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# Web Resources for the Glycoscientist

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*This article is dedicated to Dr. Claus-Wilhelm "Willi" von der Lieth, who was a pioneer in the glycobioinformatics field and who unexpectedly passed away in November 2007.*

## Introduction

Carbohydrates are the third major class of biopolymers after proteins and nucleic acids.[1] Covalently attached to proteins in protein glycosylation, they can change the properties of the glycoproteins, making them more soluble,[2] increasing protein stability, protecting them from proteolysis,[3] or providing additional recognition epitopes, which can, for example, serve as molecular addresses in protein trafficking.[4,5] Within the calnexin/calreticulin cycle, N-glycan chains participate in the protein-folding process and the tagging of incompletely folded or misfolded proteins.[6] In addition, protein–carbohydrate interactions play an important role in a variety of cell–cell and cell–matrix recognition events, ranging from fertilization and cell differentiation to host–pathogen interactions, immune responses, and diseases such as cancer, arthritis, and Alzheimer's disease.[7–10]

Carbohydrates differ from other biopolymers such as proteins or nucleic acids insofar that their monomeric building blocks, the monosaccharides, can be linked in multiple ways.[11] This includes the possibility of forming branched structures.[12] As classical bioinformatics algorithms were developed for linear protein or nucleic acid sequences and thus cannot be applied to carbohydrates, new algorithms have to be developed.[11] Furthermore, because of the complexity of carbohydrates and the fact that there is no method comparable to PCR to amplify glycan structures,[13] relatively few primary data are available to work on or to use as training and test sets for the algorithms. For these reasons, glycobioinformatics is still in its infancy and lagging behind bioinformatics applications for genomics or proteomics.[14] Nevertheless, there is a variety of tools and databases currently available to glycoscientists.

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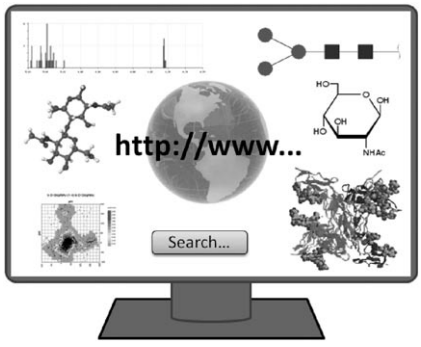
## Glycobioinformatics Resources

The subsequent sections describe web resources that are freely available to glycoscientists. They are summarized together with their URLs and references in Table 1 (portals and databases) and Table 2 (tools). Each row in those tables has a number, which is used to reference the resources within this article.




## Portals

Currently, there are three major glyco-related web portals available that offer a variety of tools and databases. These are the websites of the US Consortium for Functional Glycomics (CFG; 1), KEGG Glycan (2) as part of the Japanese KEGG (Kyoto Encyclopedia of Genes and Genomes) portal, and the GLYCOSCIENCES.de portal (3) in Germany. All of them have different focuses. The CFG portal is the main access point for the data that are produced by the consortium. These include the results of protein–carbohydrate interaction analyses with glycan arrays and of the expression of glycogenes analyzed with gene microarrays. The KEGG portal aims to integrate genomic, chemical, and systemic functional information,[15] and the KEGG Glycan portal has a special emphasis on metabolic pathways. The main focus of the GLYCOSCIENCES.de portal is carbohydrate 3D structures. RINGS (4) is related to the KEGG portal, but also features some GLYCOSCIENCES.de data. The EUROCarbDB portal (5) is currently still under development but already provides a few tools, mainly for mass spectrometry (MS) of carbohydrates.

## Databases

The first attempt to systematically collect information on carbohydrate structures from the literature was the Complex Carbohydrate Structure Database (CCSDB; 6), better known by the name of its query software CarbBank. After funding stopped in the mid-1990s, CarbBank was not further developed and CCSDB is not updated any more. Nevertheless, the data from CCSDB can still be accessed online and formed the basis for most of the current major carbohydrate structure databases. Although initially often based on the same data, most of these databases, like the web portals, have their own special focus. The main purpose of the CFG database (7) is to access the CFG experimental data via the carbohydrate structure. As the CFG data are mainly yielded from human and mouse samples, this database primarily contains

**Table 1.** Glycobioinformatics portals and databases

| No | Name | Description | URL | Ref. |
|---|---|---|---|---|
| **Web portals** | | | | |
| 1 | CFG | Websites of the Consortium for Functional Glycomics | http://www.functionalglycomics.org | [30] |
| 2 | KEGG Glycan | Carbohydrate subpart of the KEGG portal | http://www.genome.jp/kegg/glycan/ | [31] |
| 3 | GLYCOSCIENCES.de | Collection of tools and databases for glycoscientists | http://www.glycosciences.de | [32] |
| 4 | RINGS | Resource for INformatics of Glycomes at Soka | rings.t.soka.ac.jp | |
| 5 | EUROCarbDB | European Carbohydrate Database portal | http://www.eurocarbdb.org | |
| **Databases** | | | | |
| 6 | CCSDB/CarbBank | Complex Carbohydrate Structure Database, first carbohydrate database | http://www.boc.chem.uu.nl/sugabase/carbbank.html | [33] |
| 7 | CFG Database | Database of the Consortium for Functional Glycomics | http://www.functionalglycomics.org/glycomics/common/jsp/firstpage.jsp | [30] |
| 8 | BCSDB | Bacterial Carbohydrate Structure Database | http://www.glyco.ac.ru/bcsdb/ | [34] |
| 9 | GLYCOSCIENCES.de DB | Database of the GLYCOSCIENCES.de portal | http://www.glycosciences.de/sweetdb/ | [35] |
| 10 | KEGG Glycan Database | Database of the KEGG Glycan portal | http://www.genome.jp/kegg/glycan/ | [31] |
| 11 | GlycoconjugateDB:Structures | Carbohydrate 3D structures from the PDB | http://www.glycostructures.jp | [36] |
| 12 | DOUGAL | Glycoprotein structures database | http://www.cryst.bbk.ac.uk/DOUGAL/ | |
| 13 | O-GlycBase | Database of O-glycosylation sites | http://www.cbs.dtu.dk/databases/OGLYCBASE/ | [37] |
| 14 | ECODAB | *E. coli* O-antigen database | http://www.casper.organ.su.se/ECODAB/ | [38] |
| 15 | Sugabase | Carbohydrate-NMR database that combines CarbBank data with chemical shift values | http://www.boc.chem.uu.nl/sugabase/sugabase.html | [39] |
| 16 | GlycoMapsDB | Conformational maps of carbohydrates | http://www.glycosciences.de/modeling/glycomapsdb/ | [40] |
| 17 | DisaccharideDB | Conformational maps of disaccharides | http://www.cermav.cnrs.fr/cgi-bin/di/di.cgi | |
| 18 | CAZy | Carbohydrate Active enZymes database | http://www.cazy.org | [16] |
| 19 | KEGG Pathway | Carbohydrate metabolism pathways | http://www.genome.jp/kegg/pathway.html#glycan | [41] |
| 20 | KEGG Orthology | KEGG Orthology (KO) groups for glycosyltransferases | http://www.genome.jp/kegg/glycan/GT.html | [42] |
| 21 | CFG GT Database | Glycosyltransferases database of the CFG | http://www.functionalglycomics.org/static/gt/gtdb.shtml | [43] |
| 22 | CFG GBP Database | Glycan Binding Proteins database of the CFG | http://www.functionalglycomics.org/glycomics/molecule/jsp/gbpMolecule-home.jsp | [30] |
| 23 | CFG Consortium data | Experimental data from the CFG: Glycan Profiling (MS), Mouse Phenotyping, Gene Microarray and Glycan Array data | http://www.functionalglycomics.org/glycomics/publicdata/home.jsp | [44] |
| 24 | GlycoepitopeDB | Database of carbohydrate recognition motifs, recognising antibodies and glycoproteins/glycolipids carrying the motifs | http://www.glyco.is.ritsumei.ac.jp/epitope/ | |
| 25 | GGDB | Human glycogenes database | http://riodb.ibase.aist.go.jp/rcmg/ggdb/ | [45] |
| 26 | GPI Anchor Biosynthesis Report | Database of enzymes for biosynthesis of GPI anchors | http://mendel.imp.ac.at/SEQUENCES/gpi-biosynthesis/ | [46] |
| 27 | GlycoBase | Database of 2-aminobenzamide labelled released glycans and exoglycosidase digestion pathways | http://glycobase.ucd.ie | [47] |
| 28 | Elution Coordinate DB | Database of 2-aminopyridine labelled glycans | http://www.gak.co.jp/ECD/Hpg_eng/hpg_eng.html | |
| 29 | GlycomeDB | Meta-database to search various databases via one interface | http://www.glycome-db.org | [48] |
| 30 | MonoSaccharideDB | Reference database for monosaccharide notation | http://www.monosaccharidedb.org | |

mammalian carbohydrates. In contrast, the Bacterial Carbohydrate Structure Database (BCSDB; 8) in Russia targets bacterial carbohydrates, many of them being polysaccharides. It was the initial aim of the database of the GLYCOSCIENCES.de portal (9), the former SweetDB, to make CCSDB/CarbBank data available over the internet and provide computed 3D structures with its entries. Later, references to experimental data from the Protein Data Bank (PDB) and NMR chemical shift values were added. Entries in the KEGG Glycan Database (10) are linked to other KEGG resources such as pathways.

In addition to the more general databases described above, there are a number of specialized databases available. Data from the PDB, for example, were used to create the GDB:Structures database (11) and the DOUGAL database on glycoprotein structures (12). O-glycosidically modified proteins are collected in O-Glyc-Base (13), whereas antigens from *E. coli* O-glycans can be found in ECODAB (14). Sugabase (15) provides NMR data that are available for CarbBank structures. Information on conformational preferences of carbohydrate chains can be extracted from the GlycoMapsDB (16) and the disaccharides database (17).

Carbohydrate sequences are indirectly encoded in the genome by the enzymes that degrade (glycosidases), modify, or create (glycosyltransferases) glycosidic bonds.[16] The Carbohydrate-Active enZymes (CAZy) database (18) describes families of structurally-related catalytic and carbohydrate-binding modules (or functional domains) of such enzymes. Information on glycosyltransferases (GTs) or glycan-binding proteins is also provided by KEGG Glycan (19, 20), the CFG portal (21–23), GlycoEpitopeDB (24), GGDB (25), and the GPI Anchor Biosynthesis Report (26), whereas GlycoBase (27) and the Elution Coordinate Data-

**Table 2.** Tools related to glycobiology or glycochemistry.

| No | Name | Description | URL | Ref. |
|---|---|---|---|---|
| **Mass spectrometry tools** | | | | |
| 31 | Glycofragment | Calculate and display the main fragments (Band C-, Z- and Y-, A- and X-ions) of oligosaccharides that should occur in MS spectra | http://www.glycosciences.de/tools/GlycoFragments/ | [49] |
| 32 | GlycoSearchMS | Search GLYCOSCIENCES.de database for structures matching a given set of MS mass peaks | http://www.glycosciences.de/sweetdb/start.php?action=form_ms_search | [50] |
| 33 | GlycoPeakfinder | Tool for fast annotation of glycan MS spectra, results can be used for advanced database search in GLYCOSCIENCES.de | http://www.eurocarbdb.org/applications/ms-tools/ | [51] |
| 34 | GlycoWorkBench | Tool to assist the manual interpretation of MS spectra | http://www.eurocarbdb.org/applications/ms-tools/ | [52] |
| 35 | GlycoMod | Prediction of possible oligosaccharide structures that occur on proteins from their experimentally determined masses | http://www.expasy.org/tools/glycomod/ | [53] |
| 36 | GlycanMass | Calculation of the mass of an oligosaccharide structure from its composition | http://www.expasy.org/tools/glycomod/glycanmass.html | [53] |
| **NMR tools** | | | | |
| 37 | CASPER | Simulation of NMR spectra and carbohydrate sequence determination from NMR chemical shift values | http://www.casper.organ.su.se/casper/ | [54] |
| 38 | GlyNest | Estimation of NMR chemical shifts | http://www.glycosciences.de/sweetdb/start.php?action=form_shift_estimation | [55] |
| 39 | ProSpectND | Integrated NMR data processing and inspection tool | http://www.eurocarbdb.org/applications/nmr-tools | |
| 40 | CCPN | Website of the Collaborative Computing Project for NMR | http://www.ccpn.ac.uk | [56] |
| **HPLC tools** | | | | |
| 41 | autoGU | Tool to assist the interpretation of HPLC data | glycobase.ucd.ie/cgi-bin/profile_upload.cgi | [47] |
| 42 | GALAXY | Visualization of HPLC 2-D maps | http://www.glycoanalysis.info/ENG/index.html | [57] |
| **Tools for prediction/analysis of glycosylation and protein–carbohydrate interactions** | | | | |
| 43 | GECS | KEGG Gene Expression to Chemical Structure, N-glycan prediction server | http://www.genome.jp/tools/gecs/ | [58] |
| 44 | CBS Prediction servers | Prediction of posttranslational modifications of proteins, including N-glycosylation sites (NetNGlyc), O-glycosylation sites (NetOGlyc), glycation sites (NetGlycate), C-mannosylation sites (NetCGlyc), and O-GlcNAc glycosylation sites (DictyOGlyc/YinOYang) | http://www.cbs.dtu.dk/services/ | [59,60] |
| 45 | GlySeq | Statistical analysis of glycosylation sites in the PDB and SwissProt | http://www.glycosciences.de/tools/glyseq/ | [61] |
| 46 | GlyVicinity | Statistical analysis of protein–carbohydrate interactions data from the PDB | http://www.glycosciences.de/tools/glyvicinity/ | [61] |
| **3D structure/conformation tools** | | | | |
| 47 | Sweet-II | Generation of carbohydrate 3D structure models | http://www.glycosciences.de/modeling/sweet2/ | [62] |
| 48 | Glycam Biomolecule Builder | Generation of carbohydrate 3D structure models | http://www.glycam.com/CCRC/biombuilder/biomb_index.jsp | [63] |
| 49 | pdb2linucs | Detection of carbohydrate moieties in PDB structures | http://www.glycosciences.de/tools/pdb2 linucs/ | [23] |
| 50 | pdb-care | Validation of carbohydrate 3D structures | http://www.glycosciences.de/tools/pdb-care/ | [64] |
| 51 | CARP | Carbohydrate Ramachandran Plot | http://www.glycosciences.de/tools/carp/ | [61] |
| 52 | GlyTorsion | Statistical analysis of torsion angles derived from the PDB | http://www.glycosciences.de/tools/glytorsion/ | [61] |
| 53 | GlyProt | In silico glycosylation of proteins | http://www.glycosciences.de/modeling/glyprot/ | [65] |
| 54 | Dynamic Molecules | Online molecular dynamics (MD) simulations | http://www.md-simulations.de | [66] |
| **Notation and graphical representation of carbohydrates** | | | | |
| 55 | IUPAC | Official IUPAC recommendations for carbohydrate notation | http://www.chem.qmul.ac.uk/iupac/2carb/ | [67] |
| 56 | LINUCS | Linear notation for carbohydrate structures | http://www.glycosciences.de/tools/linucs/ | [68] |
| 57 | LiGraph | Graphical representation of carbohydrate structures | http://www.glycosciences.de/tools/LiGraph/ | [14] |
| 58 | KEGG CSM | Composite Structure Map, graphical query tool for KEGG databases | http://www.genome.jp/kegg-bin/draw_csm | [69] |
| 59 | Glycan Builder | Graphical input of carbohydrate structures | http://www.eurocarbdb.org/applications/structure-tools/ | [70] |
| 60 | SuMo | Sugar Motif Search | http://www.glycosciences.de/tools/sumo/ | |
| 61 | Glyde-II | XML exchange format for carbohydrates | glycomics.ccrc.uga.edu/GLYDE-II/ | [71] |

base (28) list exoglycosidase digestion pathways and glucose unit (GU) values. Of course, the classical protein databases such as SwissProt[17] also contain information on these proteins, and are often linked by the glyco-specific databases. Links from the proteomics resources to glycomics databases, however, are usually not present.

Most of these databases use their own notation to store the carbohydrate structures, which makes direct crosslinking difficult. Nevertheless, there have been attempts to enable users to simultane-

ously query the BCSDB and the GLYCOSCIENCES.de databases[18] and to cross-link structures of the CFG and the GLYCOSCIENCES.de databases. Therefore, users who are exploring an entry in one of these two databases, for which there is also information in the other database, can easily access all of the data in both resources. However, the situation in the glycomics databases is still far from that in, for example, proteomics databases,[19] where a lot more links between the various resources are established. To help the user to find as much information as possible about a single carbohydrate structure without having to learn the query mechanisms of the various databases, glycome-db (29) was introduced as a *meta*-search database, where the user can receive links to the respective entries in various databases with one single query. An attempt to offer information on monosaccharide residues together with unique notation is made by MonoSaccharideDB (30).

## Tools

In addition to the databases, there are various online tools available which are summarized in Table 2. Many of them are independent applications, whereas some are connected to databases and serve as a convenient way to query a database or use database content as a basis for calculations. This especially applies to software that is developed to assist researchers with the analysis or interpretation of experimental data, such as mass spectrometry (MS; 31–36), nuclear magnetic resonance (NMR; 37–40), or high-performance liquid chromatography (HPLC; 41, 42) data. Most of these tools compute or estimate expected experimental values such as fragment masses (MS) or chemical shift values (NMR) for a given carbohydrate structure, or compare experimental values provided by the user with the predicted values of the structures present in a database or directly with experimental data that are stored in a database.

Other tools deal with the prediction or analysis of glycosylation sites. Based on information about the GTs that are expressed in an organism or a tissue, the KEGG GECS server (43) predicts N-glycan structures that might be present in that sample. Such GT expression data can be obtained from the consortium data of the CFG (23). The CBS Prediction Servers (44) estimate the occupancy of potential glycosylation sites in a given protein sequence. When using the prediction results, one should keep in mind that the occupancy of some glycosylation sites can be influenced by the state of a cell (for example, physiological age, tissue, health, etc.).[20] A statistical analysis of occupied glycosylation sites extracted from the PDB[21] and SwissProt[17] is performed by the GlySeq web interface (45). A similar analysis of amino acids in the spatial vicinity of carbohydrates in the PDB is accomplished by GlyVicinity (46).

Various tools are related to the 3D structure of carbohydrates. Sweet-II (47) and the Glycam Biomolecule Builder (48) create 3D structure models of carbohydrate chains. To check single PDB files for experimentally resolved carbohydrate 3D structures, the pdb2linucs software (49) can be used, whereas a search for PDB entries that contain a certain carbohydrate structure should be done by querying the GLYCOSCIENCES.de (9) or the GDB:Structures (11) databases. The former is automatically updated every week with new PDB entries and thus always provides access to the current PDB release.[22] Unfortunately, a rather high error rate is found within the carbohydrate moieties of PDB entries.[23,24] A validation of carbohydrate residue names and connectivities in PDB entries is performed by pdb-care (50). In addition, the GDB:Structures database (11) offers a service that tries to match N-glycan structures that are detected in a PDB structure with entries from the KEGG Glycan database (10) and thus helps to identify structures for which there is no biological pathway available. The conformation of carbohydrate chains, which is mainly determined by the torsions of the glycosidic linkages, can be evaluated in a way similar to the Ramachandran plot with CARP (51). For comparison, torsion data from other PDB entries, provided by GlyTorsion (52), or computed conformational maps from the GlycoMapsDB (16) can be used. In most PDB entries, however, only a short part of N- and O-glycan chains is present. About 90% of these chains consist of no more than three residues.[22] The glyProt software (53) carries out an in silico glycosylation to provide models of glycoproteins with larger glycan chains. All these tools deal with static 3D structures. Carbohydrates, however, are highly flexible molecules,[25,26] and therefore a static 3D structure only represents a snapshot of its conformational space.[27] The Dynamic Molecules server (54) allows online molecular dynamics (MD) simulations to examine the conformational behavior of carbohydrates and other molecules in time.

The complexity of carbohydrates is also reflected in the various notations that are used. There are IUPAC recommendations available (55), but these often are not unique and therefore not suited for computational purposes. Therefore, many different notations have been developed by the various resources. For LINUCS, the notation used within GLYCOSCIENCES.de, a conversion tool for translation from CarbBank/IUPAC notation is available online (56). The RINGS portal (4) provides tools to translate between LINUCS and KCF, the format used within the KEGG portal. Conversion from LINUCS to IUPAC is done by the LiGraph tool (57), which can also create graphical representations of carbohydrate chains. A graphical representation of multiple chains in one graph is KEGG CSM (58), which can also be used to query the KEGG databases (10, 19, 20). The Glycan Builder (59), a tool for a graphical input of glycan structures is, for example, used by GlycomeDB (29) to enable the user to enter queries graphically. The Sugar Motif Search tool (60), which finds frequent carbohydrate substructure motifs such as Lewis antigens in a given carbohydrate structure, is used to classify entries of the GLYCOSCIENCES.de database (9).

## Conclusions

Although bioinformatics for glycobiology is still lagging behind the genomics and proteomics areas, considerable progress has been made in recent years. However, many of the applications are still rather like disconnected islands. Only recently, have some efforts been made to estab-

lish cross-links between them and provide common interfaces to some of the resources. The agreement on Glyde-II (61) as a common data-exchange format[19] was a first step towards unifying the information provided by the major databases, which will increase the possibilities for data exchange.[13] This will lead to synergetic effects and provide users with easier access to the data. Another problem that many of the applications encounter is the fact that relatively few primary data, such as MS or NMR spectra, are publicly available to the developers to test their algorithms.[13,28]

Computational analysis of these data, combined with data from other resources, will help to extract information about the link between carbohydrate structures and diseases. This enables the identification of carbohydrates as biomarkers for diseases and as potential drug targets.[19,29]

**Keywords:** bioinformatics · carbohydrates · cheminformatics · databases · glycosylation

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