



Web resources for the Carbohydrate Chemist

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glycosciences.de

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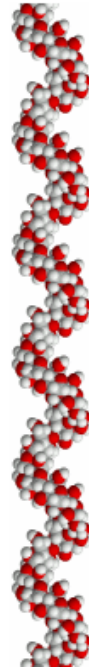
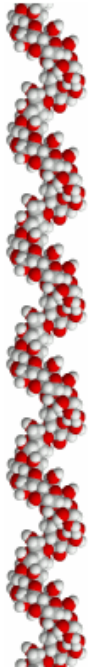
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This site provides **databases** and bioinformatics **tools** for glycobiology and glycomics.

Background

The human genome seems to encode for not more than 30,000 to 40,000 proteins. A major challenge is to understand how posttranslational events, such as glycosylation, affect the activities and functions of these proteins in health and disease. The importance of protein glycosylation is becoming widely realized through studies on protein folding, protein localization and trafficking, protein solubility, biological half-life as well as studies on cell-cell interactions. The progressing Glycomics projects will dramatically accelerate the understanding of the roles of carbohydrates in cell communication and lead to novel therapeutic approaches for treatment of human disease. The MIT's magazine of innovation (January 21 2003) has identified Glycomics as one of the top ten technologies that will change the future.

To support the upcoming Glycomics projects we focus our research activities on the development of bioinformatic tools and databases for glycobiology.



Consortium for Functional Glycomics

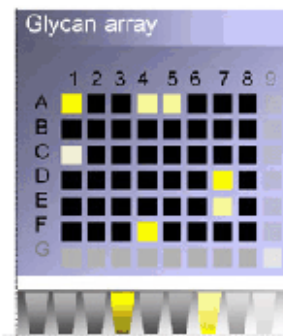
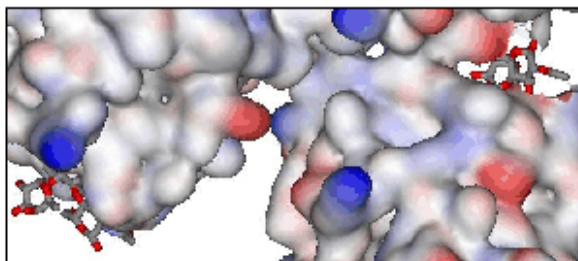
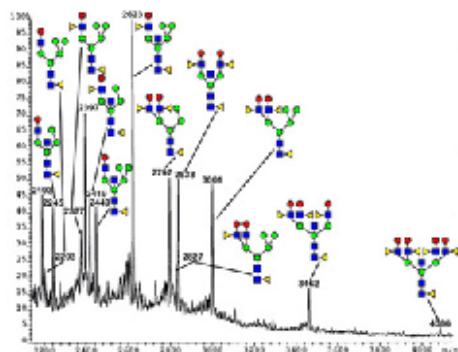
CFG

CONSORTIUM FOR FUNCTIONAL GLYCOMICS
funded by National Institute of General Medical Sciences

CONSORTIUM HOME DATABASES SITE MAP CONTACT US

Home Search By: [Sub Structure](#) | [Mol.Wt.](#) | [Composition](#) | [Linear Nomenclature](#) | [Multiple Criteria](#)

Glycan Database



Updates

- First cut version of glycan structures database
- Contains nearly 7500 entries
- Each entry contains structural and chemical information as well as related references

Search for glycans

- **Sub-structure**
- **Molecular weight**
- **Composition**
- **Linear nomenclature**
- **Use multiple search criteria**

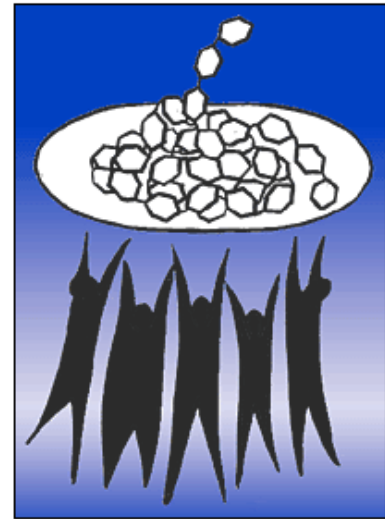
JCGG

日本糖鎖科学コンソーシアム (JCGG) Japan Consortium for Glycobiology and Glycotechnology

- 理事長あいさつ
- 趣旨および会則
- 沿革
- コンソーシアム構想
- 第1回シンポジウム
- 第2回シンポジウム

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Glyco3D



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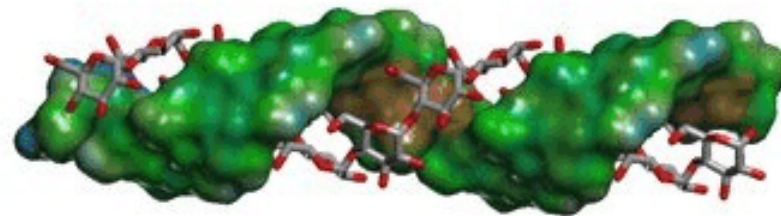
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GLYCO3D

A site for glycosciences



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38400 St Martin d'Hères - France

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Conformation

PDB – Protein Data Bank, “Brookhaven DB”

Protein structures, incl. glycoproteins

www.rcsb.org/pdb

GlycoMaps Database, SWEET-II etc...

Conformational databases and applications for oligosaccharides

www.glycosciences.de

Disaccharide Database

Conformational maps for some disaccharides

www.cermav.cnrs.fr/databank/disaccharides

PDB ligands

HIC-Up

alpha2.bmc.uu.se/hicup/

Het-PDB Navi

daisy.bio.nagoya-u.ac.jp/golab/hetpdbnavi.html

Image Library of Biological Macromolecules

www.imb-jena.de/ImgLibPDB/pages/carb.html

Enzymes, Lectins and Glycoproteins

CAZy – Carbohydrate Active Enzymes

afmb.cnrs-mrs.fr/CAZY/

3D Lectin Database

www.cermav.cnrs.fr/lectines/

BPGD - Bacterial Polysaccharide Gene Database

www.microbio.usyd.edu.au/BPGD/default.htm

KEGG

Kyoto Encyclopedia of Genes and Genomes



KCaM Documents

[Main](#)

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■ Published Papers

["Efficient Tree-Matching Methods for Accurate Carbohydrate Database Queries,"](#)

[Aoki, K. F. et al.](#)

■ Online Documents

[KCF format for glycans](#)

CBS Prediction Servers

Protein glycosylation

Post-translational modifications of proteins

[DictyOGlyc](#)

O-(alpha)-GlcNAc glycosylation sites
 (trained on *Dictyostelium discoideum* proteins).

[NetAcet](#) - new -

N-terminal acetylation in eukaryotic proteins.

[NetCorona](#)

Coronavirus 3C-like proteinase cleavage sites in proteins.

[NetNGlyc](#)

N-linked glycosylation sites in human proteins.

[NetOGlyc](#)

O-GalNAc (mucin type) glycosylation sites in mammalian proteins.

[NetPhos](#)

Serine, threonine and tyrosine phosphorylation
 sites in eukaryotic proteins.

[NetPicoRNA](#)

Posttranslational cleavage by picornaviral proteases.

[ProP](#)

Arginine and lysine propeptide cleavage sites in eukaryotic protein
 sequences.






[YinOYang](#)

O-(beta)-GlcNAc glycosylation and *Yin-Yang* sites
 (intracellular/nuclear proteins).



ExPASy

Protein identification and characterization

- [AACompIdent](#)  - Identify a protein by its amino acid composition
- [FindMod](#)  - Predict potential protein post-translational modifications and potential single amino acid substitutions in peptides. Experimentally measured peptide masses are compared with the theoretical peptides calculated from a specified Swiss-Prot entry or from a user-entered sequence, and mass differences are used to better characterize the protein of interest.
- [GlycoMod](#)  - Predict possible oligosaccharide structures that occur on proteins from their experimentally determined masses (can be used for free or derivatized oligosaccharides and for glycopeptides)
- [GlycanMass](#)  - Calculate the mass of an oligosaccharide structure
- [FindPept](#)  - Identify peptides that result from unspecific cleavage of proteins from their experimental masses, taking into account artefactual chemical modifications, post-translational modifications (PTM) and protease autolytic cleavage
- [ProteinProspector](#) - A variety of tools from UCSF (MS-Fit, MS-Tag, MS-Digest, etc.) for mining sequence databases in conjunction with mass spectrometry experiments [Mirrors at [UCL-Ludwig](#), UK / [Ludwig Institute Melbourne](#) (Australia)]
- [PROWL](#) - Protein chemistry and mass spectrometry resource from Rockefeller and NY Universities [or from [Genomic Solutions](#)]

Structural analysis



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Structural analysis of carbohydrates

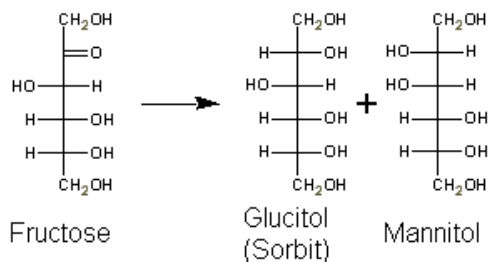


Sugar analysis using alditol acetates

Introduction

The hydrolysis of glycosides and polysaccharides to reducing sugars and the concomitant conversion to alditol acetates (borohydride reduction and acetylation) is a standard method to analyse polysaccharides containing aldoses, ketoses, deoxyaldoses, and acetamidohexoses and other related sugars. Sugars that cannot be observed with this analysis are uronic acids, ulosonic acids (*e.g.* Kdo), 4-aminosugars, or charged species like phosphorylated sugars which may arise in a hydrolysate. The acids are not observed because the sodium salt of the acid that is formed on addition of NaBH_4 is not volatile. Of special concern is the difference in rate of hydrolysis between sugars. Thus, uronic acids are seldom completely hydrolysed and the sugar that the uronic acid is linked to is underrepresented. 2-Acetamidohexoses undergo partial *N*-deacetylation and the resulting 2-aminosugars are not hydrolysed at all and both the 2-aminosugar and the sugar to which it is linked are underrepresented. Normally, yields of 60-80% are obtained. 4-acetamido sugars are hydrolysed to pyrrole derivatives which are polymerised and such sugars are therefore not observed. Methanolysis is however possible with 4-acetamido sugars.

Note that all ketoses on reduction are expected to yield approximately equal amounts of both the *R*- and the *S*-isomer, which may or may not separate on GLC analysis. Thus, fructose gives an equimolar mixture of glucitol and mannitol.



GlycoWord



Lectin



Glycogene



Proteoglycan



Structural Glycobiology



Glycoprotein



Immunity & Sugar Chain



Glycolipid



Cancer & Sugar Chain

Contemporary Carbohydrate Chemistry

"CONTEMPORARY CARBOHYDRATE CHEMISTRY" *by A M Stephen*

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**A COMPACT REVIEW OF PROGRESS THROUGH THE
NINETIES, AND INTO THE NEW MILLENNIUM**
**A Handbook For Students, Their Teachers And Those In
Industry**
By A. M. Stephen

Department of Chemistry, University of Cape Town, RSA

This work is intended as an on-line up to date Handbook with extensive coverage of all the major issues concerning the chemistry of carbohydrates, using the term chemistry in a broad sense. The level of the book is aimed at advanced students and research workers. The references cover a wide spectrum, some to major reviews and others given to illustrate the diversity of sources; Conference Proceedings constitute an important feature, it being assumed that international meetings are representative of current trends.

Future directions

Cross-linking between resources – makes it easy to find related information.

Portals – one interface to different resources.

Better interfaces – current interfaces are often too complex or too limited.

XML – allows data to be transferred directly to local applications.

Conclusion

There is a wide range of carbohydrate related resources available on the WWW.

Many provide useful information but all are rather limited in scope.

There are problems transferring data between databases. The interfaces are difficult to use. Manuals or instructions are often missing.