GlycoRDF version 0.5

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# 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# |

# glycan:glycan

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.

**Superclass:** owl:Thing

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| dcterms:identifier | xsd:string |  | entry ID in other resource |
| glycan:degraded\_by | glycan:glycosyl\_hydrolase\_reaction |  | Object is an enzyme, which degrades the subject. |
| glycan:generated\_by | glycan:glycosyltransferase\_reaction |  | Object is an enzyme, which synthesize the subject. |
| glycan:has\_affinity\_to | xsd:anyURI |  | Subject is a glycan, which binds to (or is bound by) the object. |
| glycan:has\_aglycon | glycan:aglycon |  | in case of glyco\_conjugate, define the aglycon |
| glycan:has\_component | glycan:component |  | Reference to an object (of rdf:type glyco:component) that can use has\_monosaccharide, has\_cardinality and has\_cardinality\_per\_repeat predicates. |
| 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 glyco:glycoconjugate\_sequence |
| glycan:has\_glycosequence | glycan:glycosequence |  | glycan sequence information to object of rdf:type glyco:glycosequence |
| glycan:has\_image | foaf:image |  | Object is a URI to an image instance describing a grafical 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:relation | glycan:correlation |  | Back-reference to the glyco:relation by which the subject is used. |
| owl:sameAs | xsd:anyURI |  | Reference to another RDF of exactly this carbohydrate provided by a different resource which may contain complementary information |
| rdfs:seeAlso | glycan:resource\_entry |  | Reference to other resource can be used as subject for further annotation (resource\_name and resource\_id) |

## glycan: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.

**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 glyco:repeatUnits only. Missing for non-stoichiometrical residues. |
| glycan:has\_monosaccharide | glycan:monosaccharide | yes | URI to a RDF resource describing the monosaccharide (usually MonosaccharideDB). |

## glycan:sequence

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

**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:glycosequence

Sequence of the glycan in a specified sequence format.

**Superclass:** glycan:sequence

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

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

#### glycan:carbohydrate\_format

Instances of this class are the carbohydrate sequence formats.

**Superclass:** owl:Thing

**Instances:**

|  |  |
| --- | --- |
| **URI** | **Description** |
| glycan:carbohydrate\_format\_glycoct |  |
| glycan:carbohydrate\_format\_iupac\_short |  |
| glycan:carbohydrate\_format\_iupac\_condensed |  |
| glycan:carbohydrate\_format\_csdb |  |
| glycan:carbohydrate\_format\_linearcode |  |
| glycan:carbohydrate\_format\_glyde2 |  |
| glycan:carbohydrate\_format\_iupac\_extended |  |
| glycan:carbohydrate\_format\_kcf |  |
| glycan:carbohydrate\_format\_carbbank |  |
| glycan:carbohydrate\_format\_linucs |  |

### glycan:glycoconjugate\_sequence

Sequence of the Glycoconjugate that includes the carbohydrate portion and the aglyca.

**Superclass:** glycan:sequence

## glycan:aglycon

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

**Superclass:** owl:Thing

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| foaf:name | xsd:string |  | trivial name |
| glycan:has\_attachment\_position | xsd:integer |  | atom number in aglycon to which the carbohydrate moiety is attached |
| glycan:has\_linkage | xsd:integer |  | carbon number in the glycan to which the aglycon is attached |
| glycan:has\_reference | glycan:reference |  | literature information to object of rdf:type glyco:reference |

## glycan:resource\_entry

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

**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. |

### glycan:glycan\_database

List of databases that glycans and related information.

**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:glycan\_database\_category

List of categories for the classification of glycan databases.

**Superclass:** owl:Thing

## foaf:image

Graphical representation of the molecule.

**Superclass:** owl:Thing

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| dc:format | xsd:string |  | The file format of the image. (image/svg+xml, image/png, image/gif, …) |
| glycan:has\_symbol\_format | glycan:symbol\_format | yes | URL to explanation of symbol? The display style of the glycan. (cfg, uoxf, atoms) |

### glycan:symbol\_format

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

**Superclass:** owl:Thing

**Instances:**

|  |  |
| --- | --- |
| **URI** | **Description** |
| glycan:symbol\_format\_uoxf |  |
| glycan:symbol\_format\_cfg |  |

## glycan: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.

**Superclass:** glycan:glycan

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

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

### glycan:glycan\_epitope

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

**Superclass:** glycan:glycan\_motif

## glycan:polysaccharide

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

**Superclass:** glycan:glycan

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_repeat | glycan:repeat |  | 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 glyco:repeat\_count. |

### glycan:repeat

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

**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:integer | yes | value of repeat\_attribute in resource, if known |

#### glycan:repeat\_attribute

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

**Superclass:** owl:Thing

**Instances:**

|  |  |
| --- | --- |
| **URI** | **Description** |
| glycan:repeat\_attribute\_unknown |  |
| glycan:repeat\_attribute\_min |  |
| glycan:repeat\_attribute\_max |  |
| glycan:repeat\_attribute\_exact |  |
| glycan:repeat\_attribute\_average |  |

### glycan: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.

**Superclass:** glycan:polysaccharide

### glycan:biological\_repeat\_unit

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

**Superclass:** glycan:polysaccharide

## glycan:cyclic\_glycan

Cyclic glycans are a special form of glycans which are rarely found in nature.

**Superclass:** glycan:glycan

## glycan:reaction

Class for reactions to create or degrade glycans.

**Superclass:** owl:Thing

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:catalyzed\_by | xsd:anyURI |  | Subject is an enzyme, which synthesizes the object. |
| glycan:has\_substrate | glycan:glycan | yes | URI of the Glycan that is consumed by a reaction. |

### glycan:glycosyltransferase\_reaction

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

**Superclass:** glycan:reaction

### glycan:glycosyl\_hydrolase\_reaction

Instances of this class are glycosyl hydrolase reactions which truncate glycans by releasing parts of the glycan.

**Superclass:** glycan:reaction

# glycan:monosaccharide

Instances of this class represent monosaccharides and their information. These monosaccharides are used to specify the composition of glycans.

**Superclass:** owl:Thing

**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 a monosaccharide (subject). |
| glycan:has\_linking\_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 numberic 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\_name | xsd:string | yes | Name of the subject |
| glycan:has\_substituent | glycan:substituent |  | reference to another RDF resource with URI. The substituent is linked to the basetype in this monosaccharide. |

## glycan:monosaccharide\_property

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

**Superclass:** owl:Thing

## glycan:monosaccharide\_alias

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

**Superclass:** glycan:monosaccharide\_property

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_external\_substituent | glycan:substituent |  | Reference to a glyco: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:has\_name | xsd:string | yes | Name of the subject |
| 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 glyco: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) |

## glycan:monosaccharide\_notation\_scheme

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

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |
| --- | --- |
| **URI** | **Description** |
| glycan:monosaccharide\_notation\_scheme\_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'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 | The Notation used in the Glycosciences.de web portal. It is based on the CarbBank notation. |
| glycan:monosaccharide\_notation\_scheme\_glycoct | The nomenclature that is used by EUROCarbDB. For more information see www.eurocarbdb.org/recommendations/encoding/. |
| glycan:monosaccharide\_notation\_scheme\_cfg | The LinearCode notation used by the US Consortium for Functional Glycomics (CFG). |
| glycan:monosaccharide\_notation\_scheme\_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 | 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 | 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. |

## glycan:basetype

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

**Superclass:** glycan:monosaccharide\_property

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_anomer | glycan:anomer | yes | alpha, beta, none, unknown (URI for concept to be provided). anomeric state of the basetype |
| glycan:has\_basetype\_id | xsd:integer | yes | Id of the basetype in MonosaccharideDB. |
| 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 | Assignes 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 |
| 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 |

### glycan:anomer

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

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |
| --- | --- |
| **URI** | **Description** |
| glycan:anomer\_unknown |  |
| glycan:anomer\_none |  |
| glycan:anomer\_beta |  |
| glycan:anomer\_alpha |  |

### glycan: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.

**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 configuraiton D or L |

#### glycan:absolute\_configuration

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

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |
| --- | --- |
| **URI** | **Description** |
| glycan:absolute\_configuration\_unknown |  |
| glycan:absolute\_configuration\_laevus |  |
| glycan:absolute\_configuration\_dexter |  |

#### glycan:relative\_configuration

List of relative monosaccharide configurations according to IUPAC.

**Superclass:** glycan:monosaccharide\_property

**Instances:**

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

### glycan:ring\_type

Ringtype of a basetype.

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |
| --- | --- |
| **URI** | **Description** |
| glycan:pyranose |  |
| glycan:furanose |  |

### glycan:core\_modification

Core modification of a monosaccharide. A core modification consist of a modification type and the position at which this modification happened.

**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 modifcation. |
| glycan:has\_position | xsd:integer |  | Carbon atom number of the monosaccharide which has been modified. |

#### glycan:core\_modification\_type

List of core modifications that can appear on a monosaccharide.

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |
| --- | --- |
| **URI** | **Description** |
| glycan:core\_modification\_type\_enx | Double bond in the basetype backbone with unknown deoxygenation pattern. |
| glycan:core\_modification\_type\_deoxy | Deoxygenation of a position: The OH group is removed and replaced by a hydrogen atom. |
| glycan:core\_modification\_type\_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 | Triple bond in the basetype backbone. |
| glycan:core\_modification\_type\_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 | Carboxyl (COOH) group. |
| glycan:core\_modification\_type\_sp | Triple bond to a substituent. |
| glycan:core\_modification\_type\_geminal | Loss of stereochemistry due to identical substituents with DEOXY and H\_LOSE linkage types at a single position. |
| glycan:core\_modification\_type\_sp2 | Double bond to a substituent. |
| glycan:core\_modification\_type\_aldi | Alditol: Reduction of the aldehyde group to CH2OH. |
| glycan:core\_modification\_type\_anhydro | Intramolecular anhydride. |

## glycan:substituent

Substition of a monosaccharide by another molecule. The substituent consists of the substituent type and the linkage between monosaccharide and substituent.

**Superclass:** glycan:monosaccharide\_property

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| 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:substituent\_type

List of substituent types possible on monosaccharides.

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |
| --- | --- |
| **URI** | **Description** |
| glycan:substituent\_type\_r\_pyruvate | CH2CCOOH |
| glycan:substituent\_type\_n\_trifluoroacetyl | NHCOCF3 |
| glycan:substituent\_type\_r\_lactate | CH3CHCOOH |
| glycan:substituent\_type\_telluro | TeH |
| glycan:substituent\_type\_s\_pyruvate | CH2CCOOH |
| glycan:substituent\_type\_n\_alanine | NHCOCHNH2CH3 |
| glycan:substituent\_type\_s\_lactate | CH3CHCOOH |
| glycan:substituent\_type\_n\_succinate | NCOCH2CH2COOH |
| glycan:substituent\_type\_n\_dimethyl | N(CH3)2 |
| glycan:substituent\_type\_n\_trimethyl | N(CH3)3 |
| glycan:substituent\_type\_ethyl | CH2CH3 |
| glycan:substituent\_type\_bromo | Br |
| glycan:substituent\_type\_n\_glycolyl | NCOCH2OH |
| glycan:substituent\_type\_hydroxymethyl | CH2OH |
| glycan:substituent\_type\_nitrat | NO2 |
| glycan:substituent\_type\_iodo | I |
| glycan:substituent\_type\_n\_sulfate | NHSO3H |
| glycan:substituent\_type\_methyl | CH3 |
| glycan:substituent\_type\_chloro | Cl |
| glycan:substituent\_type\_n\_formyl | NHCHO |
| glycan:substituent\_type\_seleno | SeH |
| glycan:substituent\_type\_amino | NH2 |
| glycan:substituent\_type\_ethanolamine | NHCH2CH2OH |
| glycan:substituent\_type\_imino | NH |
| glycan:substituent\_type\_n\_acetyl | NHCOCH3 |
| glycan:substituent\_type\_x\_lactate | CH3CHCOOH |
| glycan:substituent\_type\_phosphate | PO3H2 |
| glycan:substituent\_type\_formyl | CHO |
| glycan:substituent\_type\_n\_methyl | NHCH3 |
| glycan:substituent\_type\_thio | SH |
| glycan:substituent\_type\_x\_pyruvate | CH2CCOOH |
| glycan:substituent\_type\_sulfate | SO3H |
| glycan:substituent\_type\_n\_ethyl | NHCH2CH3 |
| glycan:substituent\_type\_s\_methyl | SCH3 |
| glycan:substituent\_type\_trifluoroacetyl | COCF3 |
| glycan:substituent\_type\_glycolyl | COCH2OH |
| glycan:substituent\_type\_acetyl | COCH3 |
| glycan:substituent\_type\_fluoro | F |

### glycan:substituent\_linkage

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

**Superclass:** glycan:monosaccharide\_property

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| 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 of the substituent |

#### glycan:linkage\_type

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

**Superclass:** glycan:monosaccharide\_property

**Instances:**

|  |  |
| --- | --- |
| **URI** | **Description** |
| glycan:linkage\_type\_s\_config | Same as R\_CONFIG, but resulting in an S-Configuration of the carbon. |
| glycan:linkage\_type\_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\_lose | The substituent is linked directly to the basetype backbone by replacing the hydrogen atom. |
| glycan:linkage\_type\_h\_at\_oh | A standard O-linked substituent, i.e. the substituent replaces the hydrogen of an OH group. |
| glycan:linkage\_type\_deoxy | The substituent is linked directly to the basetype backbone by replacing the OH group. |

# glycan:source

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

**Superclass:** owl:Thing

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:relation | glycan:correlation |  | Back-reference to the glyco:relation by which the subject is used. |

## glycan:source\_modeled

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

**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. |

### glycan:software

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

**Superclass:** owl:Thing

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

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

## glycan: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.

**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 |

### glycan:synthetic\_type

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

**Superclass:** owl:Thing

## glycan:source\_natural

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

**Superclass:** glycan:source

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| dc:name | xsd:string |  | Literal such as “Homo sapiens”. |
| 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\_taxon | xsd:anyURI | 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. |
| rdfs:subclassOf | xsd:anyURI |  | Reference to the closest taxon of which the glyco:taxon is a subclass. |

# glycan:reference

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

**Superclass:** owl:Thing

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| bibo:Series | bibo:Book |  | Series of the publication |
| bibo:abstract | xsd:string |  | Abstract of the publication. |
| bibo:chapter | xsd:string |  | Chapter in a book. |
| bibo:issue | xsd:string |  | Issue the publication was published in. |
| bibo:issuer | foaf:Organization |  | Organisation issuing the publication. |
| bibo:pageEnd | xsd:string |  | End page of the publication. |
| bibo:pageStart | xsd:string |  | Start page of the publication |
| bibo:shortTitle | xsd:string |  | Short title of the publication. |
| bibo:volume | xsd:string |  | Volumn the publication was published in. |
| dc:contributor | xsd:string |  |  |
| dc:creator | foaf:Person |  | Author of the publication. |
| dc:date | xsd:string |  | Date of publication. |
| dc:isPartOf | bibo:Journal |  | use ISSN or NLM\_id or random identifier to link to a journal entity |
| dc:publisher | xsd:string |  | Name of the publisher. |
| dc:title | xsd:string |  | Title of the publication. |
| dcterms:bibliographicCitation | xsd:string |  | Citation string. |
| dcterms:issued | xsd:string |  | Year of publication. |
| 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:relation | glycan:correlation |  | Back-reference to the glyco:relation by which the subject is used. |
| owl:sameAs | xsd:anyURI |  |  |
| rdf:type | bibo:Collection |  | Type of publication. Such as paper, book chapter etc. |

# glycan:evidence

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

**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:relation | glycan:correlation |  | Back-reference to the glyco:relation by which the subject is used. |

## glycan:evidence\_type

List of evidence types.

**Superclass:** owl:Thing

**Instances:**

|  |  |
| --- | --- |
| **URI** | **Description** |
| glycan:evidence\_type\_nmr |  |
| glycan:evidence\_type\_msms |  |
| glycan:evidence\_type\_ms |  |
| glycan:evidence\_type\_lc\_msms |  |
| glycan:evidence\_type\_lc\_ms |  |
| glycan:evidence\_type\_lc |  |
| glycan:evidence\_type\_hplc |  |
| glycan:evidence\_type\_ce |  |

## glycan:evidence\_lc

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

**Superclass:** glycan:evidence

**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 |
| glycan:used\_lc\_column\_dimension | xsd:string | yes | width x length |
| glycan:used\_lc\_column\_material | xsd:string | yes | Material of the column |
| glycan:used\_lc\_column\_type | xsd:string | yes | Type of the column (e.g. PGC) |
| glycan:used\_lc\_gradient | xsd:string | yes | Used gradient for the experiment |
| glycan:used\_lc\_run\_time | xsd:string | yes | Runtime of the LC |
| glycan:used\_solvent | xsd:string |  | brutto-formula |

## glycan:evidence\_ms

Experiments using mass spectrometry to identify the carbohydrate structures.

**Superclass:** glycan:evidence

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_ms\_ms\_peak | glycan:msms\_peak |  | Reference to an object that uses the following predicates: ms\_mass (xsd:double), ms\_intensity (xsd:double), fragment (xsd:string) which is the annotation for the peak. |
| glycan:has\_precursor\_peak | glycan:profile\_peak |  | URI of the precursor peak of a MS^n spectra. |
| glycan:has\_retention\_time | xsd:string | yes | Retention time of the molecule in the experiment |
| glycan:used\_lc\_column\_dimension | xsd:string | yes | width x length |
| glycan:used\_lc\_column\_material | xsd:string | yes | Material of the column |
| glycan:used\_lc\_column\_type | xsd:string | yes | Type of the column (e.g. PGC) |
| glycan:used\_lc\_gradient | xsd:string | yes | Used gradient for the experiment |
| glycan:used\_lc\_run\_time | xsd:string | yes | Runtime of the LC |
| glycan:used\_mass\_spectrometry\_ionisation | glycan:mass\_spectrometry\_ionisation | yes | Ionisatin type used when producing the mass spectra. |
| glycan:used\_mass\_spectrometry\_mode | glycan:mass\_spectrometry\_mode | yes | MS mode used for generating the mass spectra. |
| glycan:used\_solvent | xsd:string |  | brutto-formula |
| rdfs:seeAlso | xsd:anyURI |  | a link to a spectrum in some other database |

### glycan:mass\_spectrometry\_peak

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

**Superclass:** owl:Thing

**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\_mz | xsd:double | yes | MZ value of the MS peak |
| glycan:has\_structure | glycan:glycan |  | Annotation of the MS peak with a structure (MS profile) |

### glycan:msms\_peak

Mass spec peak in an MS^n spectra which will be annoted with a glycan fragment.

**Superclass:** glycan:mass\_spectrometry\_peak

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_fragment | xsd:string |  | GlycoWorkbench sequence as peak annotation |

### glycan:profile\_peak

Mass spec peak in an MS profiling spectra which will be annotated with a complete glycan.

**Superclass:** glycan:mass\_spectrometry\_peak

### glycan:mass\_spectrometry\_ionisation

List of ionisation techniques which are used in mass spectrometry (ESI, MALDI).

**Superclass:** owl:Thing

### glycan:mass\_spectrometry\_mode

List of modes that are used in mass spectrometry. Instances are positive mode and negative mode or a combination of both.

**Superclass:** owl:Thing

## glycan:evidence\_nmr

Experiments using NMR to identify the carbohydrate structure.

**Superclass:** glycan:evidence

**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\_nucleus | xsd:string |  | Nucleus |
| glycan:has\_subspectrum | glycan:subspectrum |  | List of references to glyco:subspectrum object |
| glycan:has\_temperature | xsd:string | yes | value or range in K (literal) |
| glycan:used\_ph | xsd:double | yes | pH of solution |
| glycan:used\_solvent | xsd:string |  | brutto-formula |
| rdfs:seeAlso | xsd:anyURI |  | refer to raw/processed data file location if available |

### glycan:subspectrum

Subspectrum of NMR data. It contains the annotated signals.

**Superclass:** owl:Thing

**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 glyco:signal |

#### glycan:signal

A signal is a NMR data point.

**Superclass:** owl:Thing

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

|  |  |  |  |
| --- | --- | --- | --- |
| **Predicate** | **Range** | **Functional** | **Description** |
| glycan:has\_carbon\_number | xsd:integer | yes | carbon atom number |
| 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\_coupling\_constant | xsd:double |  | values in Hz |
| glycan:is\_real | xsd:boolean | yes | NO if a signal can not exist, rather than its unknown |
| glycan:used\_multiplicity | xsd:string | yes | single-character literal (S,M,D,T ,Q) or combination |

## glycan:evidence\_ce

Experiments using capillary electrophoresis to identifiy carbohydrate structures.

**Superclass:** glycan:evidence

# glycan:correlation

Correlation instances connect the different pieces of information. It contains a glycan and other information (source, references, evidence) that belong to one data set. That allows to specify that a glycan, which has been found in a certain source was published by a certain publication.

**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). A evidence can be any type of experimental data. |
| glycan:has\_glycan | glycan:glycan | yes | correlates a glycan with other information that are part of the corelation instance |
| glycan:has\_source | glycan:source |  | Source annotation of the correlation. |
| glycan:has\_structure\_location | xsd:string |  | location of glycan in a publication (e.g. Figure 1) |
| glycan:published\_in | glycan:reference | yes | The information described by the correlation was pubished in a reference given by the URI. |