduct\_ion | yes |  |

## Adduct Ion

**URI:** http://purl.jp/bio/12/glyco/glycan#adduct\_ion

**Superclass:** glycan:ms\_property

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:adduct\_ion\_na | Na+ |  |
| glycan:adduct\_ion\_h | H+ |  |

## Mass Spectrometry Device

**URI:** http://purl.jp/bio/12/glyco/glycan#mass\_spectrometry\_device

**Superclass:** glycan:ms\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_ionisation\_type | http://purl.obolibrary.org/obo/MS\_1000008 |  |  |
| glycan:has\_mass\_analyzer | http://purl.obolibrary.org/obo/MS\_1000443 |  |  |
| glycan:has\_ms\_model | http://purl.obolibrary.org/obo/MS\_1000031 | yes |  |

## Mass Spectrum

**URI:** http://purl.jp/bio/12/glyco/glycan#mass\_spectrum

**Superclass:** glycan:ms\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_fragmented\_spectrum | glycan:msn\_spectrum |  |  |
| glycan:has\_mass\_spectrometry\_peak | glycan:ms\_peak |  |  |
| glycan:has\_ms\_level | xsd:integer | yes |  |

### Msn Spectrum

**URI:** http://purl.jp/bio/12/glyco/glycan#msn\_spectrum

**Superclass:** glycan:mass\_spectrum

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_retention\_time | xsd:string | yes | Retention time of the molecule in the experiment |

### Profile Spectrum

**URI:** http://purl.jp/bio/12/glyco/glycan#profile\_spectrum

**Superclass:** glycan:mass\_spectrum

## Ms Annotation

**URI:** http://purl.jp/bio/12/glyco/glycan#ms\_annotation

**Superclass:** glycan:ms\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_adduct | glycan:adduct |  |  |
| glycan:has\_fragment | xsd:string | yes | sequence as peak annotation |
| glycan:has\_fragment\_type | glycan:ms\_fragment\_type |  |  |
| glycan:has\_neutral\_loss | glycan:neutral\_loss |  |  |

## Ms Fragment Type

**URI:** http://purl.jp/bio/12/glyco/glycan#ms\_fragment\_type

**Superclass:** glycan:ms\_property

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:ms\_fragment\_type\_z | Z |  |
| glycan:ms\_fragment\_type\_y | Y |  |
| glycan:ms\_fragment\_type\_c | C |  |
| glycan:ms\_fragment\_type\_b | B |  |

## Ms Peak

Instances represent a peak in a mass spectrometry data consisting of an m/z value, intensity value and optional a charge state.

**URI:** http://purl.jp/bio/12/glyco/glycan#ms\_peak

**Superclass:** glycan:ms\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_charge | xsd:integer |  | Charge state of the MS peak |
| glycan:has\_intensity | xsd:double | yes | intensity value of the MS peak |
| glycan:has\_ms\_annotation | glycan:ms\_annotation |  |  |
| glycan:has\_mz | xsd:double | yes | MZ value of the MS peak |

## Neutral Loss

**URI:** http://purl.jp/bio/12/glyco/glycan#neutral\_loss

**Superclass:** glycan:ms\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_chemical\_formula | xsd:string | yes |  |
| glycan:has\_count | xsd:integer | yes |  |

# Polymerization Degree

A repeat is a property of a polysaccharide that specifies how often the oligomer part is repeated to form the polysaccharide.

**URI:** http://purl.jp/bio/12/glyco/glycan#polymerization\_degree

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_repeat\_attribute | glycan:repeat\_attribute | yes | (min, max, exact, average, unknown) part of repeating unit |
| glycan:has\_repeat\_count | xsd:positiveInteger | yes | value of repeat\_attribute in resource, if known |

# Reaction

Class for reaction process to create or degrade glycans or glycoconjugates.

**URI:** http://purl.jp/bio/12/glyco/glycan#reaction

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_enzyme | glycan:enzyme |  | Object is an enzyme, which performs the reaction. |
| glycan:has\_product |  |  | Object is generated by the reaction. |
| glycan:has\_substrate |  |  | Object is consumed by the reaction. |
| glycan:used\_buffer | glycan:buffer |  | Link to buffer information, such as http://en.wikipedia.org/wiki/Phosphate\_buffered\_saline. |

## Glycosyl Hydrolase Reaction

Instances of this class are glycosyl hydrolase reactions which releases monosaccharide or oligosaccharides from the glycan or glycoconjugate.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycosyl\_hydrolase\_reaction

**Superclass:** glycan:reaction

## Glycosyltransferase Reaction

Instances of this class are glycosyltransferase reactions that build up glycans or glycoconjugates by attaching additional monosaccharides or oligosaccharides to them.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycosyltransferase\_reaction

**Superclass:** glycan:reaction

## Sulfotransferase Reaction

Instances of this class are sulfotransferase reactions that modifies glycans or glycoconjugates by attaching sulfuric moiety to them.

**URI:** http://purl.jp/bio/12/glyco/glycan#sulfotransferase\_reaction

**Superclass:** glycan:reaction

# Referenced Compound

Previously correlation instances, which connects a compound class and other information (source, references, evidence) that belong to one data set. That allows to specify that a compound instance, which has been found in a certain source was published by a certain publication.

**URI:** http://purl.jp/bio/12/glyco/glycan#referenced\_compound

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:elucidated | xsd:boolean | yes | if this glycan was elucidated (rather than just studied) in this publication |
| glycan:has\_evidence | glycan:evidence |  | evidence for a given set of information (glycan, publication). An evidence can be any type of experimental data. |
| glycan:has\_glycan | glycan:saccharide | yes | The glycan object referenced by this subject. |
| glycan:has\_structure\_location | xsd:string |  | The location of the referenced compound in a publication (e.g. Figure 1). |
| glycan:is\_from\_source | glycan:source |  | Source annotation for a referenced compound. |
| glycan:published\_in | glycan:citation | yes | Reference information for the subject. |

# Repeat Attribute

List of possible attributes to specify the repeat count. Possible values are average, exact, minimum, maximum or unknown.

**URI:** http://purl.jp/bio/12/glyco/glycan#repeat\_attribute

**Superclass:** owl:Thing

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:repeat\_attribute\_unknown | unknown |  |
| glycan:repeat\_attribute\_min | min |  |
| glycan:repeat\_attribute\_max | max |  |
| glycan:repeat\_attribute\_exact | exact |  |
| glycan:repeat\_attribute\_average | average |  |

# Resource Entry

A resource entry describes an entry about the glycan in another database.

**URI:** http://purl.jp/bio/12/glyco/glycan#resource\_entry

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| dcterms:identifier | xsd:string |  | Identifier of the glycan in the database. |
| glycan:in\_glycan\_database | glycan:glycan\_database | yes | Glycan is present in the glycan database specified by the URI. |

# Sample Preparation

A process which is the syntesis or preparation of sample for glycan analysis.

**URI:** http://purl.jp/bio/12/glyco/glycan#sample\_preparation

**Superclass:** owl:Thing

## Glycan Release

A class for process of glycan release, including chemical and enzymatic reaction.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycan\_release

**Superclass:** glycan:sample\_preparation

### Chemical Release

Release of glycan that is used chemical reaction.

**URI:** http://purl.jp/bio/12/glyco/glycan#chemical\_release

**Superclass:** glycan:glycan\_release

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:reductive\_beta\_elimination | reductive beta elimination | Beta elimination that is used reducing a get for stabilize glycan. |
| glycan:beta\_elimination | beta elimination | Beta elimination that released glycan from glycoconjugate. |

### Enzymatic Release

Release of glycan that is used enzymatic reaction.

**URI:** http://purl.jp/bio/12/glyco/glycan#enzymatic\_release

**Superclass:** glycan:glycan\_release

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:PNGaseF\_release | PNGaseF release | Release of glycan that is used PNGaseF. |

# Sequence

A sequence is the textual description of a molecule. For example FASTA sequences for proteins / peptides.

**URI:** http://purl.jp/bio/12/glyco/glycan#sequence

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_sequence | xsd:string | yes | Sequence of the Glycan |
| glycan:in\_carbohydrate\_format | glycan:carbohydrate\_format | yes | carbohydrate sequence format of the sequence given in the glycosequence instance |

## Glycoconjugate Sequence

Sequence of the glycoconjugate that includes the carbohydrate and the aglyca. Predicates should be selected based on the format used to represent the structure.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycoconjugate\_sequence

**Superclass:** glycan:sequence

## Glycosequence

Sequence of the glycan in a specified sequence format.

**URI:** http://purl.jp/bio/12/glyco/glycan#glycosequence

**Superclass:** glycan:sequence

# Signal

A signal is a NMR data point.

**URI:** http://purl.jp/bio/12/glyco/glycan#signal

**Superclass:** glycan:nmr\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_chemical\_shift | xsd:double |  | chemical shift (may be multiple e.g. for CH2 groups in 1H spectra. May be missing if unknown) |
| glycan:has\_chemical\_shift\_max | xsd:double | yes | Maximum value of chemical shift. |
| glycan:has\_chemical\_shift\_min | xsd:double | yes | Minimum value of chemical shift. |
| glycan:has\_coupling\_constant | xsd:double |  | values in Hz |
| glycan:has\_multiplicity | xsd:string | yes | single-character literal (S,M,D,T ,Q) or combination |
| glycan:is\_missing | xsd:boolean | yes | If true unassigned signal. NO if a signal can not exist, rather than its unknown. |
| glycan:of\_carbon\_number | xsd:integer | yes | carbon atom number |

# Software

Software that has been utilized for the glycan. For example software used to model the glycan.

**URI:** http://purl.jp/bio/12/glyco/glycan#software

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| foaf:name | xsd:string |  | Name of the software. |
| glycan:has\_version | xsd:string | yes | Version of the software used |

# Solvent

A solvent is a substance that dissolves a solute (a chemically different liquid, solid or gas), resulting in a solution.

**URI:** http://purl.jp/bio/12/glyco/glycan#solvent

**Superclass:** glycan:role

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:H2O |  | Water |
| glycan:DMSO | DMSO | Dimethyl sulfoxide (DMSO) is an organosulfur compound with the formula (CH3)2SO. This colorless liquid is an important polar aprotic solvent that dissolves both polar and nonpolar compounds and is miscible in a wide range of organic solvents as well as water. |
| glycan:D2O | D2O | Heavy water, formally called deuterium oxide. Deuterium oxide is used in NMR spectroscopy when the solvent of interest is water and the nuclide of interest is hydrogen. |

# Source

Source of the glycan or glycoconjugate. The source can be a biological organism that the compound was found in, a synthesis procedure trying to reproduce a natural glycan or a modeling approach for the glycan.

**URI:** http://purl.jp/bio/12/glyco/glycan#source

**Superclass:** owl:Thing

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_reference | glycan:referenced\_compound |  | Reference between :compound, :citation, :evidence, :source and :referenced\_compound. |

## Source Modeled

Class for modeled source. Instance contain information about the software used for modeling and the target organism.

**URI:** http://purl.jp/bio/12/glyco/glycan#source\_modeled

**Superclass:** glycan:source

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_destination\_organism | glycan:source\_natural | yes | glycan of which organism authors wanted to synthesize or model |
| glycan:is\_fragment | xsd:boolean | yes | If the synthesised or modeled molecule is just a fragment or the complete target molecule |
| glycan:used\_software | glycan:software |  | Software used to model the molecule. |

## Source Natural

Class for sources from biological organism. Instances contain information about the species, cell type, tissue and so on.

**URI:** http://purl.jp/bio/12/glyco/glycan#source\_natural

**Superclass:** glycan:source

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_cell\_line | xsd:anyURI | yes | Cell line information of the source |
| glycan:has\_cell\_type | xsd:anyURI | yes | Cell type information of the source |
| glycan:has\_disease | xsd:anyURI |  | MESH reference for disease |
| glycan:has\_fluid | xsd:anyURI |  | either tissue or fluid |
| glycan:has\_life\_stage | xsd:anyURI | yes | Life stage information of the source. |
| glycan:has\_organ | xsd:anyURI | yes | Organ of the source. |
| glycan:has\_sample\_type | glycan:source\_sample |  | Sample type of the source. |
| glycan:has\_taxon | http://www.uniprot.org/core/Taxon | yes | Species information of the source. |
| glycan:has\_tissue | xsd:anyURI | yes | either tissue or fluid |
| glycan:hosted\_by | glycan:source\_natural | yes | Reference to another biological source representing the host organism. |
| glycan:hybrid\_with | glycan:source\_natural |  | An offspring of two different taxons. |

## Source Sample

Class for source from sample. Instance contain sample type.

**URI:** http://purl.jp/bio/12/glyco/glycan#source\_sample

**Superclass:** glycan:source

## Source Synthetic

Class for source for synthetic glycans. In contains information about the type of synthesis approach used and if applicable the original biological source that was tried to mimic.

**URI:** http://purl.jp/bio/12/glyco/glycan#source\_synthetic

**Superclass:** glycan:source

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_destination\_organism | glycan:source\_natural | yes | glycan of which organism authors wanted to synthesize or model |
| glycan:has\_synthesis\_type | glycan:synthetic\_type | yes | Allows to specify the synthesis type used to generated the glycan. |
| glycan:is\_fragment | xsd:boolean | yes | If the synthesised or modeled molecule is just a fragment or the complete target molecule |

# Subspectrum

Subspectrum of NMR data. It contains the annotated signals.

**URI:** http://purl.jp/bio/12/glyco/glycan#subspectrum

**Superclass:** glycan:nmr\_property

**Predicates that have this class as domain:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_linkage\_path | xsd:string | yes | path from the reducing end or from the rightmost residue in repeat |
| glycan:has\_residue | glycan:monosaccharide | yes | Monosaccharide annotation of the subspectrum. |
| glycan:has\_signal | glycan:signal |  | Resource to a :signal |

# Symbol Format

Graphical symbol formats used to represent glycans. This includes the symbol format form the CFG and from UOXF.

**URI:** http://purl.jp/bio/12/glyco/glycan#symbol\_format

**Superclass:** owl:Thing

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:symbol\_format\_uoxf\_bw | uoxf bw | UOXF symbol that is displayed black and white notation. |
| glycan:symbol\_format\_uoxf | uoxf | A symbol is Oxford (UOXF) notations. |
| glycan:symbol\_format\_text | text | A glycan structure is displayed by text-only form. |
| glycan:symbol\_format\_cfg\_bw | cfg bw | CFG symbol that is displaied black and white notation. |
| glycan:symbol\_format\_cfg | cfg | A symbol is Consortium for Functional Glycomics (CFG) notation. |

# Synthetic Type

Type of synthesis used for creating the glycan. Possible values are chemical synthesis, enzymatic synthesis and chemoenzymetic synthesis.

**URI:** http://purl.jp/bio/12/glyco/glycan#synthetic\_type

**Superclass:** owl:Thing

**Instances:**

|  |  |  |
| --- | --- | --- |
| **URI** | **Label** | **Description** |
| glycan:synthetic\_type\_enzymatic | enzymatic | Employing glycosyltransferases and glycosidases in a synthetic schema. |
| glycan:synthetic\_type\_chemoenzymatic | chemoenzymatic | Relying on a hybrid of chemical and enzymatic steps that typically begins with chemical synthesis and ends with enzymatic extension. |
| glycan:synthetic\_type\_chemical | chemical | Chemical synthesis that various protecting group manipulations used in the context of glycan synthesis. |