

(Bio)informační význam sacharidů  
Glykobioinformatika  
Lipidoinformatika

**C2138 Pokročilá bioinformatika, jaro 2022**

# Cukry

## 4.7.5 carbohydrate (saccharide)

*Monosaccharides*, *oligosaccharides* and *polysaccharides*, as well as substances derived from monosaccharides by reduction of the carbonyl group (alditols), by oxidation, including the oxidation of one or more terminal groups to carboxylic acids, or by replacement of one or more hydroxy groups by a hydrogen atom, an amino group, a thiol group, or by similar heteroatomic groups. This term also includes derivatives of these compounds.

Note: The term carbohydrate was applied originally to monosaccharides, in recognition of the fact that their empirical composition can be expressed as  $C_m(H_2O)_n$ . However, the term is now used generically in a wider sense.

### 4.7.35 monosaccharide

Polyhydroxy aldehyde  $H-[CHOH]_n-CHO$  or polyhydroxy ketone  $H-[CHOH]_n-CO-[CHOH]_m-H$ , with at least three or more carbon atoms, respectively.

Note 1: The generic term monosaccharide (as opposed to *oligosaccharide* or *polysaccharide*) denotes a single unit without glycosidic connection to other such units.

Note 2: Most monosaccharides exist as cyclic *hemiacetals* or *hemiketals*.

Examples: *Aldoses*, *dialdoses*, *aldoketoses*, *ketoses*, *diketoses*, as well as deoxy sugars and amino sugars, and their derivatives, provided that the compound has a (potential) carbonyl group.

### 4.7.37 oligosaccharide

Compound in which *monosaccharide* units are joined by *glycosidic linkages*.

Note: Oligosaccharides are called *disaccharides*, *trisaccharides*, *tetrasaccharides*, *pentasaccharides*, etc., according to their number of units.

### 4.7.38 polysaccharide

*Biomacromolecule* consisting of a large number of *monosaccharide* (glucose) residues joined to each other by *glycosidic linkages*.

See *glycan*

**Carbohydrate (saccharide) = cukr, sacharid = obecný termín pro celou skupinu látek**

**Glykan = složitější cukr, oligosacharid nebo polysacharid, volný nebo vázaný**

Průměrné výživové hodnoty	ø/100 g	ø/60 g*	% RI
Energetická hodnota	1485 kJ/ 352 kcal	1138 kJ/ 270 kcal	14
Tuky	6,4 g	5,8 g	8
- z toho nasycené mastné kyseliny	1,9 g	2,2 g	11
Sacharidy	59,1 g	41,5 g	16
- z toho cukr	18,5 g	17,1 g	19
Vláknina	9,2 g	5,5 g	
Bílkoviny	10,0 g	10,2 g	20
Sůl	0,08 g	0,20 g	3

\*průměr v balení/ kusová 16 výrobků na pakování

**V oboru chemie potravin jsou výrazem cukry označovány pouze monosacharidy a oligosacharidy. Dle legislativy jsou jako cukry označovány monosacharidy a disacharidy.**

**POZOR! POUŽITÍ JEDNOTLIVÝCH TERMÍNŮ SE TEDY LIŠÍ DLE VĚDNÍHO OBORU!**

## Terminology of bioanalytical methods (IUPAC Recommendations 2018)

<https://doi.org/10.1515/pac-2016-1120>  
Received November 21, 2016; accepted February 1, 2018

# Cukry

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## HLAVNÍ ŽIVINY

- Bílkoviny
- Lipidy (tuky)
- **Sacharidy**
  - množstvím ve stravě (55-60% celkového energetického příjmu) představují její základní složku
  - poskytují organizmu energii
  - jiný biologický význam je nepatrný

www.vyzivaspol.cz

## Terminology of bioanalytical methods (IUPAC Recommendations 2018)

<https://doi.org/10.1515/pac-2016-1120>  
Received November 21, 2016; accepted February 1, 2018

Zdroj energie

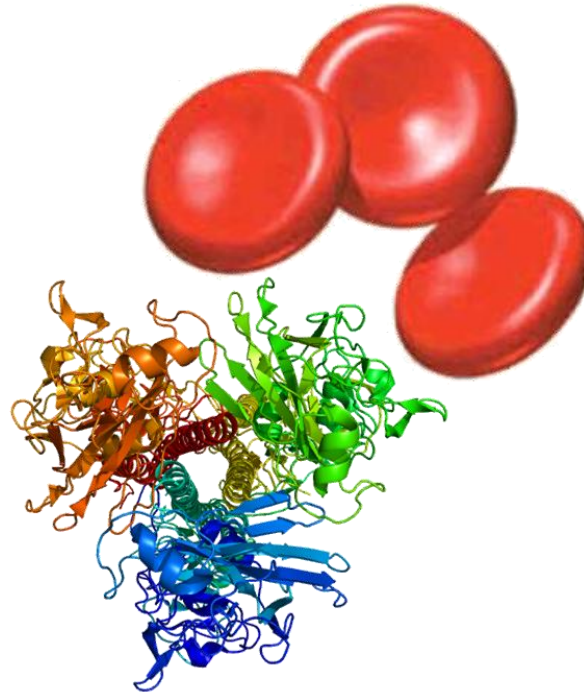


Zásoba energie

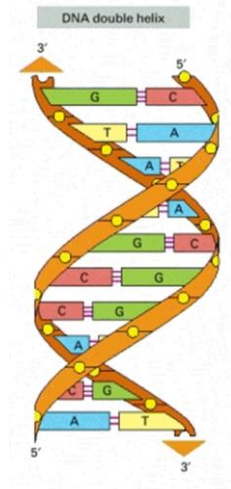


# Funkce cukrů

Nosič informace



Stavební role



...atd.  
role





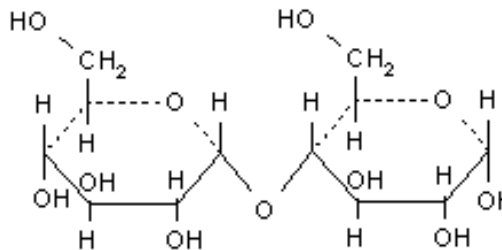
# Funkce sacharidů

Zdroj energie

- Důležitý zdroj **energie** – monosacharidy a disacharidy
- Významné sacharidy v potravě: **glukosa**, fruktosa (monosacharidy), laktosa, sacharosa, maltosa (disacharidy), **škrob** (polysacharid)



**Maltosa** – sladový cukr, disacharid glukosy, vzniká rozpadem škrobu

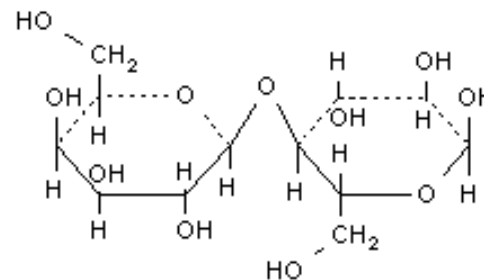


8° 10° 11° 12° ???

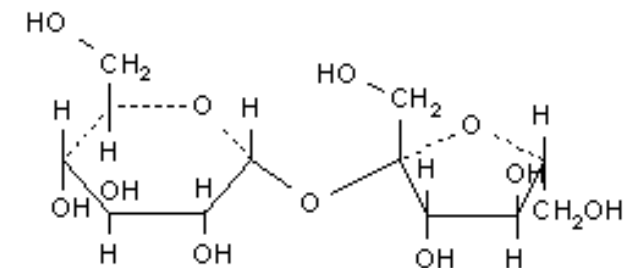
Stupňovitost piva = EMP = extrakt původní mladiny  
Hmotnostní podíl extraktivních (rozpuštěných) látek v mladině.  
Zahrnuje zkvasitelné cukernaté složky – koreluje s obsahem alkoholu ve výsledném pivu.



**Laktosa** – mléčný cukr, disacharid glukosy a galaktosy



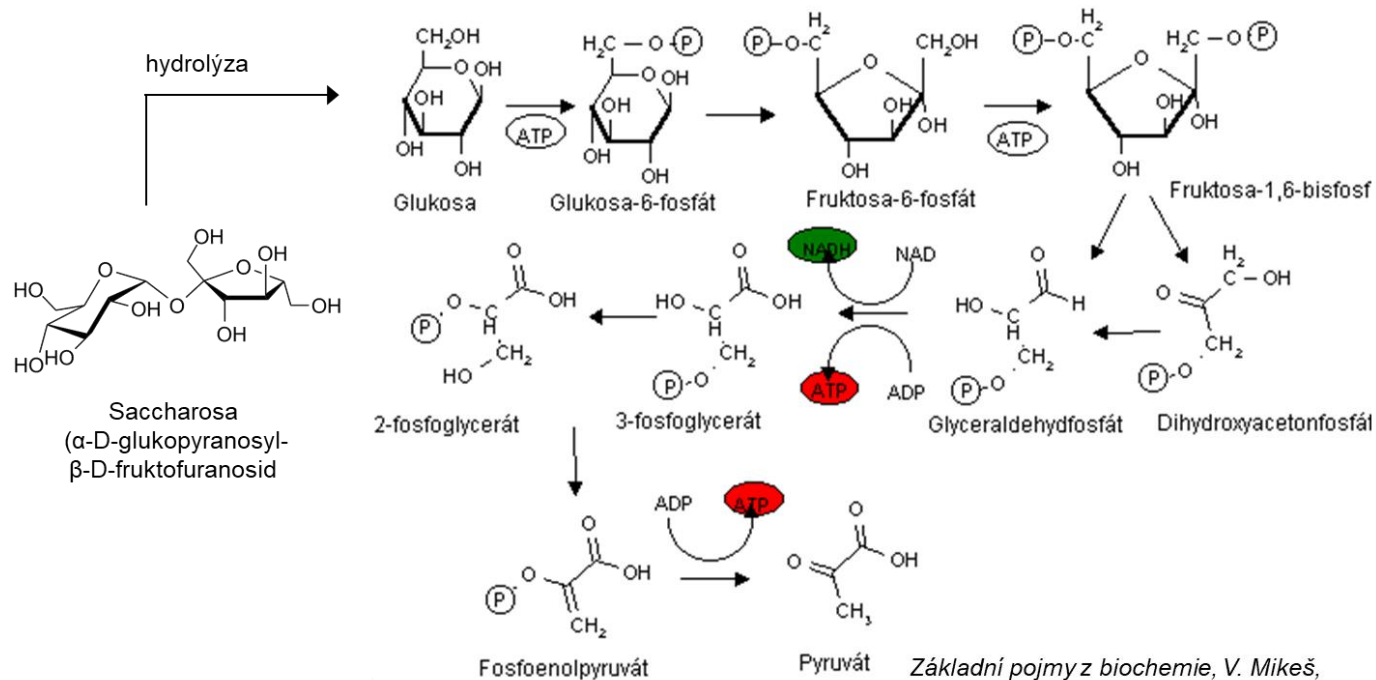
**Sacharosa** – řepný cukr, disacharid glukosy a fruktosy, potravinářské sladidlo



# Funkce sacharidů

Zdroj energie

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- Významné sacharidy v potravě: glukosa, fruktosa (monosacharidy), laktosa, sacharosa, maltosa (disacharidy), škrob (polysacharid)
- Biochemie sacharidů – **odbourávání** sacharidů a **syntéza** sacharidů
- **Glykolýza vs. glukoneogeneze**



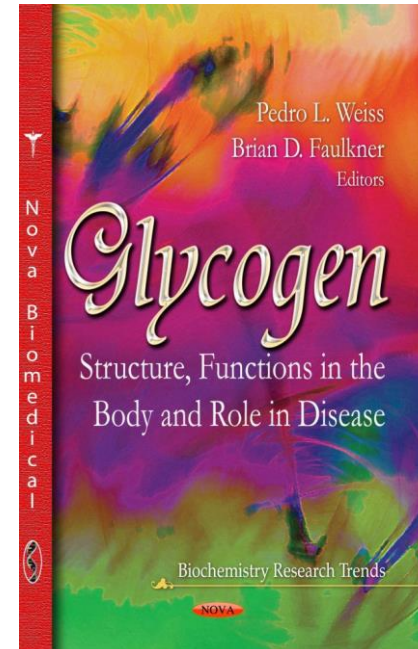
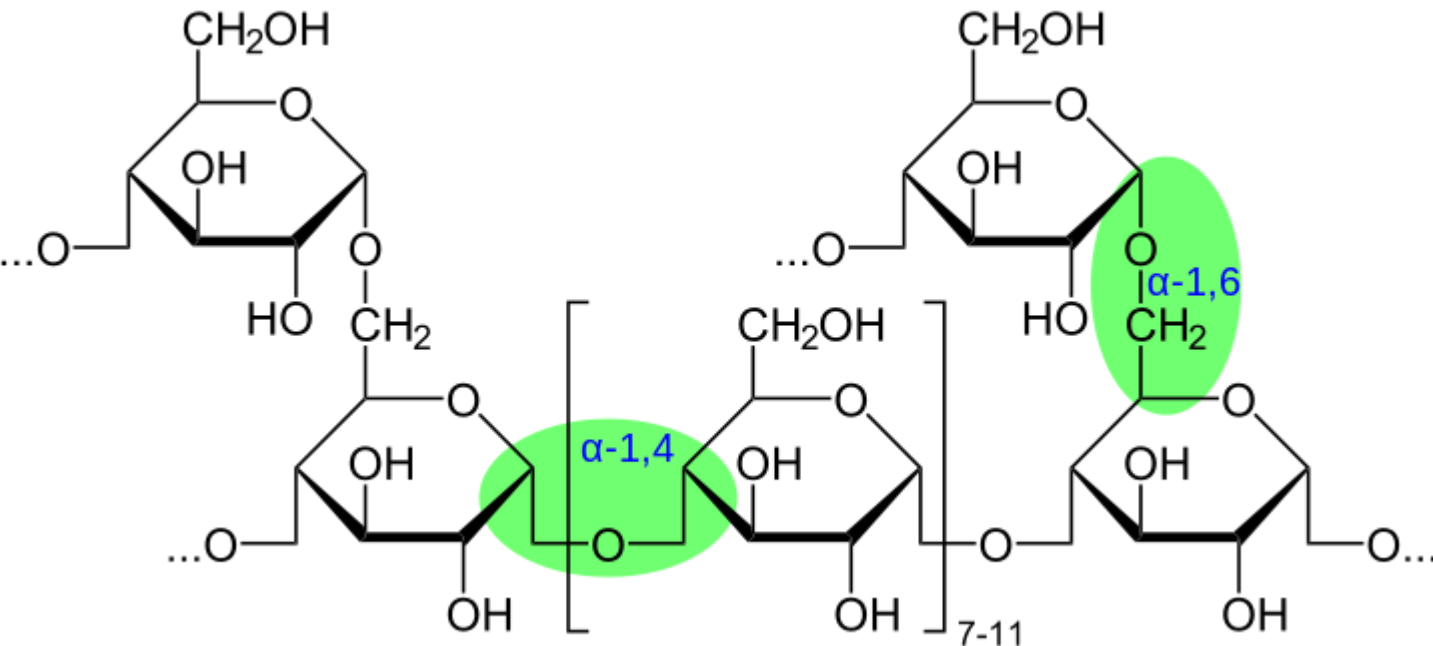
Jako u všeho, i v procesech **trávení**, **vstřebávání** a **metabolismu** sacharidů může docházet k poruchám vedoucím k více či méně závažným zdravotním potížím.

# Funkce sacharidů

Zásoba energie



- Živočichové, kvasinky, bakterie – polysacharid **glykogen**  
Glykogen tvoří glukosa spojená  $\alpha$ -1,4 glykosidovými vazbami. Je **vysoce větvený**: každých cca 10 jednotek dochází k větvení pomocí  $\alpha$ -1,6 glykosidové vazby.



**Glykogenosy** – poruchy degradace, syntézy nebo transportu glykogenu. Abnormální struktura nebo obsah glykogenu v tkáních.

# Funkce sacharidů

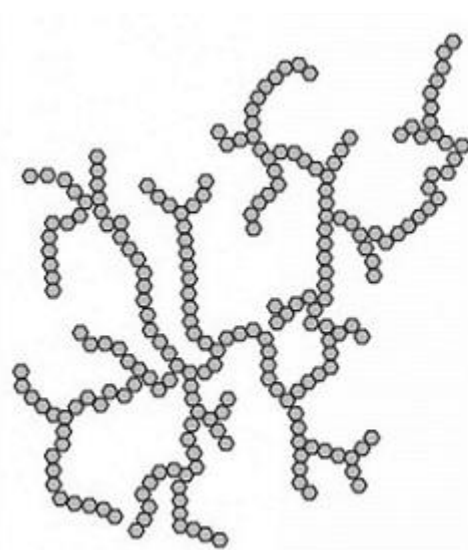
Zásoba energie

- Rostliny – **škrob**

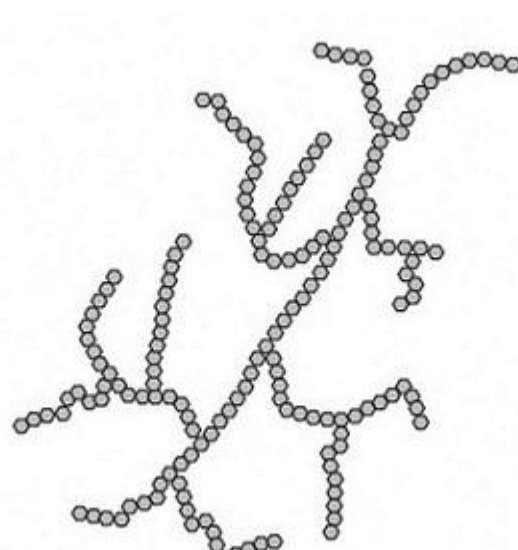
Směs polysacharidů **amylopektinu** a **amylosy**.

Amylopektin: glukosa spojená  $\alpha$ -1,4 glykosidovými vazbami. Je **větvený**, každých 25 jednotek dochází k větvení pomocí  $\alpha$ -1,6 glykosidové vazby.

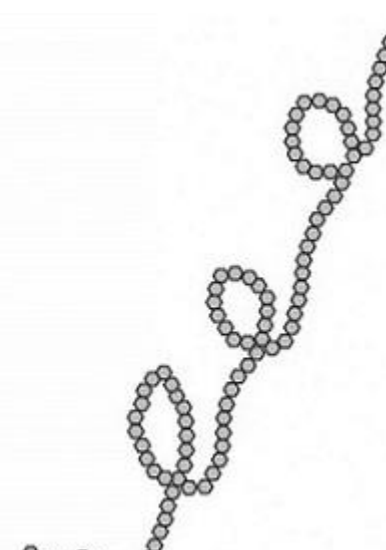
Amylosa: glukosa spojená  $\alpha$ -1,4 glykosidovými vazbami, **nevětvená**



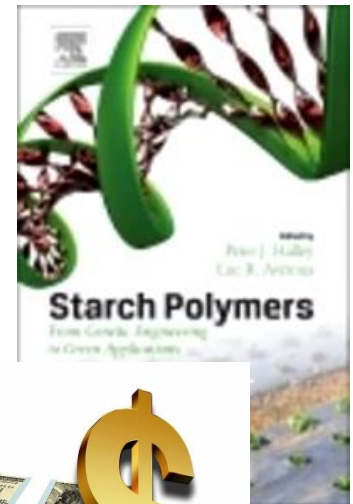
Glykogen



Amylopektin



Amylosa

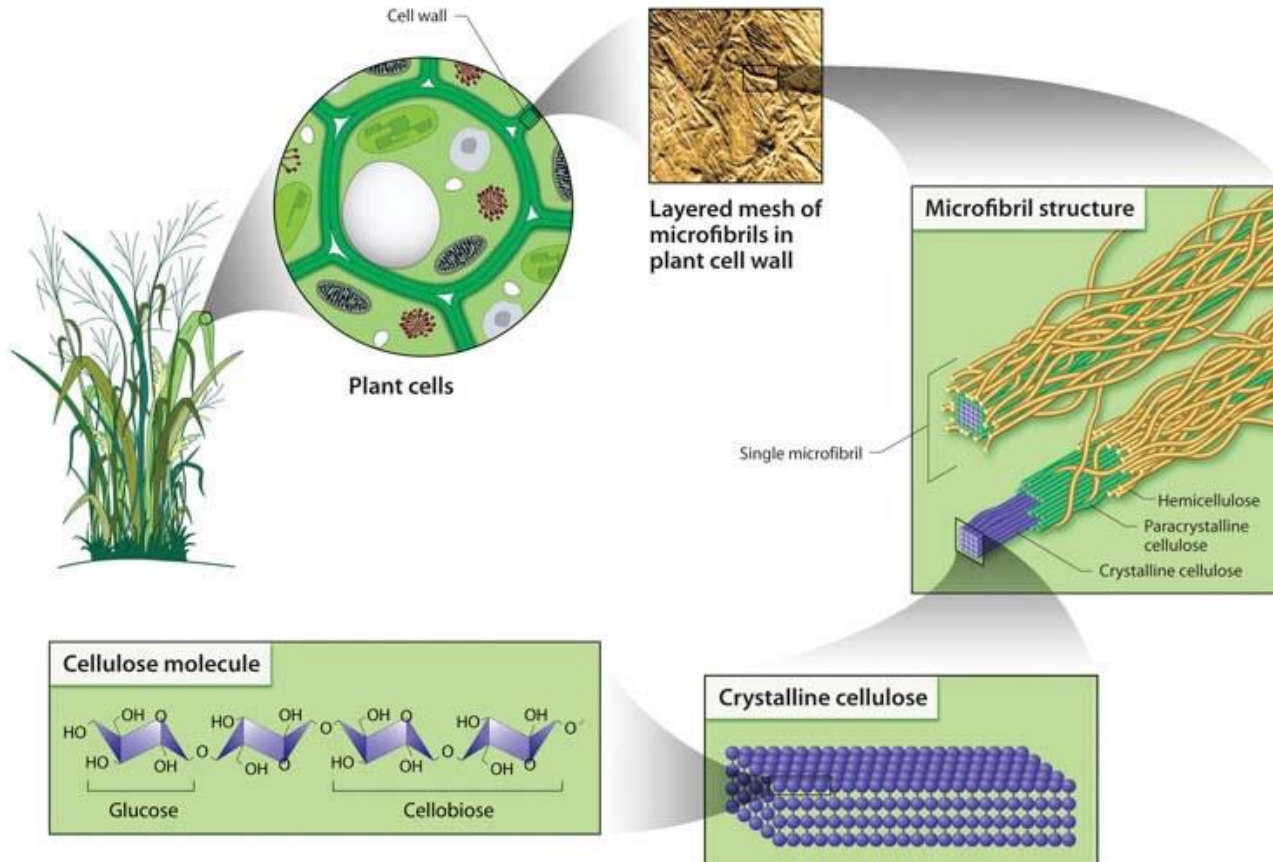
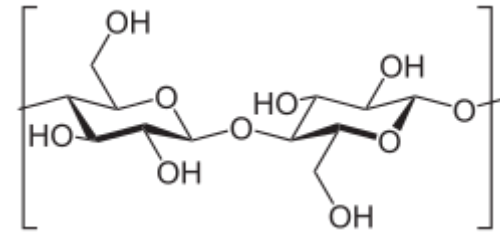




# Funkce sacharidů

Stavební  
role

- **Celulosa** – nevětvený polysacharid, glukosa spojená  $\beta$ -1,4 glykosidovými vazbami.
- Obecně považována za nejrozšířenější biopolymer na světě.
- Hlavně buněčná stěna rostlin, ale výskyt i u bakterií a živočichů.



**Pláštěnci** (Tunicata) – produkce celulosy, historicky označována jako tunicin.





# Další přírodní polysacharidy

Chitin



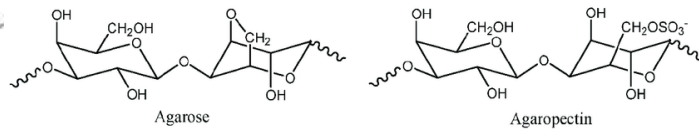
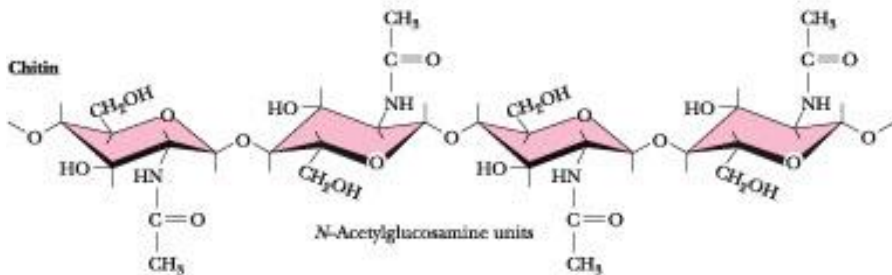
Agar



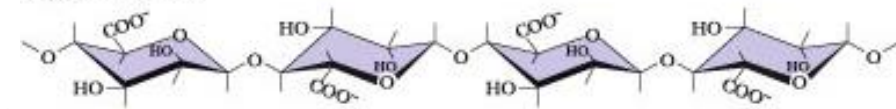
Algin



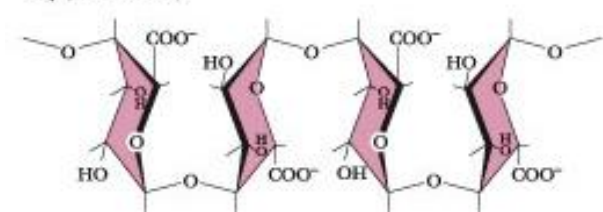
Agarosa + agaropektin



Poly (D-Mannuronate)



Poly (L-Guluronate)



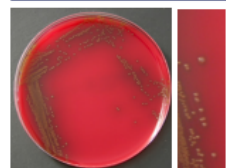
# Využití agaru/agarosy

## Agar



## Dezerty – náhražka želatiny

### Aesculin Blood Agar (modified)



*E. faecium* 24h 36°C

Kód  
Použití

*E. faecalis* ATCC® 29212  
*E. faecium* ATCC® 19434

*S. aureus* ATCC® 6538

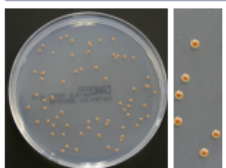
PB5023A

Modifikovaný agar s eskulinem a krví. Izolace a diferenciacie bakterií z případů bovinní mastitidy

1 - 2 mm lesklé šedé kolonie, pozitivní na eskulin  
Dobry růst, tmavě šedé kolonie, pozitivní na eskulin

Dobry růst, žluté lesklé kolonie s hemolýzou

### Biggy Agar



*C. albicans* 72h 30°C

Kód  
Použití

*C. albicans* ATCC® 10231  
*E. coli* ATCC® 25922

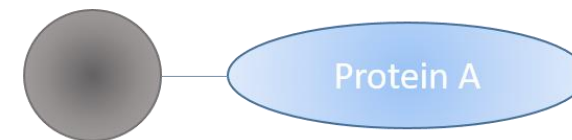
PO5011A

Médium pro izolaci a presumptivní identifikaci *Candida* sp.

1 - 2 mm světlé hnědé kolonie  
Žádný růst

## Kultivační média

## Agarosa

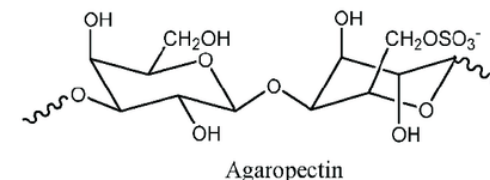
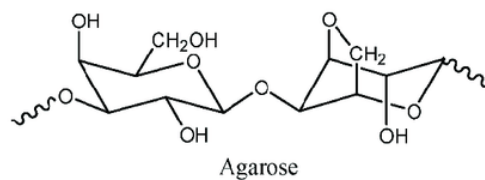


Agarose bead

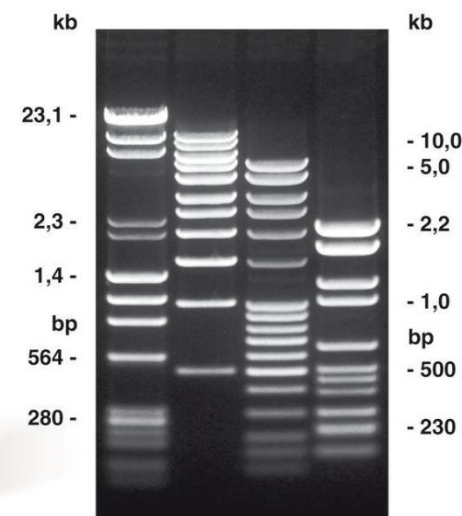
## Agar



## Agarosa + agaropektin



### 1.2 % agarose in 1 x TAE



## Purifikace proteinů Analýza DNA

# Sacharidy a nukleové kyseliny

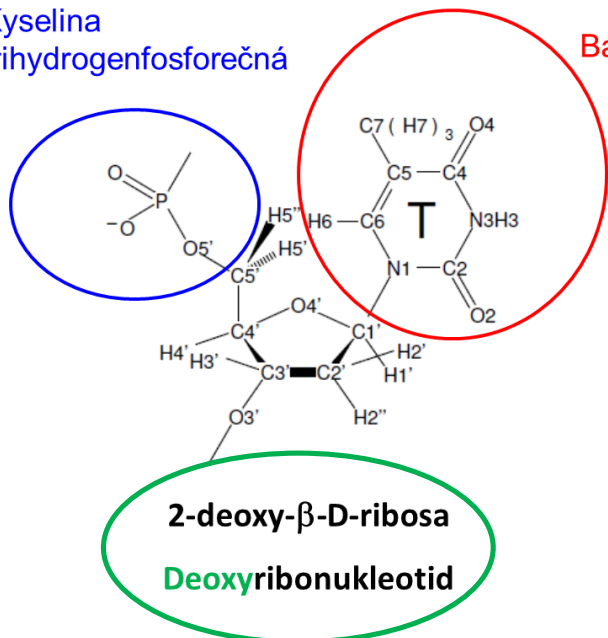
- Dlouhý, nerozvětvený polymer tvořený 4 typy monomerů. Informace je uložena v **pořadí (sekvenci)** monomerů.
- **DNA** – deoxyribonukleová kyselina – vlastní nosič genetické informace (většinou).
- **RNA** – ribonukleová kyselina.

Stavební  
role



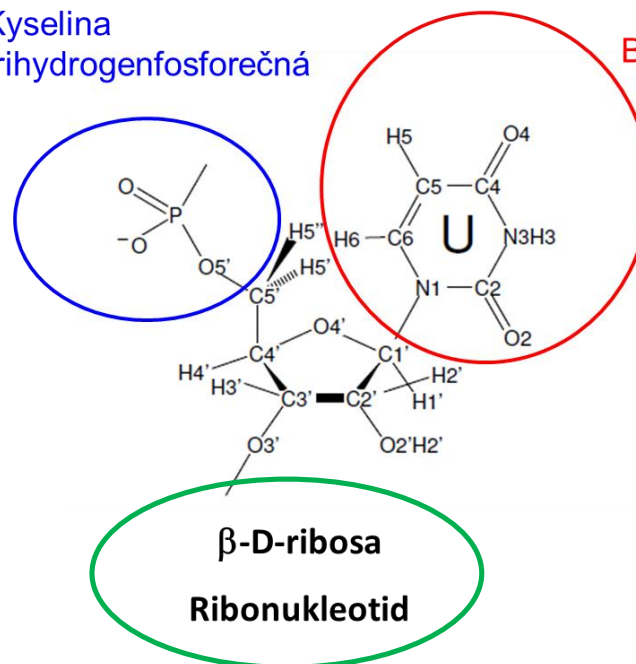
Kyselina  
trihydrogenfosforečná

Báze

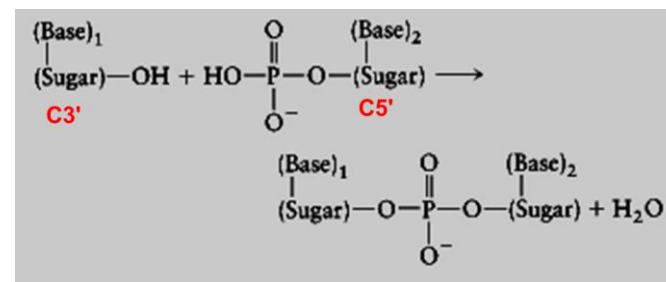


Kyselina  
trihydrogenfosforečná

Báze



**Cukr**(pentosa)fosfátová kostra  
– páteř DNA.



**3', 5' - fosfodiesterová vazba**



# Sacharidy a nukleové kyseliny

Stavební  
role

- **DNA** – deoxyribonukleová kyselina – vlastní nosič genetické informace (většinou).
- **RNA** – ribonukleová kyselina.
- Živé organismy se vyvíjejí cca 4 miliardy let, přesto všechny přechovávají genetickou informaci stejně – jako **nukleovou kyselinu**.
- **Proč** je v nukleových kyselinách (deoxy)ribosa? **Proč** vlastně NK vypadají jak vypadají?
- ?????????????????????????????



DNA AND CELL BIOLOGY  
Volume 39, Number 2, 2019  
© Mary Ann Liebert, Inc.  
Pp. 1–10  
DOI: 10.1089/dna.2019.4943

Ribose Selected as Precursor to Life

Gaspar Banfalvi

*Za daných podmínek fungovaly  
nejlíp – byly stabilní a zvládly  
přenášet informaci bez mutací  
???*

*Evoluce molekuly, která přenáší  
genetickou informaci*

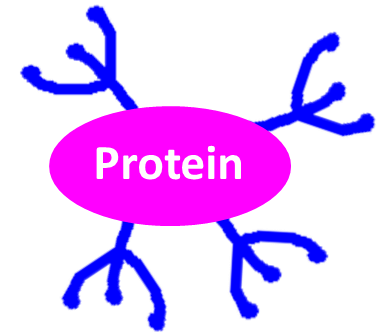
**Proč DNA obsahuje  
právě báze nukleových kyselin?**

<https://vesmir.cz/cz/casopis/archiv-casopisu/2007/cislo-8/proc-dna-obsahuje-prave-baze-nukleovych-kyselin.html>

# Glykosylace

- Kromě nukleových kyselin jsou sacharidy součástí i dalších bio(makro)molekul
- **Glykosylace** – kovalentní připojení sacharidů na jinou molekulu (protein, lipid).
- Glykosylace – významná **posttranslační modifikace**.
- Ovlivňuje **strukturu** proteinů (folding), jejich **aktivitu** i **funkci** (rozpustnost, stabilita, interakce, význam pro **imunitní systém**).
- Glykosylace probíhá u eukaryot i **prokaryot**.
- Glykosylace proteinů je **složitý proces** (syntéza aktivovaných cukrů, glykosyltransferasy, modifikace glykanů, glykosidasy), existují tedy desítky různých vrozených poruch glykosylace (**CDG, congenital disorders of glycosylation**).
- Jedna chyba v procesu glykosylace může ovlivnit funkce mnoha proteinů a projevit se **širokým spektrem** (závažných) symptomů.

Stavební  
role



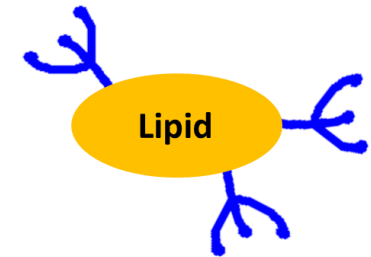
<https://www.cdgsyndrom.cz/>



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- **Glykosylace** – kovalentní připojení sacharidů na jinou molekulu (protein, **lipid**).
- **Glykolipidy** – složka eukaryotických membrán, stabilita membrány, buněčné interakce, receptory (pro viry a další patogeny).
- Lipidová složka slouží k ukotvení v membráně.
- **Lipopolysacharidy (LPS)** – složka vnějších membrán Gram-negativních bakterií, stabilizace membrány, významné antigeny – vzbuzují silnou imunitní odpověď.
- Výraz LPS je dnes používán (ne úplně správně) jako synonymum pro **endotoxin** – pyrogen, aktivace imunitního systému, poruchy srážlivosti.

Stavební  
role

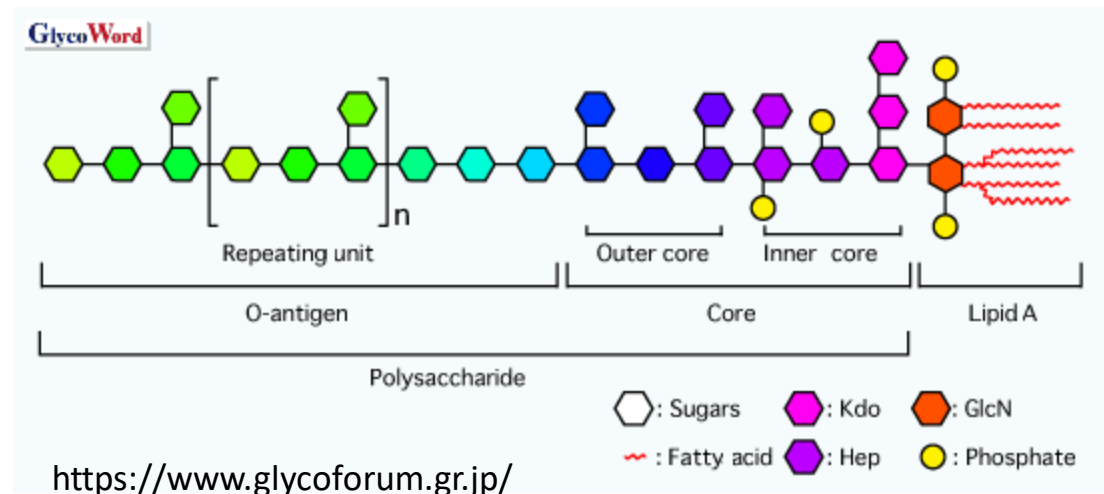


## Glycolipids: Animal

Hakomori Sen-itiroh, *Pacific Northwest Research Institute and University of Washington, Seattle, Washington, USA*

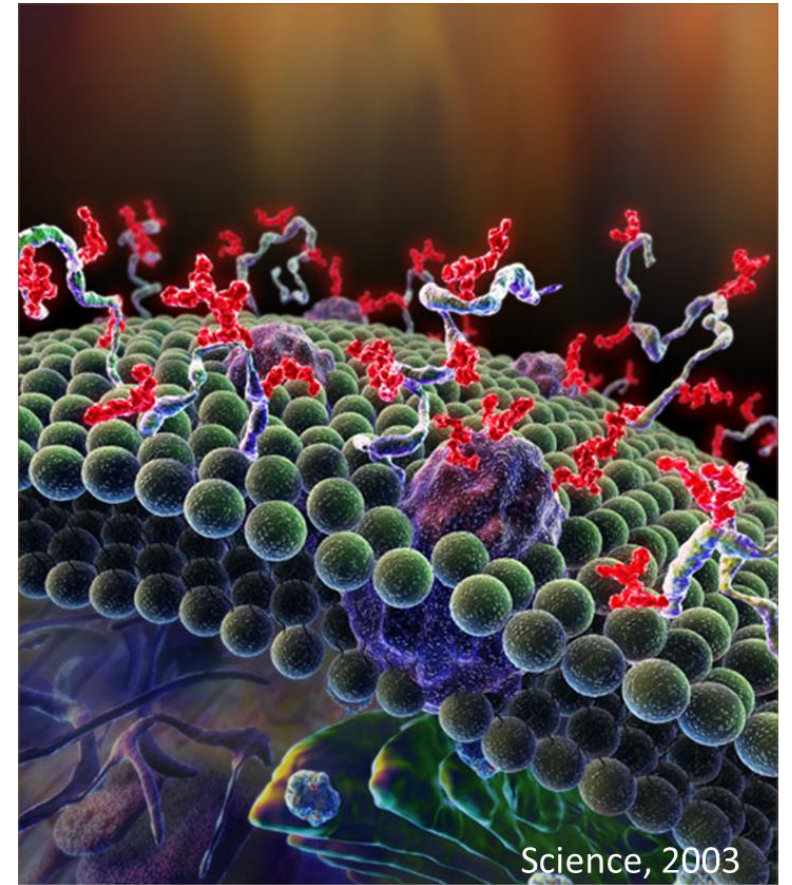
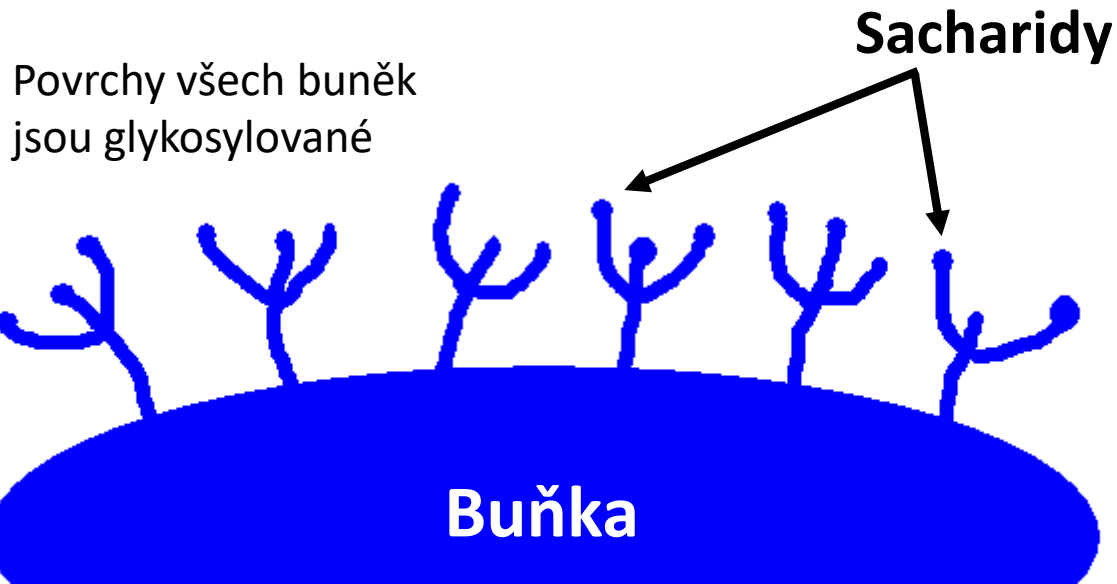
Ishizuka Ineo, *Teikyo University School of Medicine, Tokyo, Japan*

Glycolipids are carbohydrates linked to lipid (either ceramide or glyceride). They are found in animal cells and tissues.



# Výskyt sacharidů v buňce

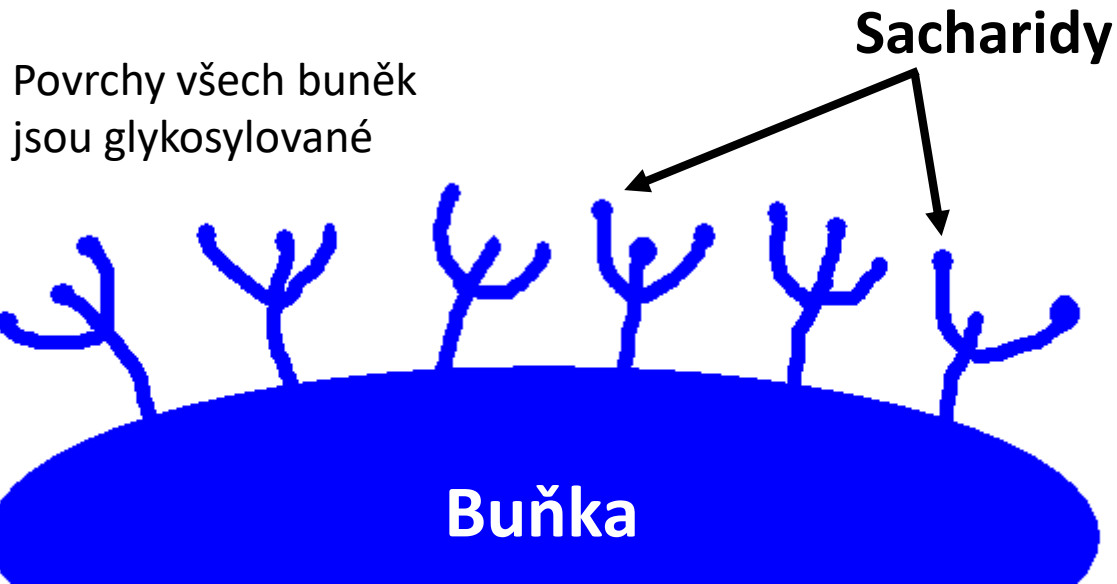
- Jádro – součást **nukleových** kyselin (ribosa, deoxyribosa)
  - Cytosol – volné monosacharidy (**metabolity**)
  - Endoplasmatické retikulum, Golgiho aparát – glykosylované proteiny
  - Buněčná **stěna** – vázané oligo a polysacharidy
  - Buněčné **membrány** – glykoproteiny, glykolipidy
  - Mimo buňku – exopolysacharidy, extracelulární matrix (ECM)
  - Jako součást glykoproteinů v podstatě všude...
- **Glykom** – soubor všech sacharidů produkovaných organismem (buňkou, tkání) v daném čase za daných podmínek.



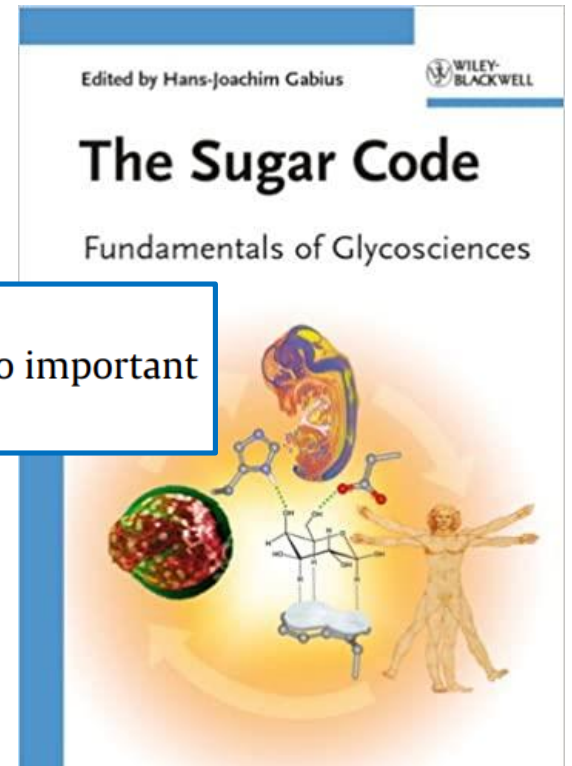
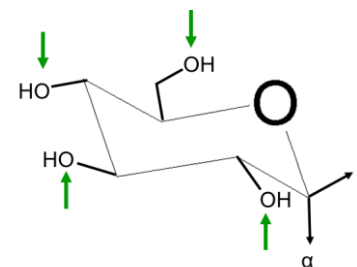
# Funkce sacharidů

- **Glykosylace buněk** – závisí na typu buněk, (zdravotním) stavu buněk, věku, prostředí.
- **Glykosylace buněk** (povrchové sacharidy) – využívá se pro komunikaci, interakce, **specifické rozpoznávání** mezi buňkami, popřípadě mezi buňkami a molekulami.
- Sacharidy mají velký potenciál pro kódování informací („**sugar code**“).

Rozpoznávací  
role



Review article  
The sugar code: Why glycans are so important  
Hans-Joachim Gabius

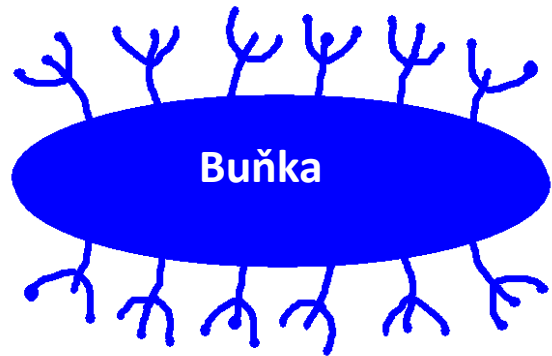


# Funkce sacharidů

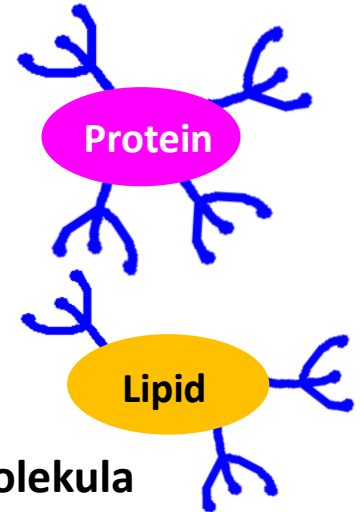
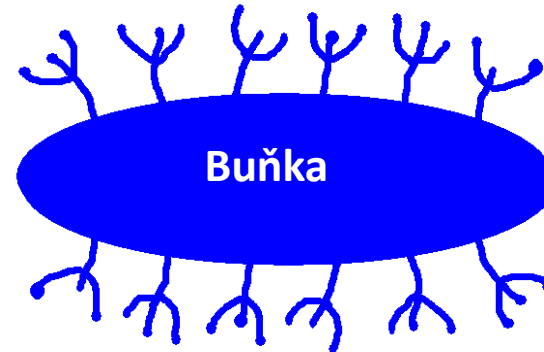
Rozpoznávací  
role

- Interakce buňka-buňka
- Interakce buňka-molekula
- Interakce buňka-patogen

- Protože se nacházejí na povrchu buněk a makromolekul, mohou se cukry uplatňovat v komunikaci a interakcích mezi buňkami a molekulami.



Patogen

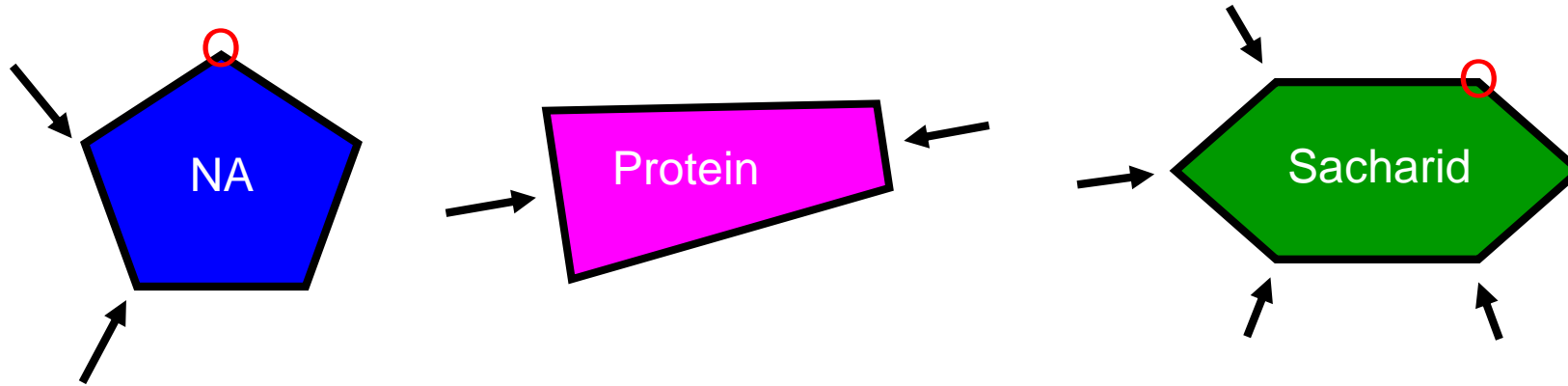


Molekula



Buňka

# Informační potenciál biomolekul



- Informační potenciál je určen množstvím „slov“ (isomerů), které je možné sestavit z jednotlivých „písmen“ (monomerů).
- Nukleotidy a aminokyseliny vytvářejí **lineární polymery**, spojované stále stejným způsobem (fosfodiesterová vazba, peptidová vazba).
- K dokonalému popisu obsažené informace stačí pouze **jednoduchá sekvence** (sled) monomerů:

ATGCTGGTGATTGTGGATGCCGTTACCCTGCTGAGCGCCTATCCGGAAGCCAGCCGTGATC  
CGGCCGCCCGACCGTGATTGATGGTCGCCACCTGTATGTTGTTAGCCCGGGCGATGCCGC

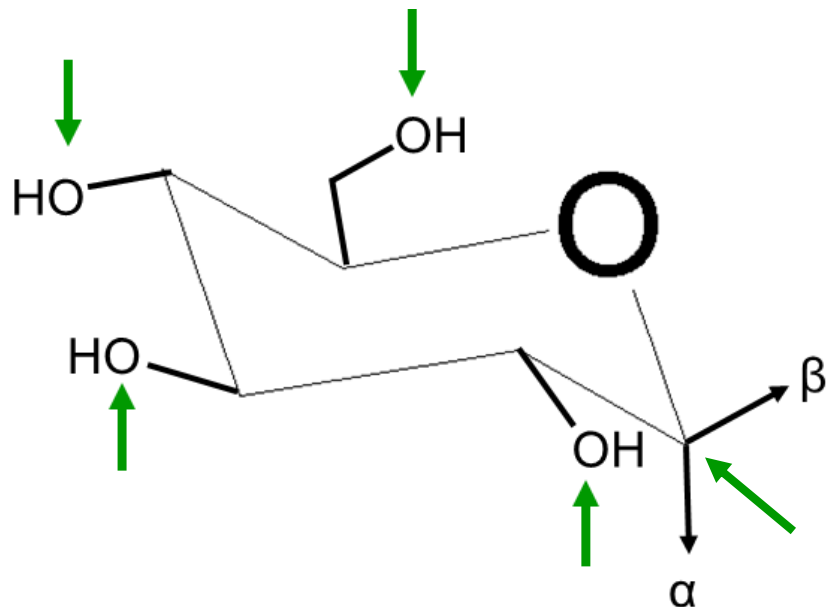
MLVIVDAVTLLSAYPEASRDPAAPTVIDGRHLYVSPGDA



# Informační potenciál sacharidů

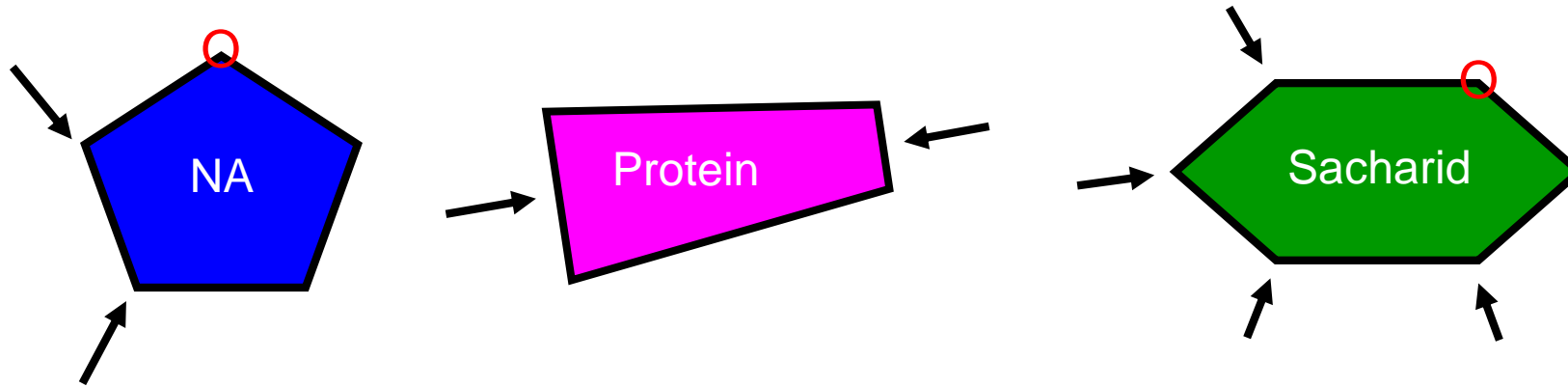
Rozpoznávací  
role

- **Glykosylace buněk** – závisí na typu buněk, (zdravotním) stavu buněk, věku, prostředí.
- **Glykosylace buněk** (povrchové sacharidy) – využívá se pro komunikaci, interakce, **specifické rozpoznávání** mezi buňkami, popřípadě mezi buňkami a molekulami.
- Sacharidy mají velký potenciál pro kódování informací („**sugar code**“).

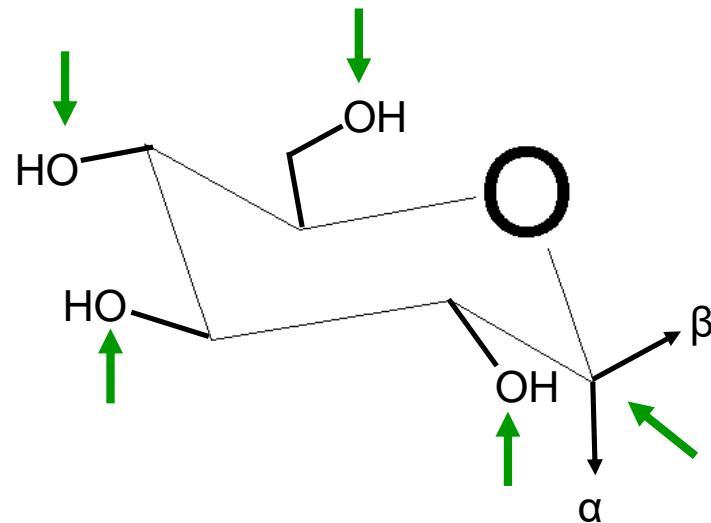


- Informační potenciál je určen množstvím „slov“ (isomerů), které je možné sestavit z jednotlivých „písmen“ (monomerů).
- Sacharidových monomerů je ve srovnání s aminokyselinami (22) a nukleotidy (4) k dispozici několik **desítek**.
- Na rozdíl od aminokyselin a nukleotidů se mohou sacharidy spojovat **různými** glykosidovými vazbami a také mohou tvořit **rozvětvené** řetězce.

# Informační potenciál cukrů



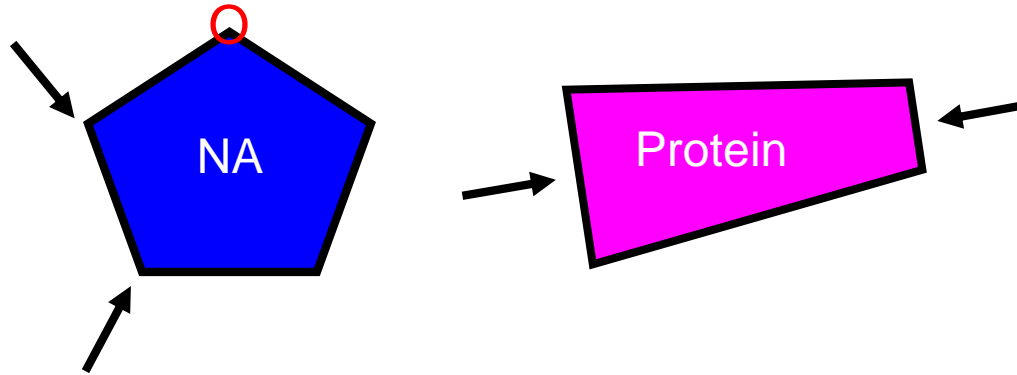
- Pro přesný popis oligo(poly)sacharidu je kromě sekvence nutné znát i typ glykosidické vazby (anomerii) a velikost kruhu.



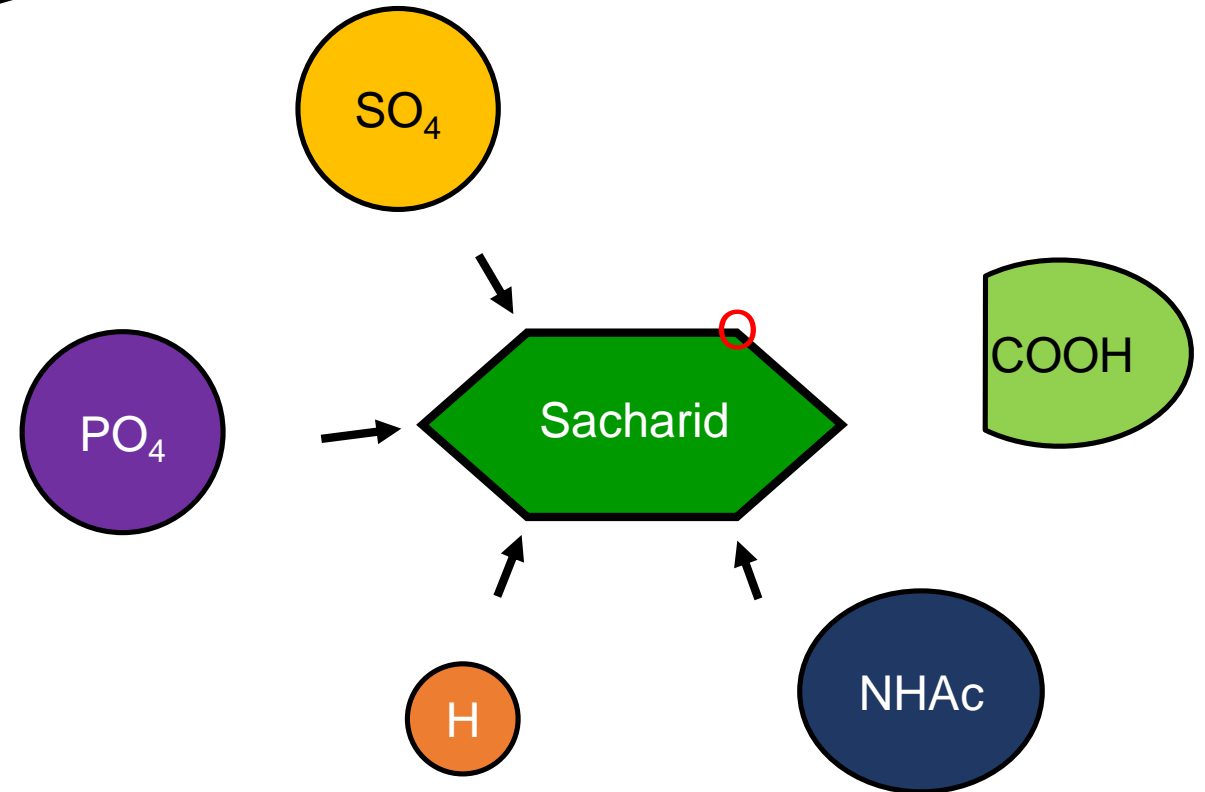
D-glukosa + D-glukosa:

$\alpha$ 1-2	kojibiosa
$\alpha$ 1-3	nigerosa
$\alpha$ 1-4	maltosa
$\alpha$ 1-6	isomaltosa
$\alpha$ 1-1' $\alpha$	trehalosa
$\beta$ 1-2	soforosa
$\beta$ 1-3	laminaribiosa
$\beta$ 1-4	cellobiosa
$\beta$ 1-6	gentibiosa

# Informační potenciál cukrů



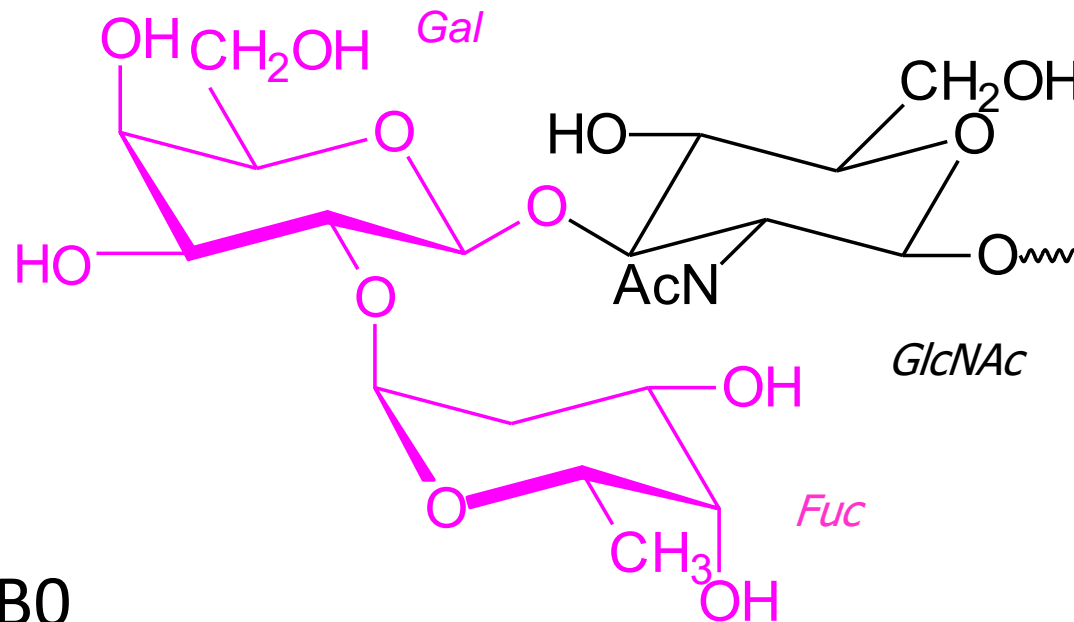
- Glykosidové vazby může tvořit i více než jedna OH skupina, vzniká **rozvětvený** oligosacharid.
- Klasickým příkladem rozvětvených oligosacharidů jsou antigeny **AB0 krevních skupin**.
- Cukry mohou být dále **modifikovány** redukcí, oxidací nebo vazbou dalších funkčních skupin.



# Krevní skupiny ABO systému

Rozpoznávací  
role

- **Glykosylace buněk** – závisí na typu buněk, (zdravotním) stavu buněk, věku, prostředí.
- **Glykosylace buněk** (povrchové sacharidy) – využívá se pro komunikaci, interakce, **specifické rozpoznávání** mezi buňkami, popřípadě mezi buňkami a molekulami.
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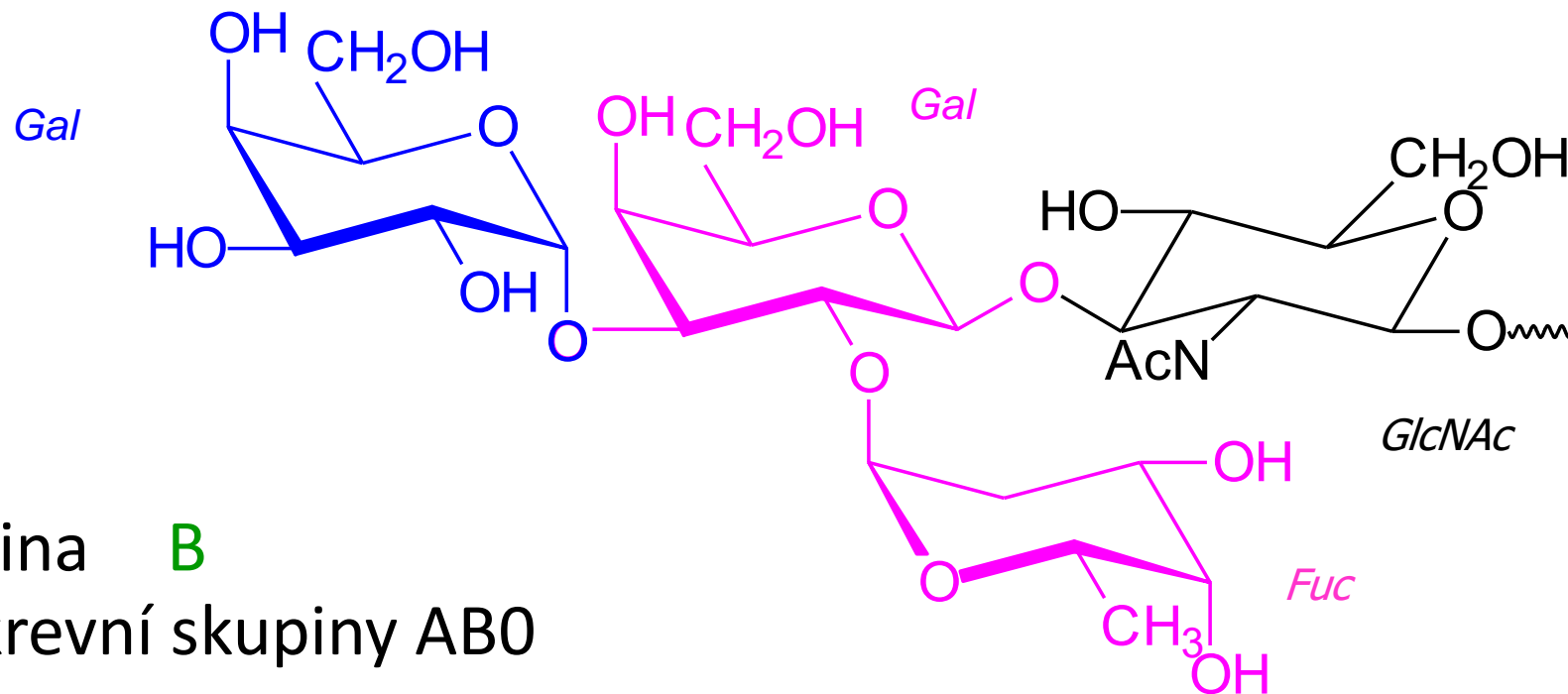


Krevní skupina **0**  
Tkáňové a krevní skupiny ABO

# Krevní skupiny ABO systému

Rozpoznávací  
role

- **Glykosylace buněk** – závisí na typu buněk, (zdravotním) stavu buněk, věku, prostředí.
- **Glykosylace buněk** (povrchové sacharidy) – využívá se pro komunikaci, interakce, **specifické rozpoznávání** mezi buňkami, popřípadě mezi buňkami a molekulami.
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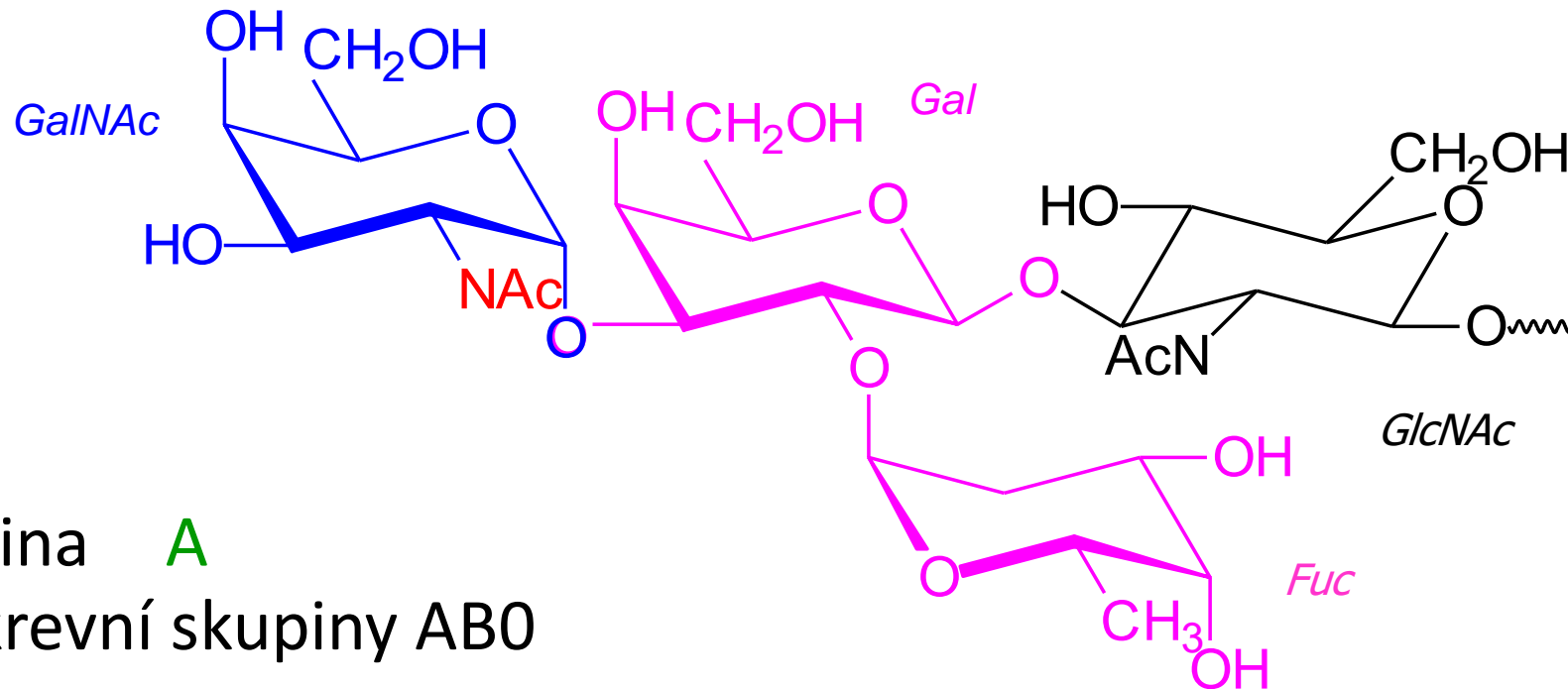
Krevní skupina **B**  
Tkáňové a krevní skupiny ABO



# Krevní skupiny ABO systému

Rozpoznávací  
role

- **Glykosylace buněk** – závisí na typu buněk, (zdravotním) stavu buněk, věku, prostředí.
- **Glykosylace buněk** (povrchové sacharidy) – využívá se pro komunikaci, interakce, **specifické rozpoznávání** mezi buňkami, popřípadě mezi buňkami a molekulami.
- Sacharidy mají velký potenciál pro kódování informací („**sugar code**“).



Krevní skupina **A**  
Tkáňové a krevní skupiny ABO

# Čtení „sacharidového kódu“

Rozpoznávací  
role

- **Protilátky** – produkt imunitní odpovědi, rozpoznávání mezi „vlastním“ a „cizím“.
- **Lektiny** – proteiny, které specificky a reverzibilně vážou mono- a oligosacharidy. Nejsou produkty imunitní odpovědi (ale významně se uplatňují v imunitním systému!).
- Lektiny plní rozpoznávací a adhezivní funkci v mnoha různých biologických procesech.
- Vyskytují se v zástupcích všech taxonů (rostliny, zvířata, houby, bakterie, viry).

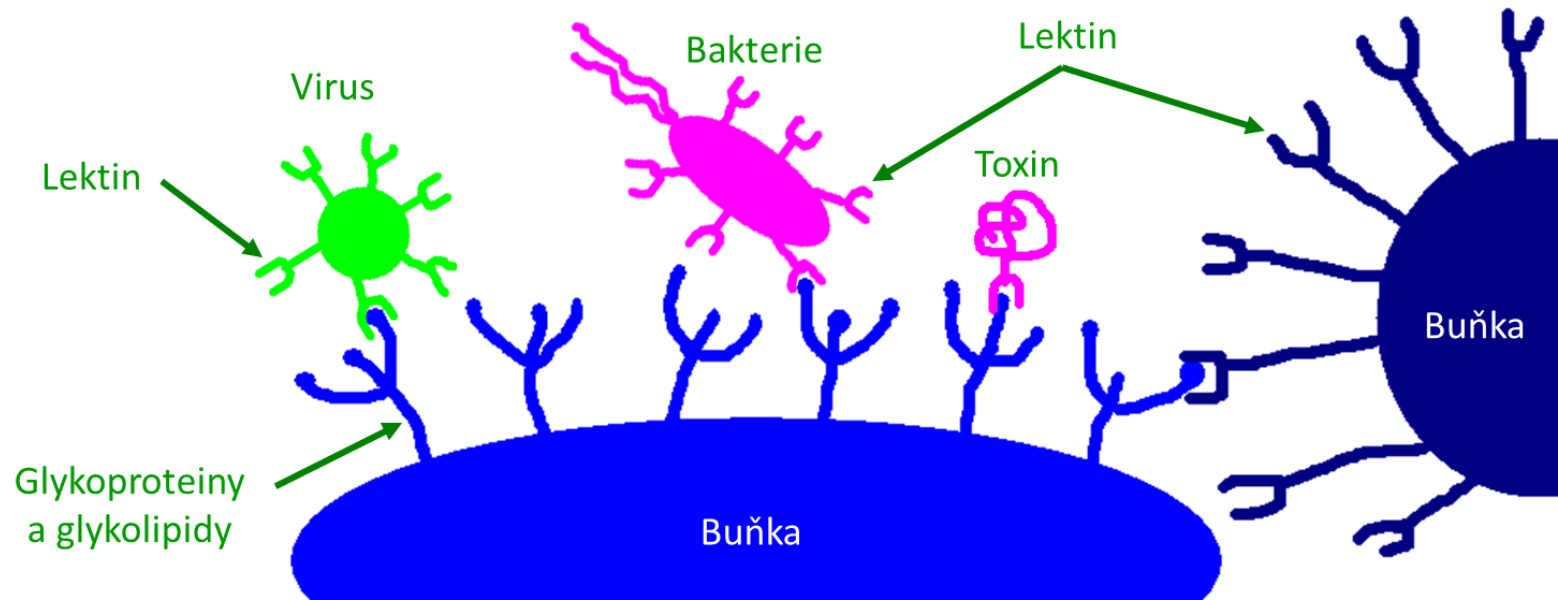


## Lectins

Nathan Sharon, Weizmann Institute of Science, Rehovot, Israel

Based in large part on the previous version of this Encyclopedia of Life Sciences (ELS) article, Lectins by Nathan Sharon and Halina Liš.

- **Interakce buňka-buňka**
- **Interakce buňka-molekula**
- **Interakce buňka-patogen**

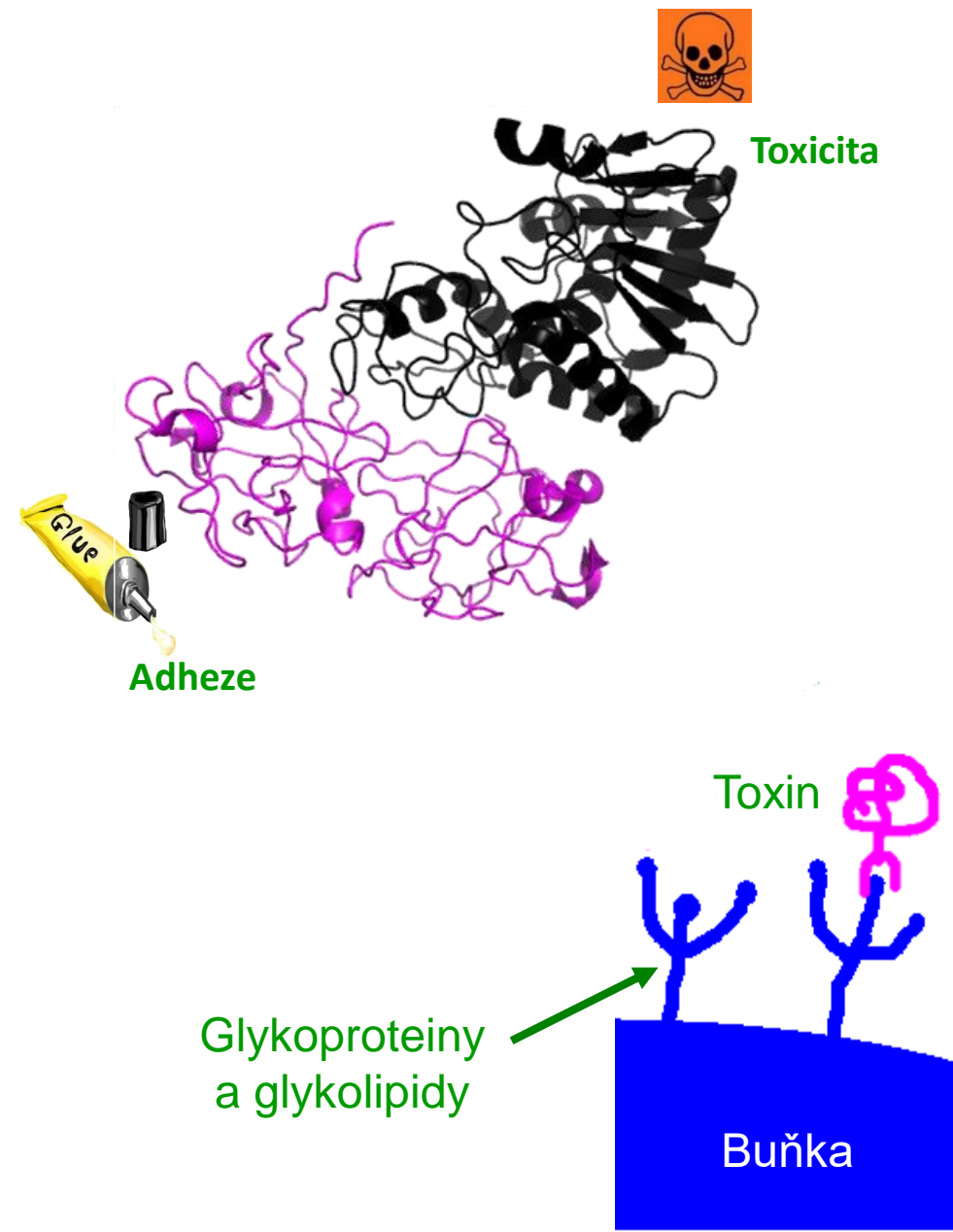


# Ricin

- **Ricin** je toxin produkovaný rostlinou *Ricinus communis* (skočec obecný, Ricín obyčejný).
- Často využíván jako **okrasná rostlina**.
- Ricin se vyskytuje nejvíce v **semenech**.
- Pro otrávení jsou celá semena nevhodná, je nutné je pořádně rozžvýkat.



Ribosome-inactivating proteins (RIPs) – proteiny inaktivující ribosomy  
Ricin, abrin, volkensin



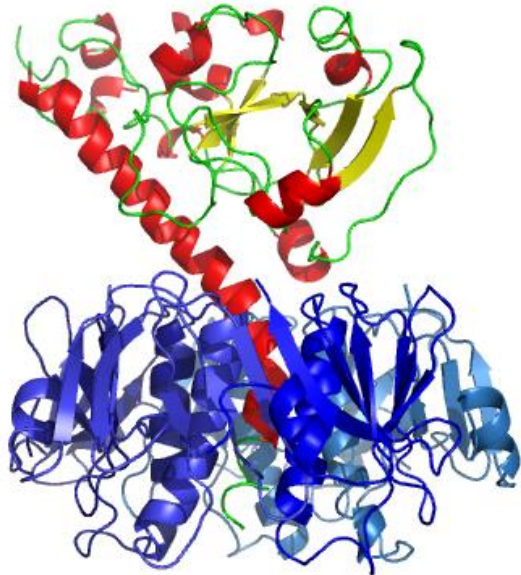
# Cholera toxin/shiga toxin

Rozpoznávací  
role

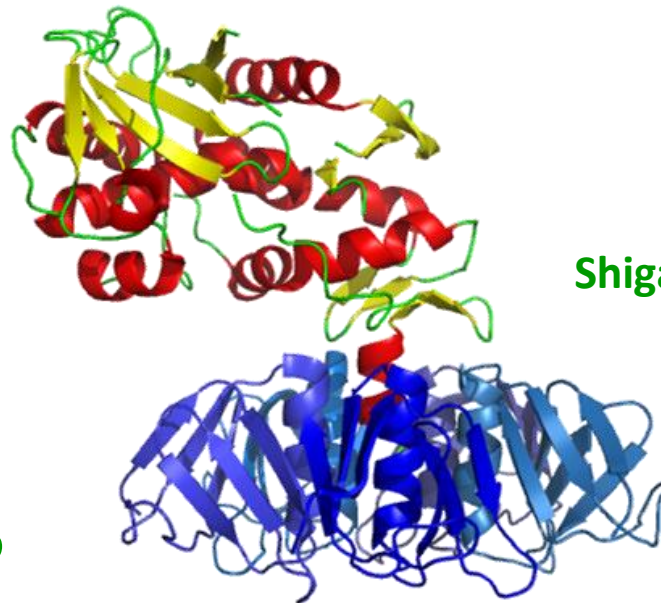
- Bakterie *Vibrio cholerae* a *Shigella dysenteriae*.
- **AB<sub>5</sub>** – katalytická (**toxická**) podjednotka A + lektinová (**vazebná**) podjednotka B.
- Lektiny jsou často součástí větších komplexů, kde zastávají adhezivní, rozpoznávací a vazebné funkce.



Cholera  
toxin



A



Shiga toxin

B<sub>5</sub>

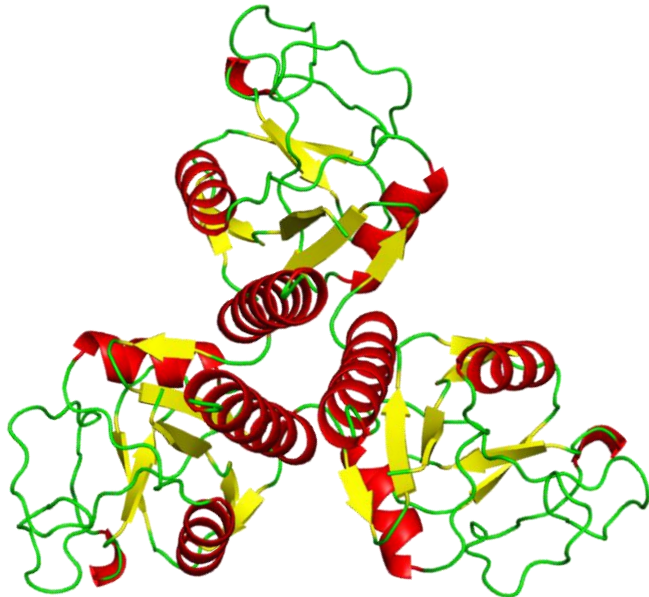
- Cholera
- Shigelóza (bacilární úplavice)
- Obě průjmová onemocnění, úplně jiný mechanismus
- **Dehydratace!** Při choleře je možné ztratit 1 litr vody za hodinu, dehydratace za pár hodin
- Náhrada vody a minerálů, antibiotika



# MBL – mannose-binding lectin

Rozpoznávací  
role

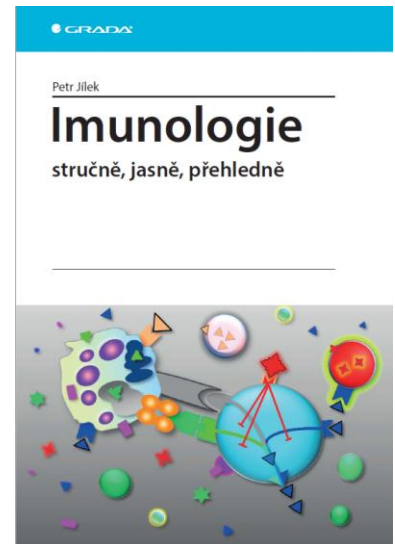
- Mannose-binding lectin; mannan-binding lectin, mannan-binding protein.
- **Lektin vázající mannosu.**
- Významná složka **nespecifické imunity** – rozeznává sacharidy na povrchu patogenních mikroorganismů.
- **Lektinová cesta aktivace komplementu.**



## 3 Komplementový systém

Komplement (zkratka C) je tvořen **systémem bílkovin**, které se kaskádovitým způsobem přeměňují z neaktivní formy do podoby enzymů, které působí na další složky kaskády. Smyslem tohoto děje je především **likvidace tělu nežádoucích buněk** prostřednictvím jejich lýzy buď samotným komplementem, nebo během **zánětu**, jehož je komplement významnou humorální složkou.

Komplement je významnou součástí přirozené humorální imunity, kam zařazujeme také látky tvořené fagocytujícími buňkami, např. lysozym nebo defenziny. Jim byla věnována pozornost už v předchozí kapitole.



# Další funkce sacharidů

...atd.  
role

- **Mechanická ochrana** – muciny (hlen, sliz) na povrchu tkání, brání průniku patogenů.
- **Rozpustnost** biomakromolekul – koncentrace proteinů v plazmě může být až 70 mg/ml!
- **„Nemrznoucí kapalina“** – ochrana před vznikem krystalků ledu v tělních tekutinách.

REVIEW ARTICLE

## 'Antifreeze' glycoproteins from polar fish

Margaret M. Harding<sup>1</sup>, Pia I. Anderberg<sup>1</sup> and A. D. J. Haymet<sup>2</sup>

<sup>1</sup>School of Chemistry, The University of Sydney, New South Wales, Australia; <sup>2</sup>CSIRO Marine Research, Hobart, Tasmania, Australia

- **Lubrikace** (snížení tření) – porucha funkce slinných žláz (tvorba mucinů) může vést k omezení schopnosti **polykat potravu a mluvit** (vypadá to jako samozřejmost až do doby, kdy to najednou nejde...).  
**Hyaluronan** – synoviální (kloubní) tekutina, kloubní maz.



- **SJÖGRENŮV SYNDROM (SS)** je systémové autoimunitní onemocnění se zhoršenou funkcí žláz s vnější sekrecí.
- Dochází k postižení především buněk **slinných a slzných žláz**.
- Syndromem může být zasažen i jícen, žaludek, slinivka břišní, potní žlázy, hlenové žlázy střev, bronchů a pochvy u žen. Může se objevit onemocnění kloubů, Raynaudův fenomén (poruchy prokrvení rukou a nohou), celková únava snižující fyzickou výkonnost. Komplikací může být riziko vzniku lymfomu (onemocnění buněk mízních uzlin).

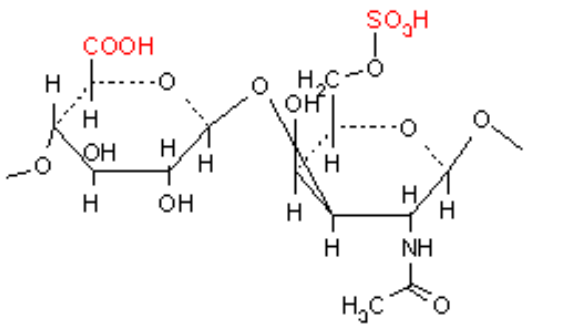
### PORUCHY POLYKÁNÍ (DYSFAGIE), PORUCHY PŘÍJMU POTRAVY:

- Nedostatek slin způsobuje suchost v ústech, v krku, suchost rtů a polykací obtíže, váznutí soust v ústech, přilnavost k patru, pocity změněné chuti, nesnášenlivost kyselého a kořeněného jídla a zejména neschopnost jíst suchou potravu či mluvit déle než 5 minut.

# Glykosaminoglykany

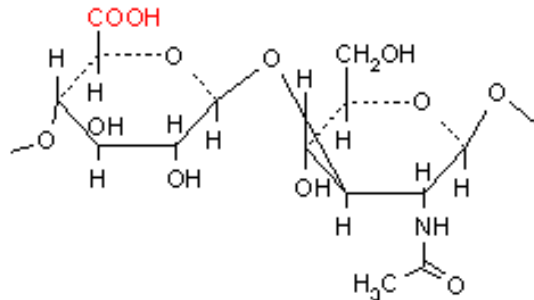
...atd.  
role

- **Glykosaminoglykany (mukopolysacharidy)** – dlouhé nevětvené polysacharidy obsahující uronové kyseliny.
- Důležitá složka mezibuněčné hmoty, vysoce polární
- **Hyaluronan (kyselina hyaluronová)**
- **Chondroitin sulfát** – mezibuněčná hmota chrupavek



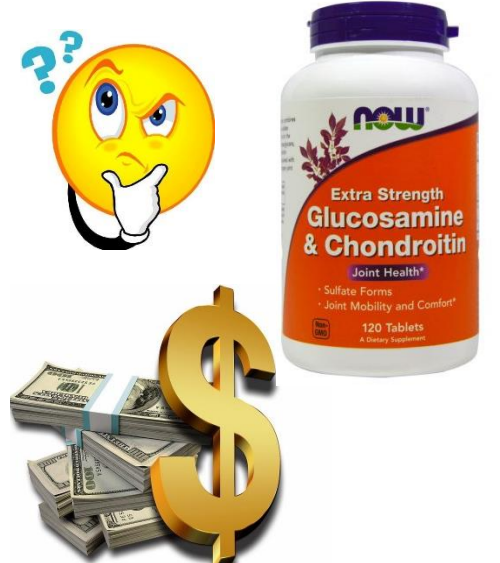
$\beta$ -D-glukuronát N-Ac- $\beta$ -D-galaktosamin

**chondroitin-6-sulfát**



$\beta$ -D-glukuronát N-Ac- $\beta$ -D-glukosamin

**hyaluronát**



„Although glucosamine and chondroitin sulfate have showed beneficial effects on joint tissues in osteoarthritis (OA), their therapeutic use in the clinical setting is still debatable. Oral supplementation with glucosamine or chondroitin sulfate reduces pain in knee OA. However, there is no additional effect using both therapeutic agents in combination for the management of symptomatic knee OA.“

Effect of glucosamine and chondroitin sulfate in symptomatic knee osteoarthritis: a systematic review and meta-analysis of randomized placebo-controlled trials

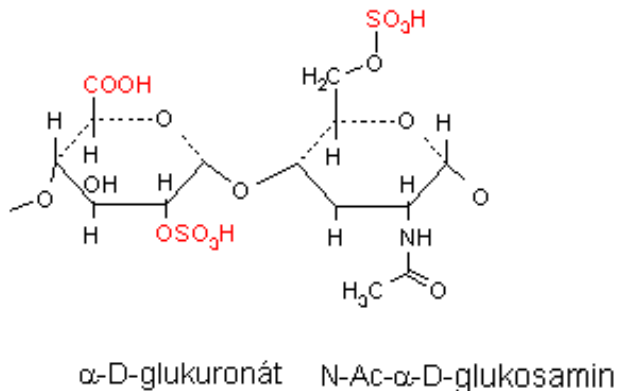
# Glykosaminoglykany

...atd.  
role

- **Glykosaminoglykany (mukopolysacharidy)** – dlouhé nevětvené polysacharidy obsahující uronové kyseliny.
- Důležitá složka mezibuněčné hmoty, vysoce polární.
- **Hyaluronan (kyselina hyaluronová).**
- **Chondroitin sulfát** – mezibuněčná hmota chrupavek.
- **Heparin** – antikoagulant, fyziologická funkce nejasná, ovlivnění průběhu zánětu a alergických reakcí?



<https://trombofilik.cz/>



heparin

Nejzávažnějším případem české kriminální současnosti je i v této publikaci zmíněný případ tzv. „heparinového vraha“ Petra Zelenky. Sám jsem se byl na soudní proces u Krajského soudu v Hradci Králové podívat a jde skutečně o kauzu, která je zajímavá zejména z psychologického hlediska. Zarážející totiž je, že podle znalců-psychologů vraždil zřejmě Zelenka „pro radost“.

Andrej Drbohlav

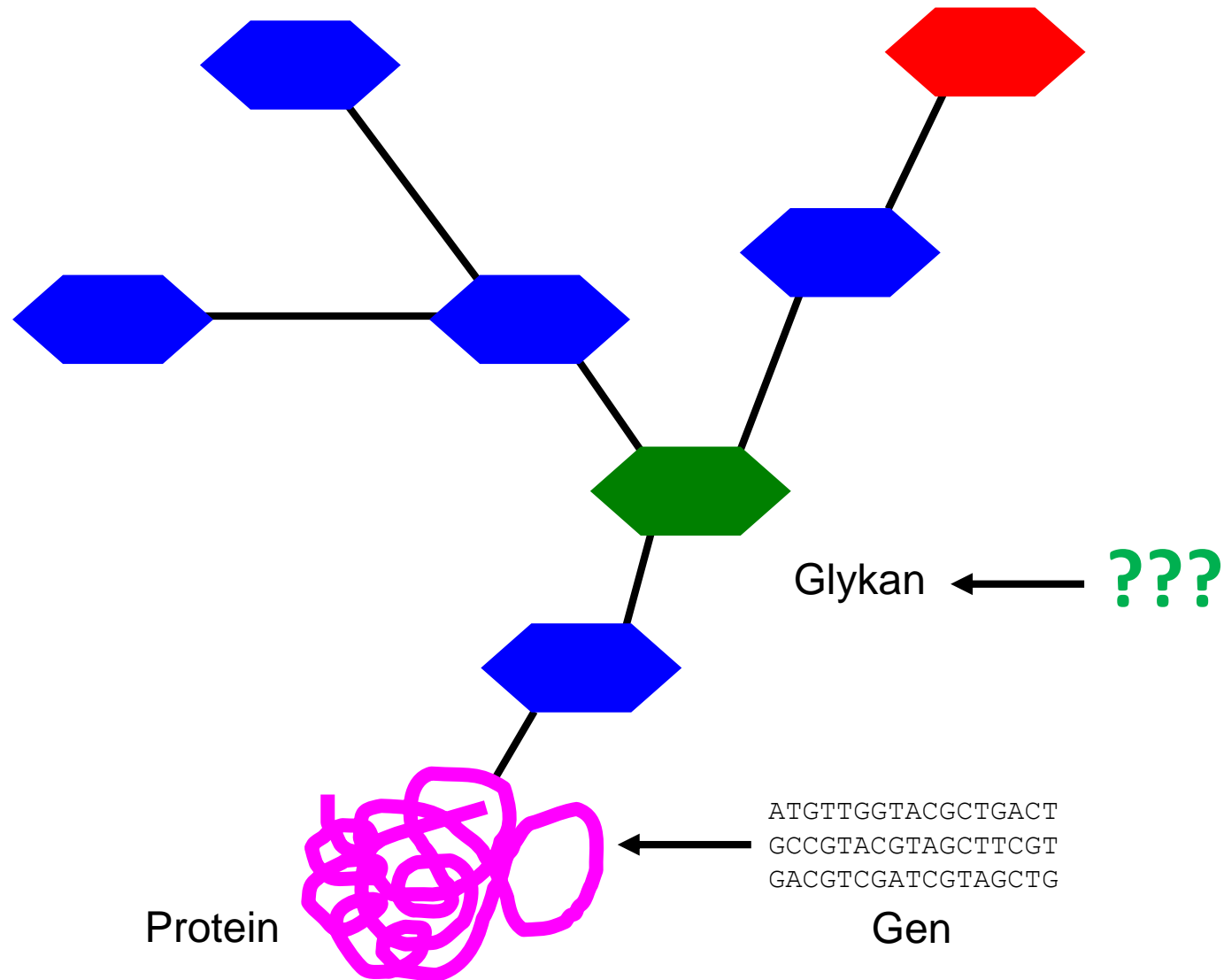
**PSYCHOLOGIE  
SÉRIOVÝCH VRAHŮ**

200 skutečných případů brutálních činů  
sériových vrahů současnosti



GRADA

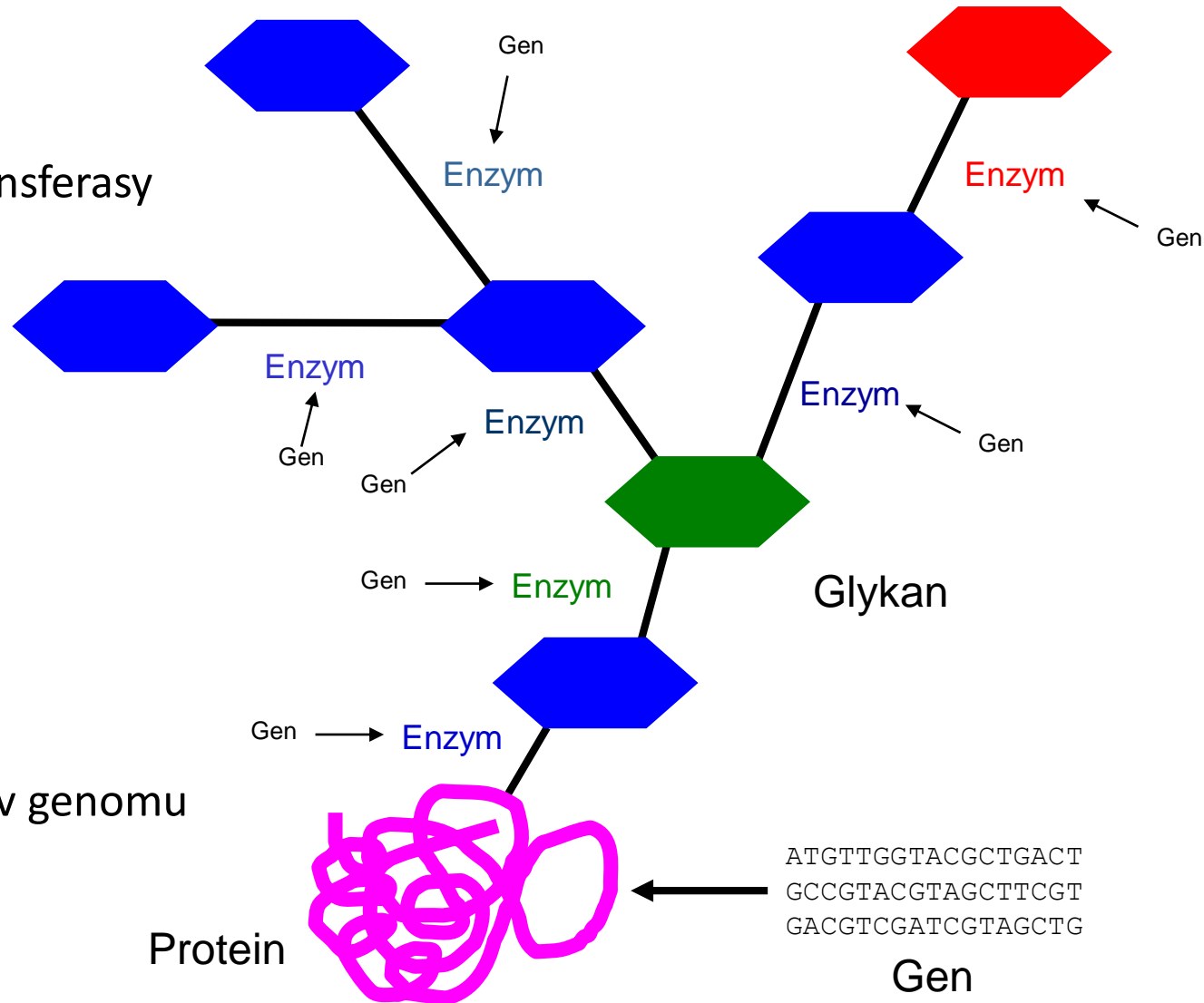
# Jak jsou glykoproteiny kódovány v genomu?





# Jak jsou glykoproteiny kódovány v genomu?

Enzymy = glykosyltransferasy



Struktura glykanů je v genomu kódována nepřímo

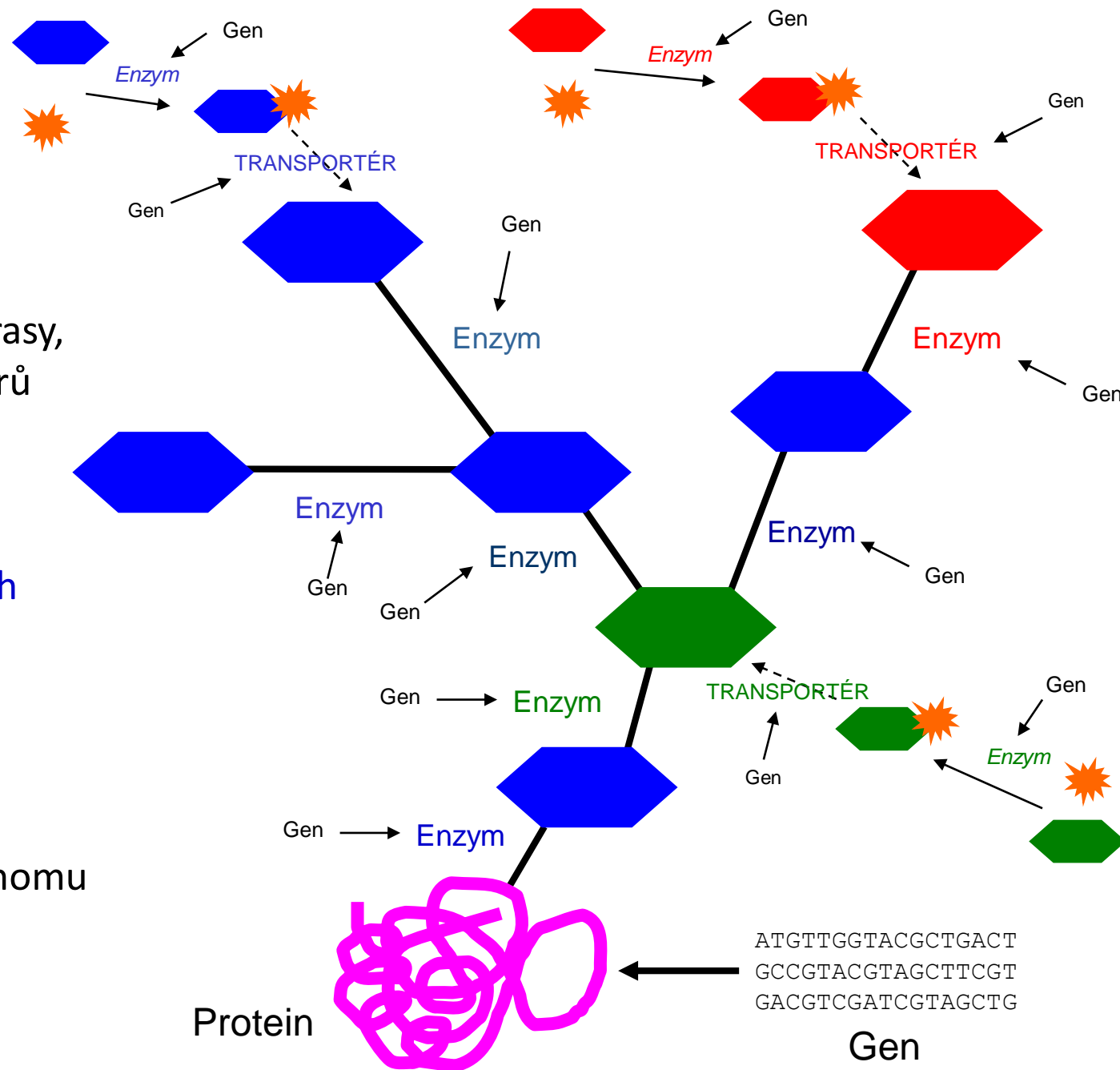
```
ATGTTGGTACGCTGACT  
GCCGTACGTAGCTTCGT  
GACGTCGATCGTAGCTG
```

Gen

Enzymy = glykosyltransferasy,  
syntéza aktivovaných cukrů

Nutná účast transportních  
proteinů!

Struktura glykanů je v genomu  
kódována nepřímo

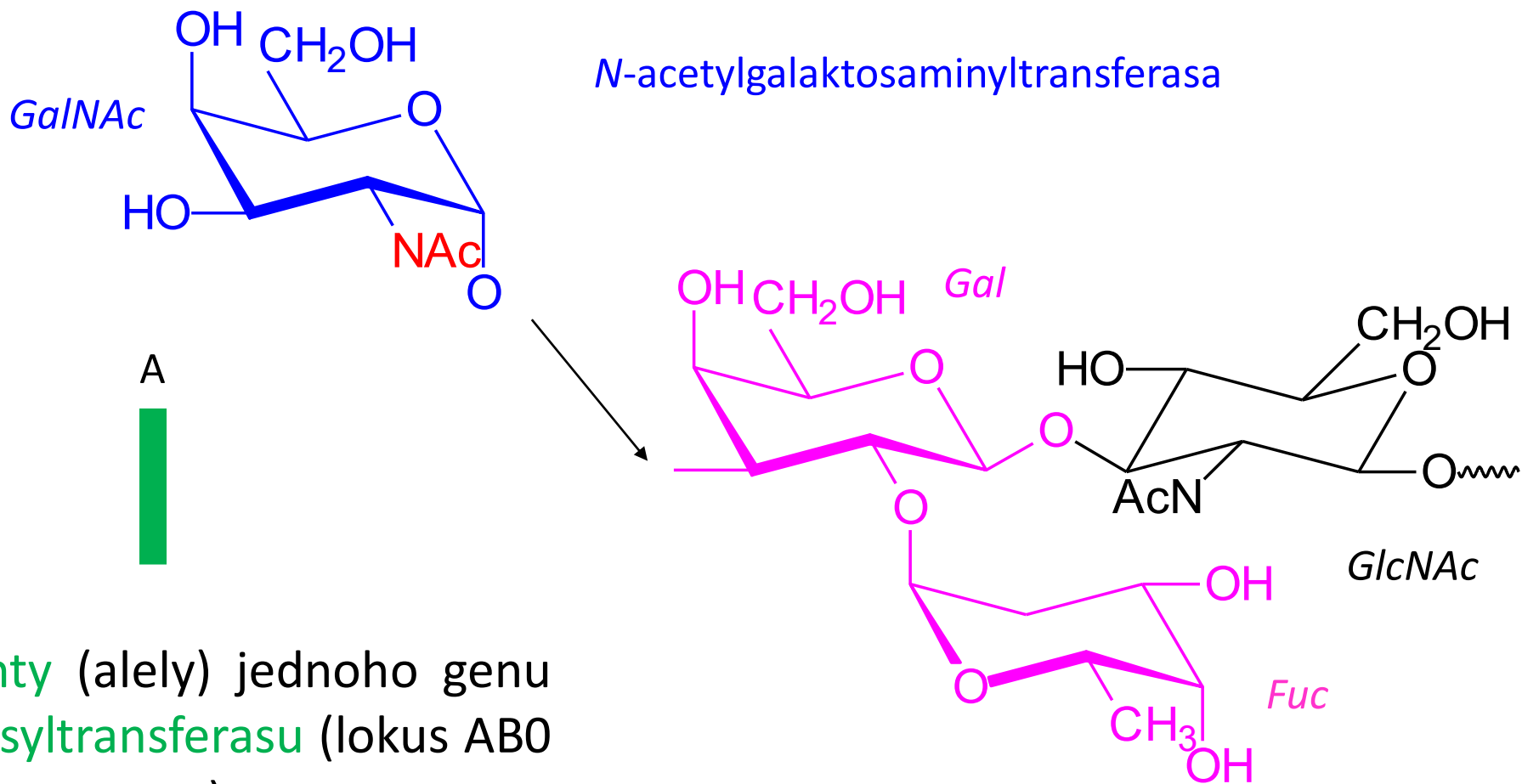


Protein

Gen

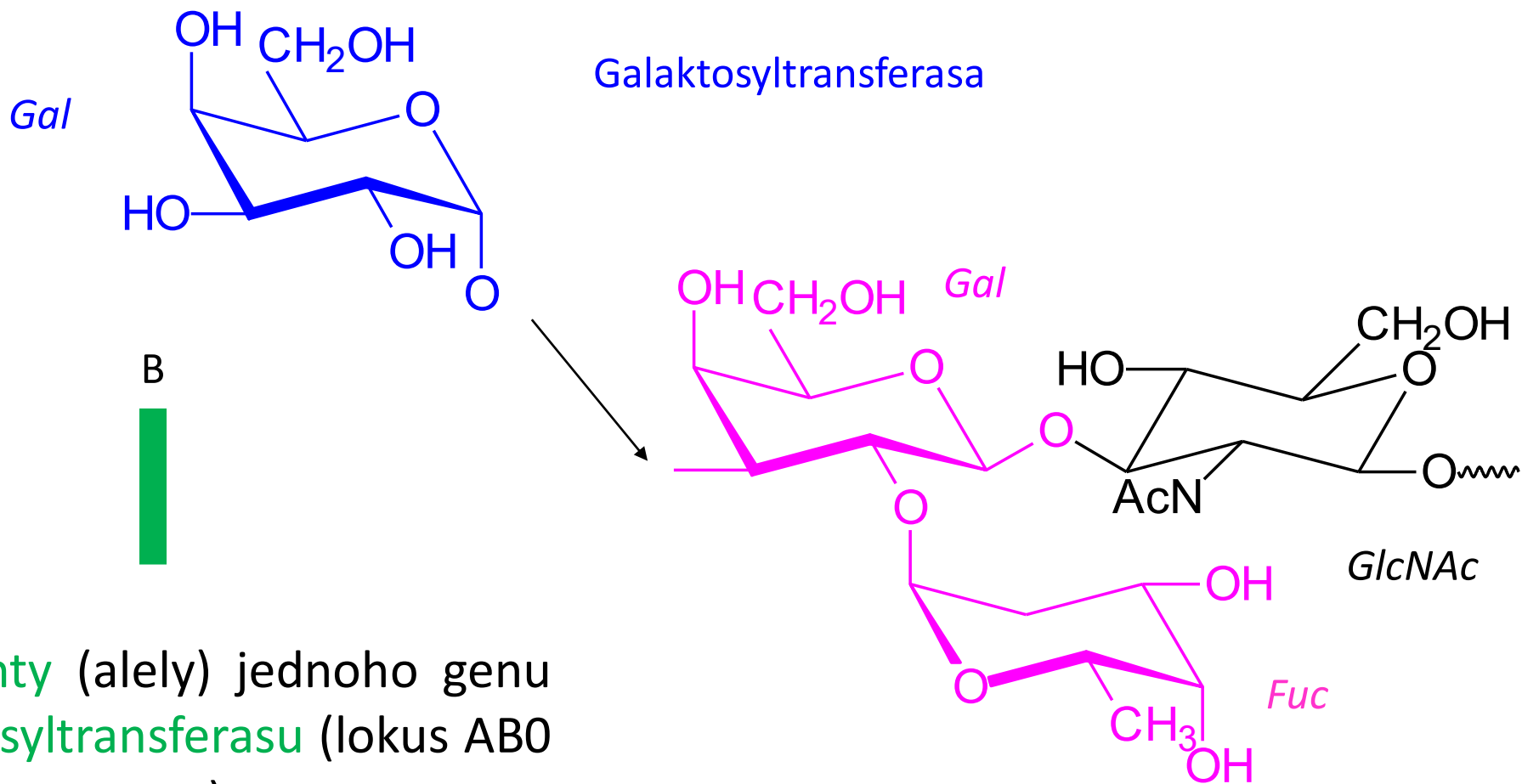
```
ATGTTGGTACGCTGACT
GCCGTACGTAGCTTCGT
GACGTCGATCGTAGCTG
```

# Dědičnost krevních skupin



Tři varianty (alely) jednoho genu pro glykosyltransferasu (lokus ABO na 9. chromozomu)

# Dědičnost krevních skupin



Tři varianty (alely) jednoho genu pro glykosyltransferasu (lokus ABO na 9. chromozomu)

**Abstract** The majority of all proteins are glycosylated and glycans have numerous important structural, functional and regulatory roles in various physiological processes. While structure of the polypeptide part of a glycoprotein is defined by the sequence of nucleotides in the corresponding gene, structure of a glycan part results from dynamic interactions between hundreds of genes, their protein products and environmental factors. The composition of the glycome attached to an individual protein, or to a complex mixture of proteins, like human plasma, is stable within an individual, but very variable between individuals. This variability stems from numerous common genetic polymorphisms reflecting in changes in the complex biosynthetic pathway of glycans, but also from the interaction with the environment. Environment can affect glycan biosynthesis at the level of substrate availability, regulation of enzyme activity and/or hormonal signals, but also through gene-environment interactions. Epigenetics provides a molecular basis how the environment can modify phenotype of an individual. The epigenetic in formation (DNA methylation pattern and histone code) is especially vulnerable to environmental effects in the

early intrauterine and neo-natal development and many common late-onset diseases take root already at that time. The evidences showing the link between epigenetics and glycosylation are accumulating. Recent progress in high-throughput glycomics, genomics and epigenomics enabled first epidemiological and genome-wide association studies of the glycome, which are presented in this mini-review.

**Keywords** Glycosylation · Glycome · Genome-wide association study · Epigenetics · Gene-environment interactions

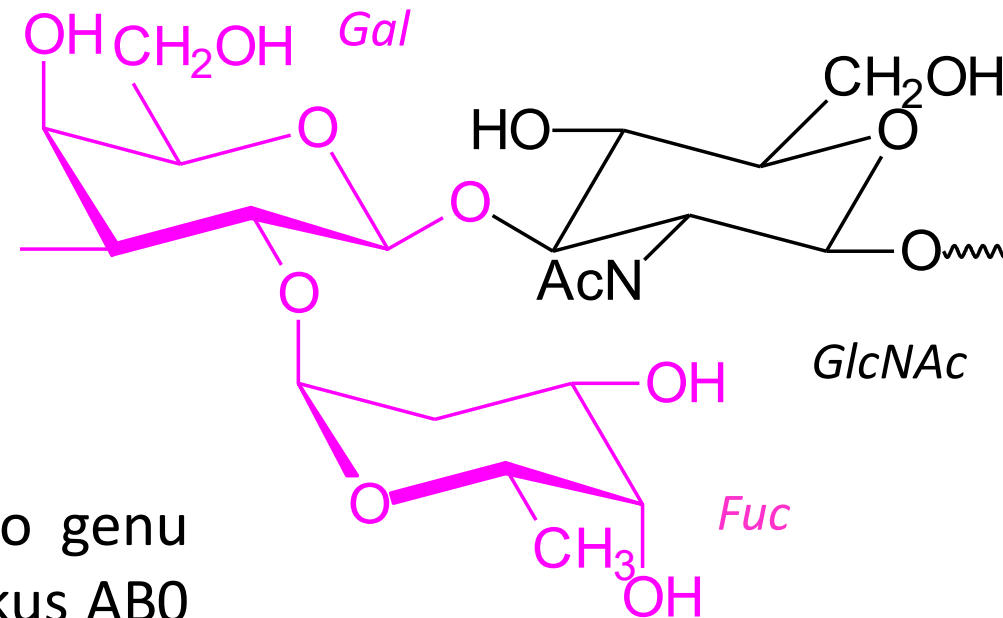
**Genetics of protein glycosylation is very complex**

According to the central dogma of molecular biology, function of each protein is determined by its structure, which is defined by the nucleotide sequence in the corresponding gene. However, in the case of glycan moieties of glycoproteins, there are several additional layers of complexity between genes and the final glycan structure. The final structure of each glycan is therefore not encoded directly in the genome

# Dědičnost krevních skupin

Zkrácená (nefunkční) varianta genu, způsobeno delecí jednoho nukleotidu a následným posunutím čtecího rámce

0  

Tři varianty (alely) jednoho genu pro glykosyltransferasu (lokus ABO na 9. chromozomu)



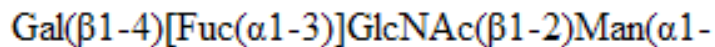
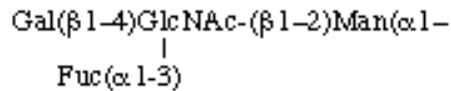
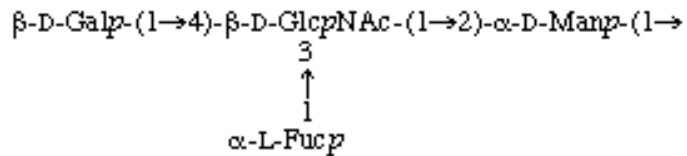
# Cukry – zkratky a symboly

- Základní jednotky složitějších sacharidů jsou **monosacharidy**.
- NA/proteiny – základní jednotky (nukleotidy, aminokyseliny) jsou jasně definovány a jejich počet není velký.
- Monosacharidů je **mnoho**, proto u glykanů nelze (jednoduše) použít jednopísmenný kód. Problém: **vazby, větvení, modifikace**
- Vyvinuto a používáno mnoho způsobů, jak sacharidy znázornit.
- Na rozdíl od NA/proteinů se u cukrů velmi často využívá **grafické znázornění**.

# Cukry – zkratky a symboly

UNION OF PURE AND APPLIED CHEMISTRY

<https://www.qmul.ac.uk/sbcs/iupac/2carb/>



- Tři IUPAC způsoby jak pomocí zkratk znázornit oligosacharid.

Linear	<b>IUPAC</b>	{ $\alpha\text{-D-GalpNAc-(1}\rightarrow\text{3)-}[\alpha\text{-L-Fucp-(1}\rightarrow\text{2)]-}\beta\text{-D-Galp-(1}\rightarrow\text{4)-}\beta\text{-D-GlcpNAc-(1}\rightarrow\text{3)-}\beta\text{-D-Galp-(1}\rightarrow\text{4)-}\beta\text{-D-Glcp}$ }																								
	<b>LINUCS</b>	[][ $\beta\text{-D-Glcp}$ ]{[( $4+1$ )] $\beta\text{-D-Galp}$ }{[( $3+1$ )] $\beta\text{-D-GlcpNAc}$ }{[( $4+1$ )] $\beta\text{-D-Galp}$ }{[( $2+1$ )] $\alpha\text{-L-Fucp}$ }{[( $3+1$ )] $\alpha\text{-D-GalpNAc}$ }{}}																								
	<b>LinearCode</b>	ANa3 (Fa2) Ab4 GNb3 Ab4 Gb4 (spaces added for clarity)																								
	<b>GLYCAM</b>	0LN (0fA) ZLB 4Gn 3LB 4GB (with LinearCode precedence rules for branching)																								
Graphical	<b>CFG</b>																									
	<b>Oxford</b>																									
	<b>GLYCAM/Oxford</b>																									
		<table border="0"> <thead> <tr> <th></th> <th>CFG</th> <th>Oxford</th> <th>GLYCAM</th> </tr> </thead> <tbody> <tr> <td>D-Galp</td> <td></td> <td></td> <td>L</td> </tr> <tr> <td>D-GalpNAc</td> <td></td> <td></td> <td>LN</td> </tr> <tr> <td>D-Glcp</td> <td></td> <td></td> <td>G</td> </tr> <tr> <td>D-GlcpNAc</td> <td></td> <td></td> <td>GN</td> </tr> <tr> <td>L-Fucp</td> <td></td> <td></td> <td>f</td> </tr> </tbody> </table> <p>Oxford-type linkage:</p> <p> <math>\alpha</math>-linkage</p> <p> <math>\beta</math>-linkage</p>		CFG	Oxford	GLYCAM	D-Galp			L	D-GalpNAc			LN	D-Glcp			G	D-GlcpNAc			GN	L-Fucp			f
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D-Glcp			G																							
D-GlcpNAc			GN																							
L-Fucp			f																							

# Cukry – zkratky a symboly

## Standardizace symbolů:

## Symbol Nomenclature for Glycans (SNFG)

<https://www.ncbi.nlm.nih.gov/glycans/snfg.html>

SHAPE	White (Generic)	Blue	Green	Yellow	Orange	Pink	Purple	Light Blue	Brown	Red
Filled Circle	Hexose	Glc	Man	Gal	Gul	Alt	All	Tal	Ido	
Filled Square	HexNAc	GlcNAc	ManNAc	GalNAc	GulNAc	AltNAc	AllNAc	TalNAc	IdoNAc	
Crossed Square	Hexosamine	GlcN	ManN	GalN	GulN	AltN	AllN	TalN	IdoN	
Divided Diamond	Hexuronate	GlcA	ManA	GalA	GulA	AltA	AllA	TalA	IdoA	
Filled Triangle	Deoxyhexose	Qui	Rha		6dGul	6dAlt		6dTal		Fuc
Divided Triangle	DeoxyhexNAc	QuiNAc	RhaNAc			6dAltNAc		6dTalNAc		FucNAc
Flat Rectangle	Di-deoxyhexose	Oli	Tyv		Abe	Par	Dig	Col		
Filled Star	Pentose		Ara	Lyx	Xyl	Rib				
Filled Diamond	Deoxynonulosonate		Kdn				Neu5Ac	Neu5Gc	Neu	Sia
Flat Diamond	Di-deoxynonulosonate		Pse	Leg		Aci		4eLeg		
Flat Hexagon	Unknwnr									
Pentagon	Assigned									

Symboly pro jednotlivé monosacharidy. Vzhledem k počtu monosacharidů je nutné využívat různé **barvy i tvary**.

Linear	IUPAC	$\{\alpha\text{-D-GalpNAc-(1}\rightarrow\text{3)-}[\alpha\text{-L-Fucp-(1}\rightarrow\text{2)]-}\beta\text{-D-Galp-(1}\rightarrow\text{4)-}\beta\text{-D-GlcpNAc-(1}\rightarrow\text{3)-}\beta\text{-D-Galp-(1}\rightarrow\text{4)-}\beta\text{-D-Glcp}\}$																								
	LINUCS	$[[[b\text{-D-Glcp}]\{[(4+1)][b\text{-D-Galp}]\{[(3+1)][b\text{-D-GlcpNAc}]\{[(4+1)][b\text{-D-Galp}]\{[(2+1)][a\text{-L-Fucp}]\}\{[(3+1)][a\text{-D-GalpNAc}]\}\}\}\}\{]]]$																								
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# Cukry – zkratky a symboly

## Standardizace symbolů:

## Symbol Nomenclature for Glycans (SNFG)



<https://www.ncbi.nlm.nih.gov/glycans/snfg.html>

Významná část glykobiinformatických nástrojů je zaměřená na grafické znázornění cukrů.

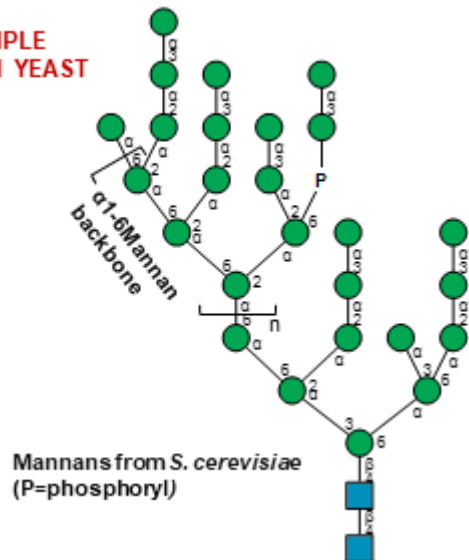
## Symbol Nomenclature for Glycans (SNFG)

Standardization in drawing glycan structures is essential for efficient communication. The tools and methodology illustrated here have become widely accepted by the scientific community. Use of these symbols to represent monosaccharides is now strongly recommended for all manuscripts submitted to major journals and other publications.

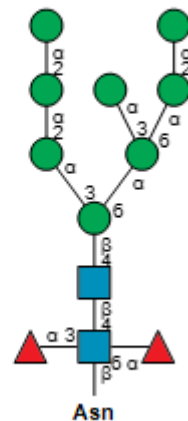
### Citation:

- Symbol Nomenclature for Graphical Representation of Glycans, *Glycobiology* 25: 1323-1324, 2015. [Citation link](#)  (PMID 26543186).
- Updates to the Symbol Nomenclature for Glycans guidelines, *Glycobiology* 29:620-624, 2019. [Citation link](#)  (PMID 31184695).

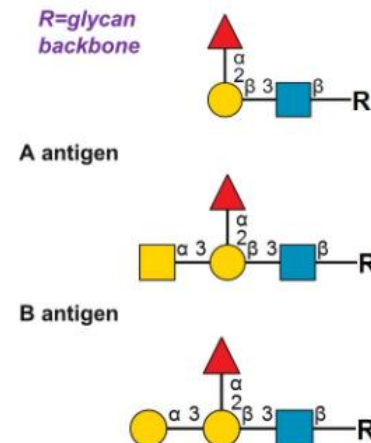
### EXAMPLE FROM YEAST



### EXAMPLES FROM SLIME MOLD

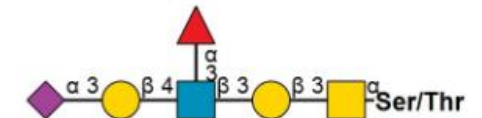


### Blood group antigens: H antigen on Type-1 lactosamine chain

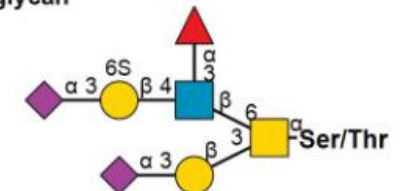


### O-linked glycans (GalNAc type)

#### Extended core-1 glycan



#### 6'sulfo-sialyl Lewis-X on core-2 glycan



# Cukry – zobrazovací nástroje



## DrawGlycan-SNFG

Render glycans and glycopeptides with fragmentation info. using the Symbolic Nomenclature for Glycans [SNFG]

<http://www.virtualglycome.org/DrawGlycan/>

IUPAC-condensed Input (glycan or glycopeptide):

Man(a2)Man(a6)[Man(a2)Man(a3)]Man(a6)Gal(a3)Fuc(a6)Man(a2)Man(a6)  
[Man(a2)Man(a3)]Man(a6)Gal(a3)

### Basic options:

Display Linkage:  ON Linkage font size:  Text font size:

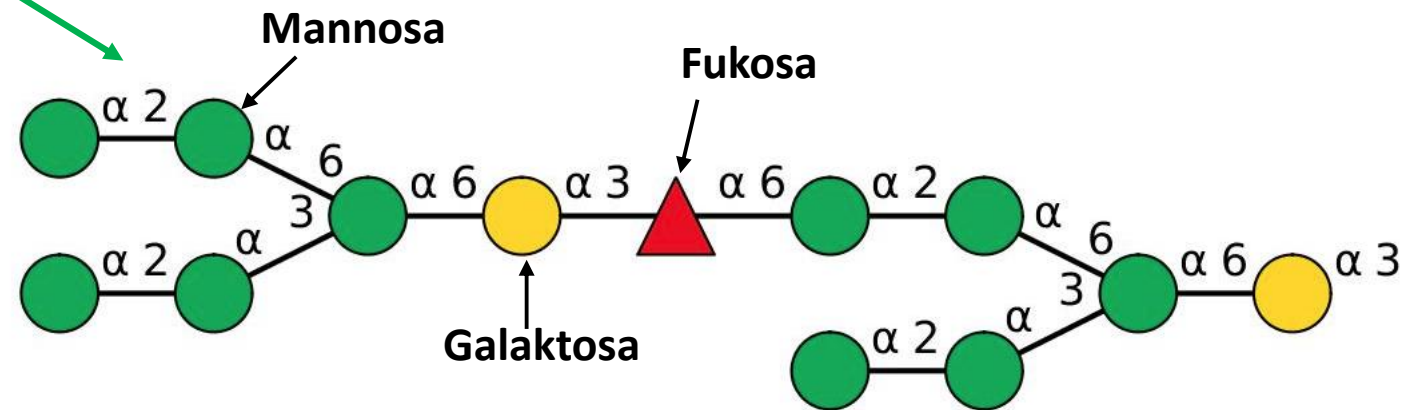
Symbol Size:  Orientation:

Other options (show/hide)

Mass Option:  Adduct:

Draw

Molecular Weight: 2254.7562








# Cukry – zobrazovací nástroje

The screenshot shows the SugarSketcher interface. At the top, there is a toolbar with icons for different sugars: Hex (white), Glc (blue), Man (green), Gal (yellow), Gul (orange), Alt (pink), All (purple), Tal (light blue), and Ido (brown). Below the toolbar is a large drawing area containing a glycan structure with green circles and blue squares connected by dashed lines. The structure includes labels like  $\alpha 1,6$ ,  $\alpha 1,5$ ,  $\beta 1,4$ , and  $\alpha 2,3$ . Below the drawing area is a toolbar with buttons numbered 1 through 6, with a question mark button circled in red. At the bottom, there are buttons for "Load Structure", "Toggle Quick Mode", and "GlycoCT/SVG".

The screenshot shows the SugarSketcher interface with a dropdown menu open. The menu lists various glycan symbols: ncorebisect, ncorebisectfuc, ncorehyb, ncorehybfuc, ncorehybbis, ncorehybbisfuc, ncoreman (highlighted), ocore1, ocore2, ocore3, ocore4, ocore5, ocore6, ocore7, ocore8, gslarthro, gslgala, gslganglio, gslglobo, gslisoglobo, and ncoreman. Below the menu is a "Submit" button. To the right of the menu is a glycan structure with green circles and blue squares connected by dashed lines. The structure includes labels like  $\alpha 1,6$ ,  $\alpha 1,3$ ,  $\alpha 1,6$ ,  $\beta 1,4$ ,  $\beta 1,4$ ,  $\beta 1,4$ ,  $\beta 1,?$ , and  $\alpha 1,2$ . At the top, there are buttons for "Add Node", "Repeat Unit", and "Update Node". At the bottom, there are buttons for "Toggle Quick Mode" and "GlycoCT/SVG".

Technical Note

## SugarSketcher: Quick and Intuitive Online Glycan Drawing

Davide Alocci <sup>1,2</sup>, Pavla Suchánková <sup>3,4</sup>, Renaud Costa <sup>5</sup>, Nicolas Hory <sup>5</sup>, Julien Mariethoz <sup>1,2</sup> ,  
Radka Svobodová Vařeková <sup>3,4</sup>, Philip Toukach <sup>6</sup>  and Frédérique Lisacek <sup>1,2,7,\*</sup> 

<https://glycoproteome.expasy.org/sugarsketcher/>

# Glykosylace

- **Glykosylace** je významná posttranslační modifikace.
- Ovlivňuje **strukturu** proteinů, jejich **aktivitu** i **funkci** (rozpustnost, stabilita, interakce, význam pro **imunitní systém**).
- Glykosylace probíhá u eukaryot i **prokaryot**.

A Repository of Experimentally Characterized Glycoproteins and Protein Glycosyltransferases of Prokaryotes



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<http://www.proglycprot.org/>

**ProGlycProt**  
*Protein Glycosylation in Prokaryotes*

## Sweet new world: glycoproteins in bacterial pathogens

M. Alexander Schmidt<sup>1</sup>, Lee W. Riley<sup>2</sup> and Inga Benz<sup>1</sup>

<sup>1</sup>Institut für Infektiologie, Zentrum für Molekularbiologie der Entzündung (ZMBE), Von-Esmarch-Str. 56, D-48149 Münster, Germany

<sup>2</sup>Division of Infectious Diseases and Immunity, School of Public Health, University of California, 140 Warren Hall, Berkeley, CA 94720, USA

In eukaryotes, the combinatorial potential of carbohydrates is used for the modulation of protein function. However, despite the wealth of cell wall and surface-associated carbohydrates and glycoconjugates, the accepted dogma has been that prokaryotes are not able to glycosylate proteins. This has now changed and protein glycosylation in prokaryotes is an accepted fact. Intriguingly, in Gram-negative bacteria most glycoproteins are associated with virulence factors of medically significant pathogens. Also, important steps in pathogenesis have been linked to the glycan substitution of surface proteins, indicating that the glycosylation of bacterial proteins might serve specific functions in infection and pathogenesis and interfere with inflammatory immune responses. Therefore, the carbohydrate modifications and glycosylation pathways of bacterial proteins will become new targets for therapeutic and prophylactic measures. Here we discuss recent findings on the structure, genetics and function of glycoproteins of medically important bacteria and potential applications of bacterial glycosylation systems for the generation of novel glycoconjugates.

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ProGP ID	ProGP470 (Putative uncharacterized protein)
Validation Status	Characterized
Organism Information	
Organism Name	Burkholderia cenocepacia K56-2
Domain	Bacteria
Classification	Family: Burkholderiaceae Order: Burkholderiales Class: Betaproteobacteria Division or phylum: "Proteobacteria"
Taxonomic ID (NCBI)	985075
Protein Information	
Protein Name	Putative uncharacterized protein
UniProtKB/SwissProt ID	B4EB72
NCBI RefSeq	WP_006486887.1.
EMBL-CDS	CAR53291.1.
UniProtKB Sequence	>tr B4EB72 B4EB72_BURCJ Putative exported protein OS=Burkholderia cenocepacia (strain ATCC BAA-245 / DSM 16553 / LMG 16656 / NCTC 13227 / J2315 / CF5610) GN=BCAL2973 PE=4 SV=1 MKSLVQAVVVAALVAPVVSFAQSGSTITRAQVRAELVQLQQAGYNSARGEDPHYPEAIQ AATARIAEQQRSALAQAGADVSGYGAQAQASASGSRAMGVRPASAEMKSLYRGS
Sequence length	117 AA
Subcellular Location	Outer membrane
Glycosylation Status	
Glycosylation Type	O- (Ser/Thr) linked
Experimentally Validated Glycosite(s) in Full Length Protein	S106
Glycosite(s) Annotated Protein Sequence	>tr B4EB72 B4EB72_BURCJ Putative exported protein OS=Burkholderia cenocepacia (strain ATCC BAA-245 / DSM 16553 / LMG 16656 / NCTC 13227 / J2315 / CF5610) GN=BCAL2973 PE=4 SV=1 MKSLVQAVVVAALVAPVVSFAQSGSTITRAQVRAELVQLQQAGYNSARGEDPHYPEAIQ AATARIAEQQRSALAQAGADVSGYGAQAQASASGSRAMGVRPASA*(106)AEMKSLYRGS
Sequence Around Glycosites (21 AA)	GSRAMGVRPASAEMKSLYRG
Technique(s) used for Glycosylation Detection	ZIC-HILIC, immunoblotting, tryptic digestion, and MS/MS analysis
Technique(s) used for Glycosylated Residue(s) Detection	MS/MS analysis
Glycan Information	
Glycan Annotation	Trisaccharide HexNAc-HexNAc-Hex.
BCSDB ID	12058
GlyTouCan	G71937MV

<http://www.proglycprot.org/>

**ProGlycProt**  
Protein Glycosylation in Prokaryotes

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Organism Information	
Organism Name	Campylobacter jejuni subsp. jejuni serotype O:2 (strain ATCC 700819 / NCTC 11168)
Clinical Implication	Pathogenic
Domain	Bacteria
Phylum	Proteobacteria
Classification	Family: Campylobacteraceae Order: Campylobacterales Class: Epsilonproteobacteria Division or phylum: "Proteobacteria"
Taxonomic ID (NCBI)	192222
Protein information	
Protein Name	PglB
UniProtKB/ SwissProt ID	Q0P9C8
NCBI Ref Seq	YP_002344519.1
UniProtKB Sequence	>sp Q0P9C8 PGLB_CAMJE Undecaprenyl-diphosphooligosaccharide--protein glycotransferase OS=Campylobacter jejuni subsp. jejuni serotype O:2 (strain ATCC 700819 / NCTC 11168) GN=pglB PE=1 SV=1 MLKKEYLKNPYLVLFAMIVLAYVFSVFCRFYWWWASEFNFFNNQLMISNDGYAFAE GARDMIAGFHQPNDLSYGGSSLSTLTWLYKITPFSFESIILYMSTFLSSLVPIILLA NEYKRPLMGFVAALLASVANSYYNRTMSGYYDTMLVIVLPMFILFFMVRMILKKDFFSL IALPLFIGIYLWWYSSYTLNVALIGLFLIYTLIFHRKEKIFIVAVILSSLTLSNIAWFY QSAIIVILFALFALEQKRLNFMIIIGLGSATLIFLILSGGVDPIYLQKFIYFRSDESAN LTQGFMYFNVNQTIQEVENVDFSEFMRRISGSEIVFLFSLFGFVWLLRKHKSMIMALPIL VLGFLALKGGLRFTIYSVPVMALGFGFLLSEFKAILVKKYSQLTSNVCIVFATILTAPV FIHIYNYKAPTVFSQNEASLLNQLKNIANREDYVVTWWDYGYPVRYSDVKTLVDGGKHL GKDNFFPFSLSKDEQAAANMARLSVEYTEKSFYAPQNDILKSDILQAMMKDYNQSNVDL FLASLSKPDFKIDTPKTRDIYLYMPARMSLIFSTVASFNFILDTGVLDKPFSTAYPL DVKNGEILSNGVWLSDDFRSFKIGDNVSVNSIVEINSIKQGEYKITPIDDKAQFYIFY LKDSAIPYAQFILMDKTMFNSAYVQMFFLGNVDKDLVINSRDAKVFKLKI
EMBL CDS	CAL35243.1
Sequence length	713 AA
Subcellular Location	Membrane (Integral component of membrane)
Function in Native Organism	1) The PglB is OSTase which transfer an heptasaccharide to N of D/E-N-X-T/S consensus sequence of the protein in Campylobacter jejuni.
String	192222.Cj1126c.
Potential Application	1) PglB can be used to create artificial glycopeptides because it has relaxed substrate specificity of accepting peptide substrates over the full-length protein. 2) PglB can transfer undecaprenyl pyrophosphate-linked saccharides of various lengths (277 saccharides) adds to the promise of using PglB in the synthesis of diverse glycopeptide products.
Additional Information	1) PglB requires an acetamido group at the C-2. 2) R331 of C.lari and R328 of C.jejuni form a salt bridge with acidic amino acid. 3) PglB can transfer several structurally different O-antigen saccharides to protein.



# Glykosylace

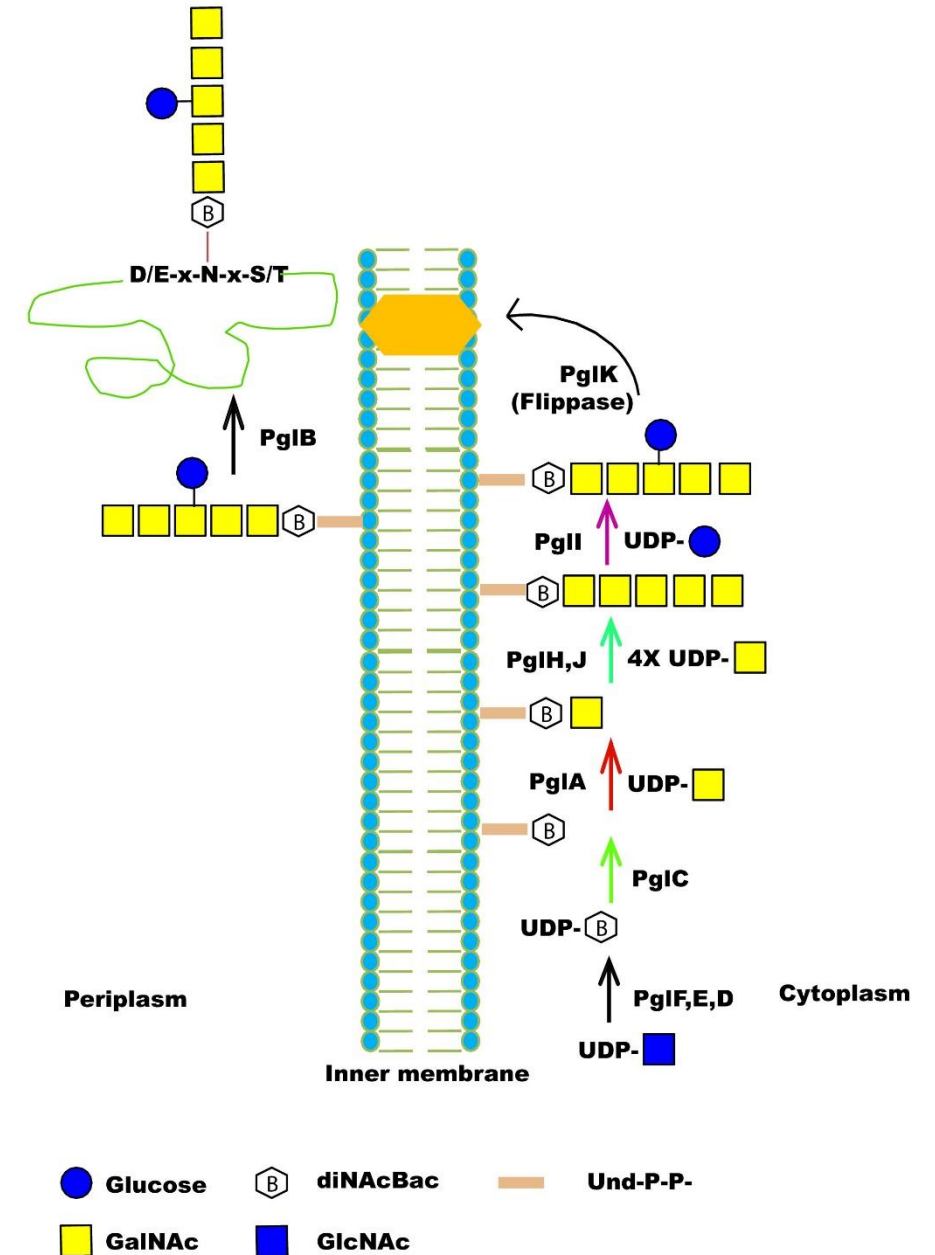
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Glycosyltransferases Database

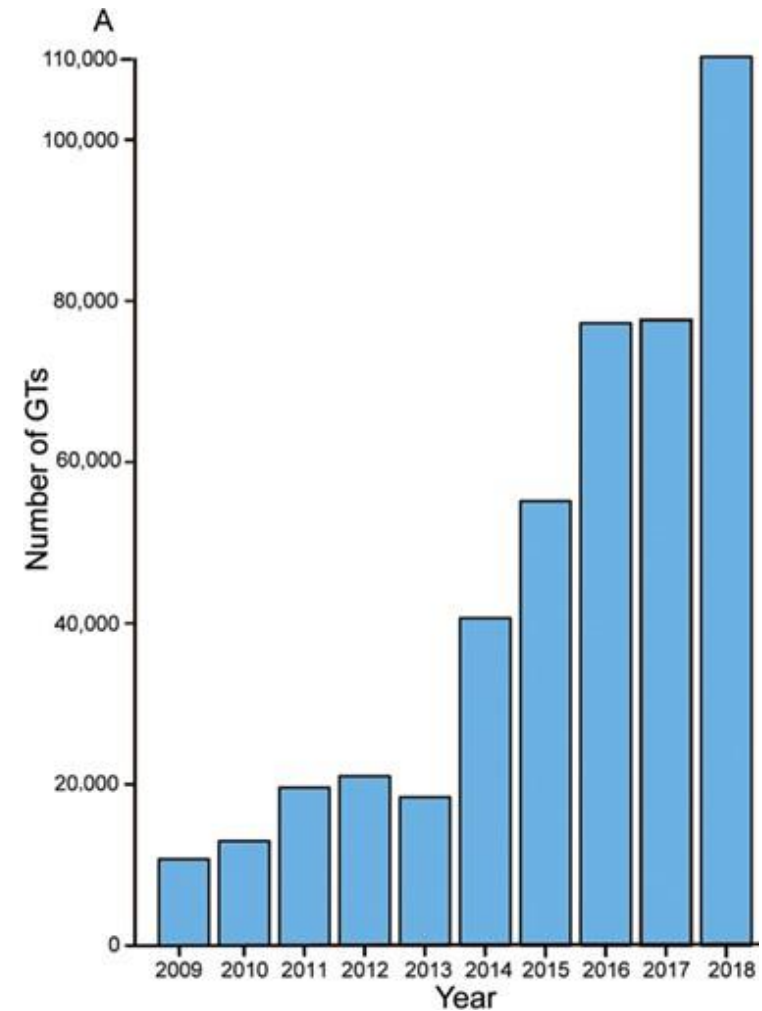
Ⓞ GTDB is an integrated repository of glycosyltransferases, which collects comprehensive information, including amino acid sequences, coding region sequences, available tertiary structures, protein classification families, catalytic reactions and metabolic pathways involved, from distinct well-known databases or predictions.

Ⓞ Search—advanced search provides various queries to specify users' concerns accurately.

Ⓞ Browse—browse data by diverse classifications and download those data in batches.

Ⓞ BLAST—sequence search of GTDB to annotate query glycosyltransferases' functions.

Ⓞ GTdock—performs several glycosyltransferases docking with the same one acceptor easily by AutoDock Vina.



Archaea (8985)  Eukaryota (49594)  Bacteria (457667)  Viruses (2497)  Unclassified (1436)  All (520179)

# Predikce glykosylace

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## NetCGlyc - 1.0

### C-mannosylation sites in mammalian proteins

The NetCGlyc 1.0 produces neural network predictions of C-mannosylation sites in mammalian proteins.

## NetNGlyc - 1.0

### N-linked glycosylation sites in human proteins

The NetNGlyc server predicts N-Glycosylation sites in human proteins using artificial neural networks that examine the sequence context of Asn-Xaa-Ser/Thr sequons.

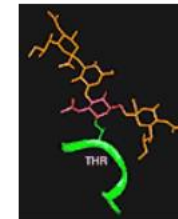
## NetOGlyc - 4.0

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

The NetOGlyc server produces neural network predictions of mucin type GalNAc O-glycosylation sites in mammalian proteins.

## DictyOGlyc - 1.1

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



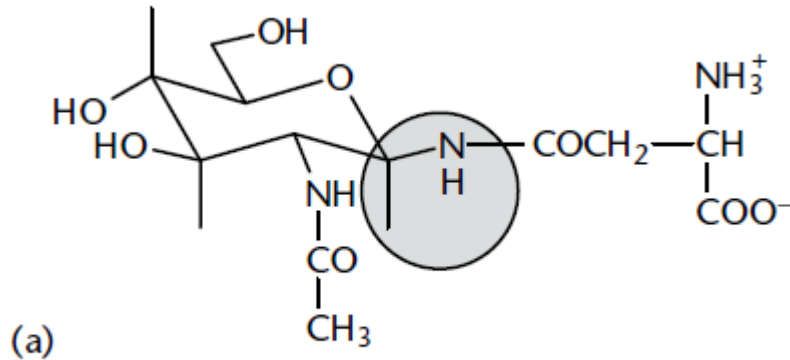
The DictyOGlyc server produces neural network predictions for GlcNAc O-glycosylation sites in *Dictyostelium discoideum* proteins.

## MINI REVIEW

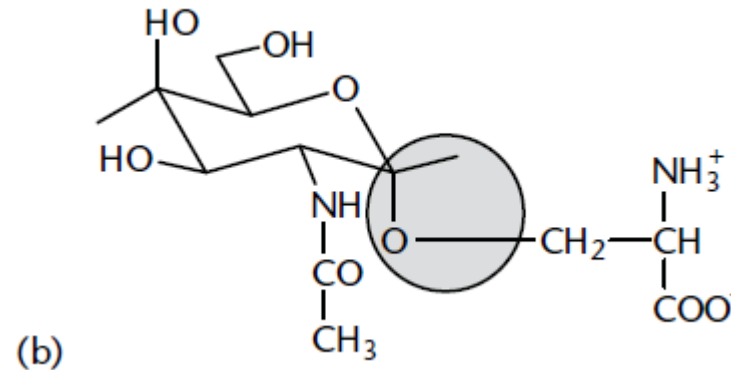
**Protein glycosylation: nature, distribution, enzymatic formation, and disease implications of glycopeptide bonds**

# Predikce glykosylace

- Predikce glykosylace: N-glykosylace x O-glykosylace



N-glykosylace aminoskupiny **asparaginu**



O-glykosylace hydroxylové skupiny **serinu nebo threoninu**

## Glycoproteins

Tony Merry, *University of Manchester, Manchester, UK*

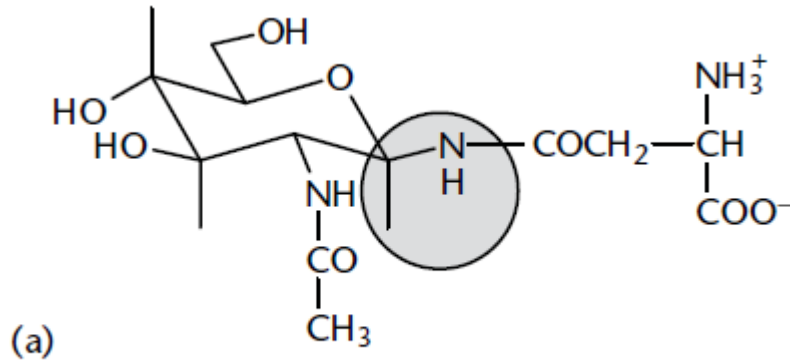
Sviatlana Astrautsova, *Grodno State Medical University, Grodno, Belarus*

*Based in part on the previous version of this Encyclopedia of Life Sciences (ELS) article, "Glycoproteins" by "Terry D Butters".*

Glykosylace chrání proteiny před proteolýzou, ovlivňuje strukturu a interakce proteinů, uplatňuje se v interakcích imunitního systému.

# Predikce glykosylace

- Predikce glykosylace: *N*-glykosylace x *O*-glykosylace

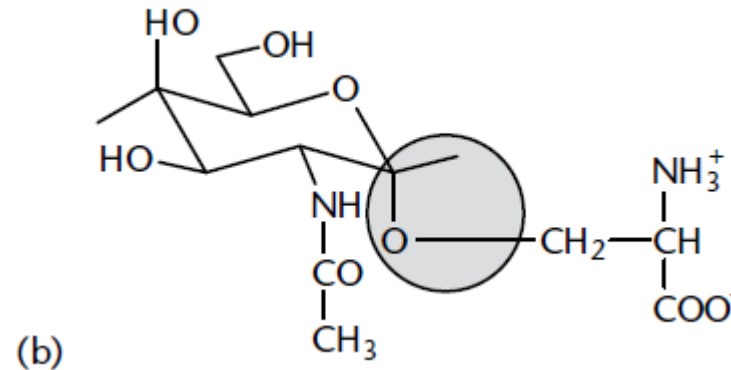


*N*-glykosylace aminoskupiny **asparaginu**

**Asn-X-Ser(Thr)**, X nesmí být Pro

Asn-X-C – nekanonický motiv

Záleží i na sousedních aminokyselinách,  
charakteru aminokyseliny „X“,  
konformaci místa.

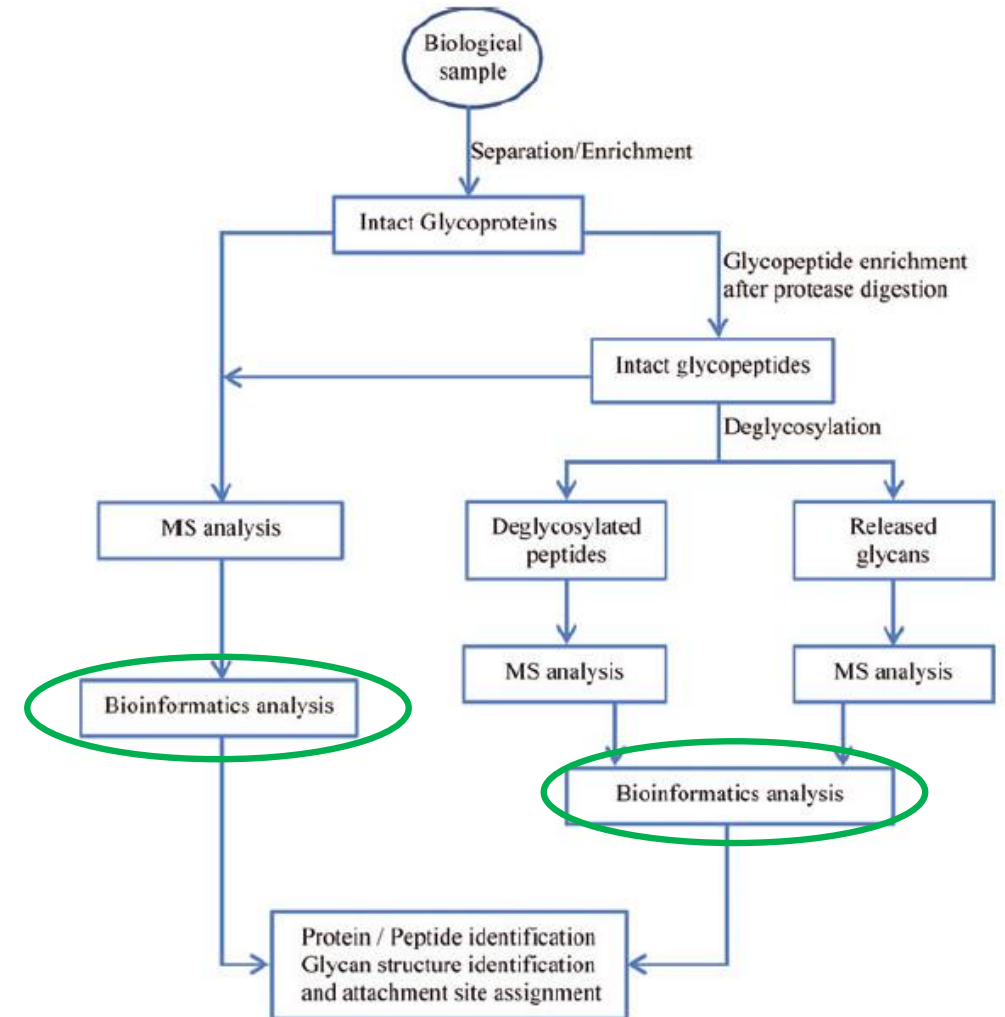
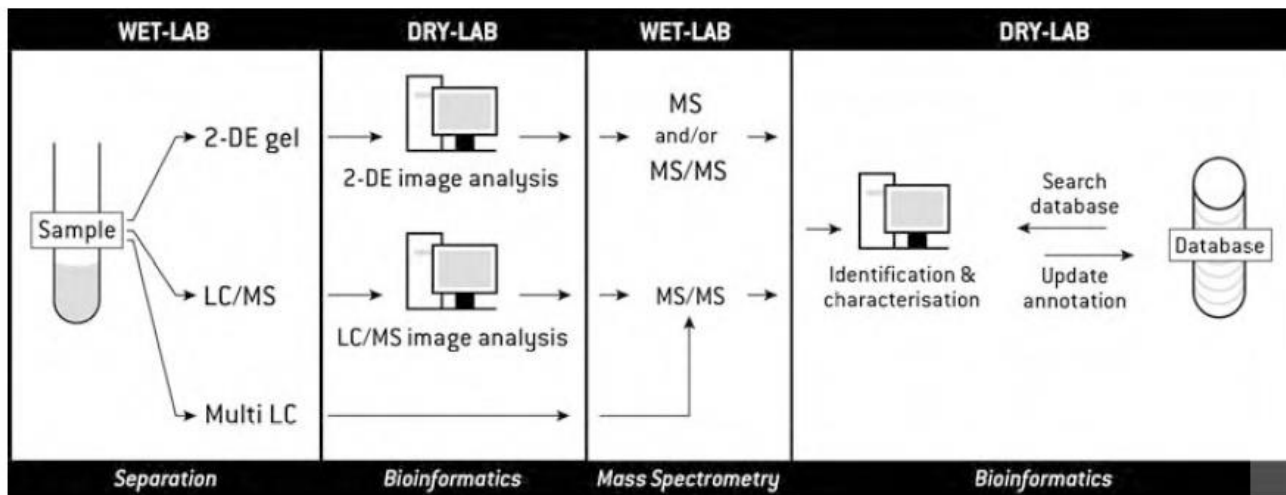


*O*-glykosylace hydroxylové skupiny  
**serinu nebo threoninu**

Nemají jasně definovaný motiv

# Analýza glykanů

- Charakterizace glykanů: hmotnostní spektroskopie (**MS**), vysokoučinná kapalinová chromatografie (**HPLC**), nukleární magnetická rezonance (**NMR**).
- Velká část softwarových nástrojů je zaměřena na zpracování a interpretaci experimentálních dat, **analýza glykanů je bez využití bioinformatiky velmi obtížná (prakticky nemožná)...**





https://web.expasy.org/glycomod/

GlycoMod Tool

GlycoMod is a tool that can predict the possible oligosaccharide structures that occur on proteins from their experimentally determined masses. The program can be used for free or derivatized oligosaccharides and for glycopeptides [Documentation / Mass values / Reference / Disclaimer].

Note: You can use GlycanMass to calculate the mass of an oligosaccharide structure from its oligosaccharide composition.

Enter a list of experimental masses:

1041.72 1080.03 1093.73  
1101.62 1111.77 1142.07  
1153.01 1157.91 1192.88  
1230.23 1274.33 1286.18  
1356.47 1371.45 1386.38  
1418.45 1430.67 1485.42

All mass values are  
 average or  monoisotopic.

Or upload a file, containing one mass per line, from your computer:

Soubor nevybrán

Mass tolerance: +/-  Dalton

```
>pdb|1TKA|A Chain A, 1 Transketolase
QFTDIDKLA VSTIRILAVDTVSKANS GHPGAPLGMAPAAHV LWSQMRMNPTNPDWINRDRFVLSNGHAVA
LLYSMLHLTGYDLSIEDLKQFRQLGSRTPGHPEFELPGVEVTTGPLGQGISNAVGMAMAQANLAATYNKP
GFTLSDNYTYVFLGDGCLQEGISSEASSLAGHLKLG NLI A IYDDNKITIDGATSISFDEDVAKRYEAYGW
EVLYVENGNEDLAGIAKAI AQA KLSKDKPTLIKMTT TIGYGS LHAGSHSVHGAPLKADDVKQLKSKF GFN
PDKSFVVPQEVYDHYQKTI LKPGVEANNKWNKLFSEYQKKFP ELGAELARRLSGQLPANWESKLP TYTAK
DSAVATRKLSETVLEDVYNQLPELIGGSADLTPSNL TRWKEALDFQPPSSSGSGNYSGRYIRYGI REHAMG
AIMNGISAFGANYPYGGTFLNFVSYAAGAVRLSALS GHVPVIWVATHDSIGVGEDGPTHQPIETLAHF RS
LPNIQVWRPADGNEVSAAYKNSLESKHTPSII ALSRQNL PQLGESSIESASKGGYV LQDVANPDIILVAT
GSEVSLSVEAAKTLAAKNIKARVVS LPDFFTFDKQPLEYR LSVLPDNVPI MSVEVLATTCW GKYAHQSFG
IDRFGASGKAPEVFKFFGF TPEGVAERAQKTI AFYKGDKLI SPLKCAF
```

1041.72 1080.03 1093.73 1101.62 1111.77 1142.07  
1153.01 1157.91 1192.88 1230.23 1274.33 1286.18  
1356.47 1371.45 1386.38 1418.45 1430.67 1485.42  
1531.45 1608.79 1628.84 1653.89 1670.17 1688.12  
1708.08 1740.03 1766.29 1790.98 1869.04 1899.45  
1960.28 2028.53 2047.74 2056.13 2105.32 2184.15  
2201.95 2261.71 2316.35 2388.56 2429.00 2446.39  
2457.63 2473.35 2545.02 2553.75 2604.07 2623.41  
2702.62 2718.76 2761.27 2779.97 2805.59 2851.70  
2867.83 2944.29 2975.04 3016.44 3028.57 3045.25  
3113.17 3221.73 3245.86 3268.72 3345.42 3373.80  
3535.19 3852.99 3868.36 3945.84

Peptides containing the motif 'N-X-S/T/C (X not P)':

position	#MC	peptide mass [M]	peptide	modifications
98-174	0	7900.79848	TPGHPEFELPGVEVTTGPLG QGISNAVGMAMAQANLAATY NKP GFTLSDNYTYVFLGDGC LQEGISSEASSLAGHLK	
359-388	0	3245.58768	LSETVLEDVYNQLPELIGGS ADLTPSNL	TR
391-408	0	1868.93408	EALDFQPPSSSGSGNYSGR	

User mass: 2761.27  
Adduct ([M+H]<sup>+</sup>): 1.00727

glycoform mass	Δmass (Dalton)	structure	type	peptide mass [M]	peptide sequence	theoretical glycopeptide mass	mod.	Links
892.281	0.148	(Hex) <sub>1</sub> (NeuAc) <sub>1</sub> (NeuGc) <sub>1</sub> (Pent) <sub>1</sub>	-	1867.834	391-408 EALDFQPPSSSGSGNYSGR	2761.122		
892.317	0.112	(Hex) <sub>3</sub> (HexNAc) <sub>2</sub>	-	1867.834	391-408 EALDFQPPSSSGSGNYSGR	2761.158		GlyConnect

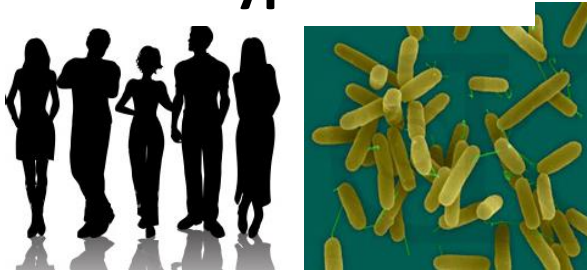
2 structures found in 1 peptide.

# Lektiny

Lektiny jsou proteiny, které vážou sacharidy. Uplatňují se v mnoha adhezivních a rozpoznávacích biologických procesech.



Všudypřítomné



## Vazba sacharidu



Specifická



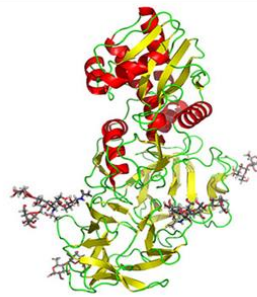
Reverzibilní



Nemodifikující

Plants

Ricin  
(*Ricinus communis*)



Obrana  
Zásobní role

Animals

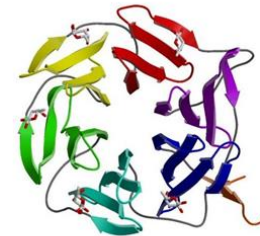
MBP  
(*Homo sapiens*)



Adheze buněk  
Rozpoznávání buněk

Fungi

AAL  
(*Aleuria aurantia*)



Mykorhiza  
Obrana

Bacteria

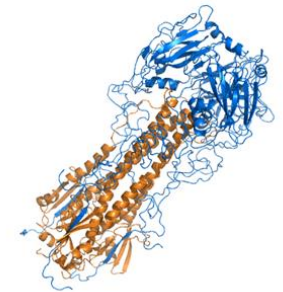
PA-IIL  
(*Pseudomonas aeruginosa*)



Rozpoznání hostitele  
Adheze na povrch hostitele

Viruses

Hemagglutinin  
(*Influenza virus*)



# UniLectin3D curated database

## What is UniLectin3D ?

The UniLectin3D module provides curated information on 3D structures of lectins. Lectins are grouped into families based on the carbohydrate binding domains.

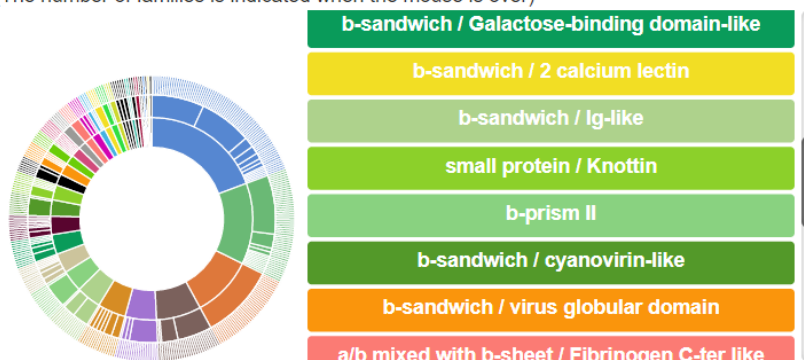
## How many lectins and structures ?

**2369** 3D XRay structures (**1519** with interacting glycan), **572** distinct lectin sequences, **248** distinct glycans, **1025** articles

Last update the 2022-04-13 21:59:35

Browse by Fold > Class > Family

(The number of families is indicated when the mouse is over)



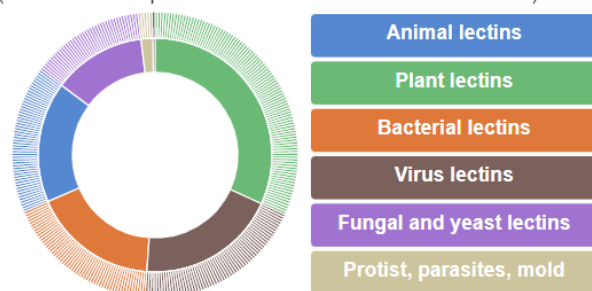
## UniLectin3D, a database of carbohydrate binding proteins with curated information on 3D structures and interacting ligands

François Bonnardei<sup>1,2,3</sup>, Julien Mariethoz<sup>2,3</sup>, Sebastian Salentin<sup>4</sup>, Xavier Robin<sup>5,6</sup>, Michael Schroeder<sup>4</sup>, Serge Perez<sup>7</sup>, Frédérique Lisacek<sup>2,3,8,\*</sup> and Anne Imberty<sup>1,\*</sup>

<https://doi.org/10.1093/nar/gky832>

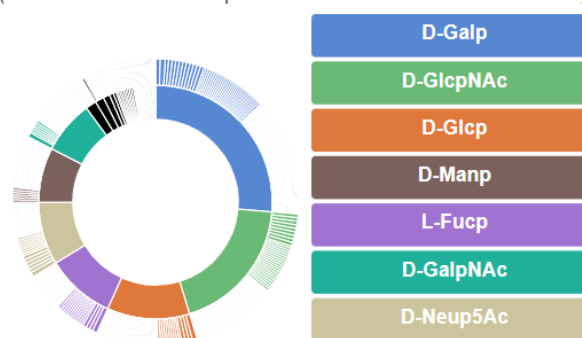
Browse by Origin > Species

(The number of species is indicated when the mouse is over)



Browse by monosaccharide and associate IUPAC sequence

(The number of distinct iupac is indicated when the mouse is over)



<https://www.unilectin.eu/unilectin3D/>

# UniLectin3D curated database

Search for a lectin by name, species, structure and glycan

ie. human, propeller, 1TL2 (PDB accession number), Q47200 (UniProt accession number), GalNAc, Lewis

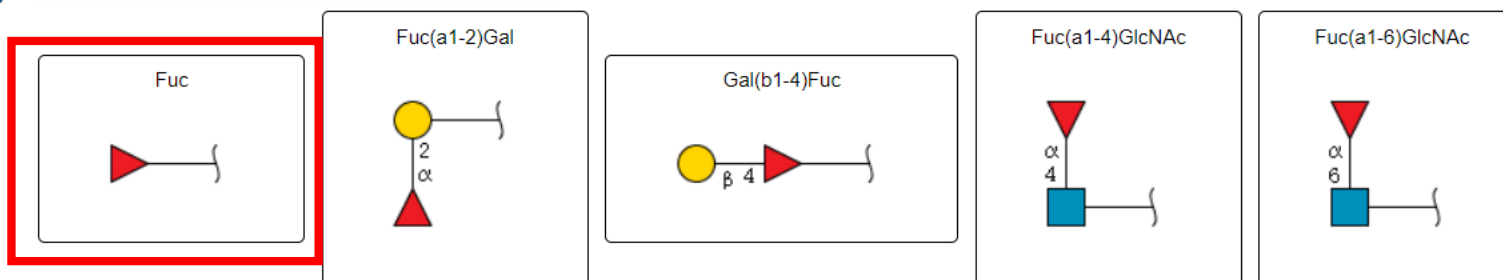
Search

## UniLectin3D glycan search

D-Abep	D-Arap	D-Fruf	D-Frup	D-Fucp	D-Galn
D-Galp	D-Galp	D-GalpNAc	D-Glcp	D-GlcpN	D-GlcpNAc
D-Manp	D-ManpN	D-ManpNAc	D-Murp	D-Neup5Ac	D-Neup5Gc
D-Talp	D-Tyyp	D-Xyyp	DD-manHepp	L-Fucp	L-Galp
L-Rhap	LD-manHepp				

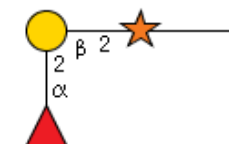
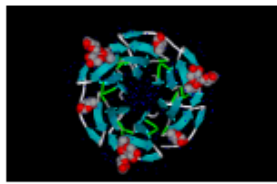
## Search fields in UniLectin3D

PDB	origin
UniProt AC	species
Fold	resolution threshold (Å)
Class	monosaccharide (ie. L-Fucp, D-Galp, D-GlcpNAc, D-Neup5Ac ...)
Family	IUPAC condensed (ie. Gal(b1-4)GlcNAc(b1-3)Gal(b1-4)Glc)
	Fuc <input type="button" value="exact motif occurrence"/>

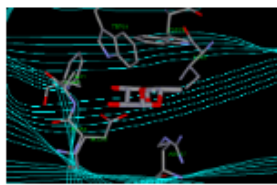
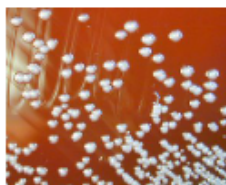


2BS6 RSL, BamBL *Ralstonia solanacearum*[View the 3D structure and information](#)

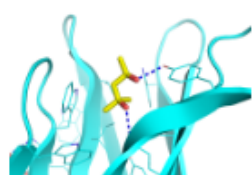
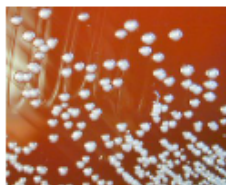
fold	b-propeller	origin	Bacterial lectins
class	AAL-like (PropLec6A)	species	<i>Ralstonia solanacearum</i>
family	RSL, BamBL	comments	N77G/G84S double mutant complexed with xyloglucan fra
resolution (Å)	1.8	IUPAC condensed	Fuc(a1-2)Gal(b1-2)Xyl

2BT9 RSL, BamBL *Ralstonia solanacearum*[View the 3D structure and information](#)

fold	b-propeller	origin	Bacterial lectins
class	AAL-like (PropLec6A)	species	<i>Ralstonia solanacearum</i>
family	RSL, BamBL	comments	
resolution (Å)	0.94	IUPAC condensed	Fuc

3ZI8 RSL, BamBL *Ralstonia solanacearum*[View the 3D structure and information](#)

fold	b-propeller	origin	Bacterial lectins
class	AAL-like (PropLec6A)	species	<i>Ralstonia solanacearum</i>
family	RSL, BamBL	comments	R17A mutant with glycerol in mutated site and fucose in n
resolution (Å)	1.5	IUPAC condensed	Fuc

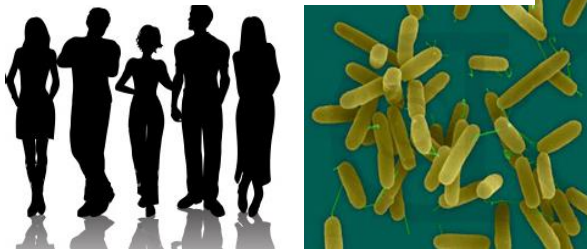




# Lektiny



**Všudypřítomné**



## Vazba sacharidu



Specifická

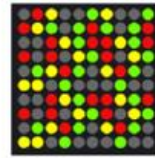


Reverzibilní



Nemodifikující

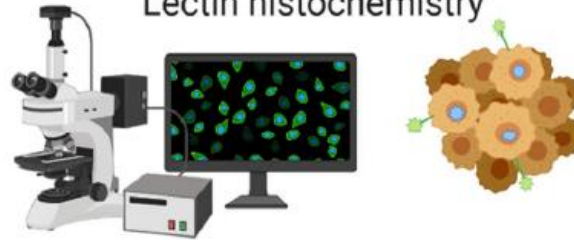
Lectin array



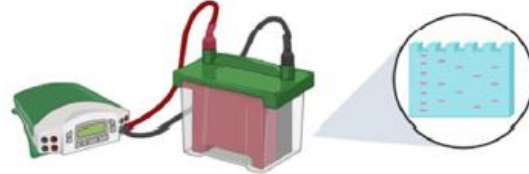
Lectin affinity chromatography



Lectin histochemistry



SDS-PAGE & Western Blot with lectins

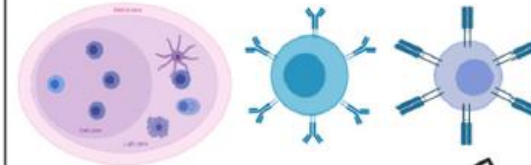


Enzyme-linked lectin assay (ELLA)



Biological activity

Mitogenic



Anticancer

Apoptotic



Necrotic

Antibacterial



Antiviral



Antifungal



Antihelminthic



# LectomeXplore - A database of predicted lectins

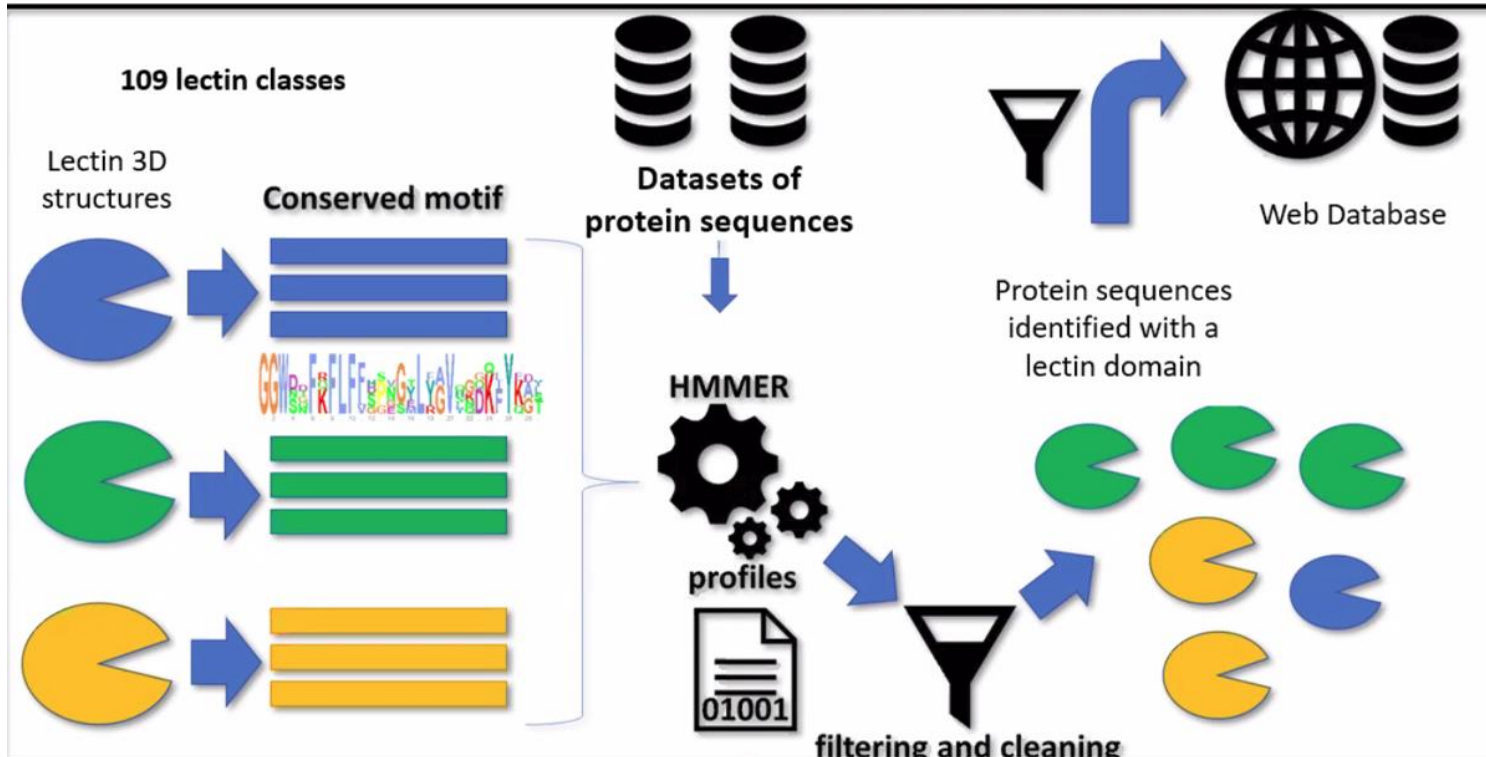
## What is LectomeXplore ?

LectomeXplore is a module dedicated to the exploration of predicted lectins for each class from UniLectin3D classification. Translated genomes (proteomes) released in the UniProtKB and RefSeq sequence databases and in the PDB structure database were screened to identify the lectome (complete set of lectins) of the corresponding species.

## How many predicted lectins ?

Proteins with a specific lectin domain: **993249** candidate lectins in **24156** species

## Workflow of lectin domains prediction



<https://www.unilectin.eu/predict/>

## TrefLec

Predicted  $\beta$ -trefoil lectins

<https://unilectin.eu/trefoil/>

## PropLec

Predicted  $\beta$ -propeller lectins

<https://unilectin.eu/propeller/>

## MycoLec

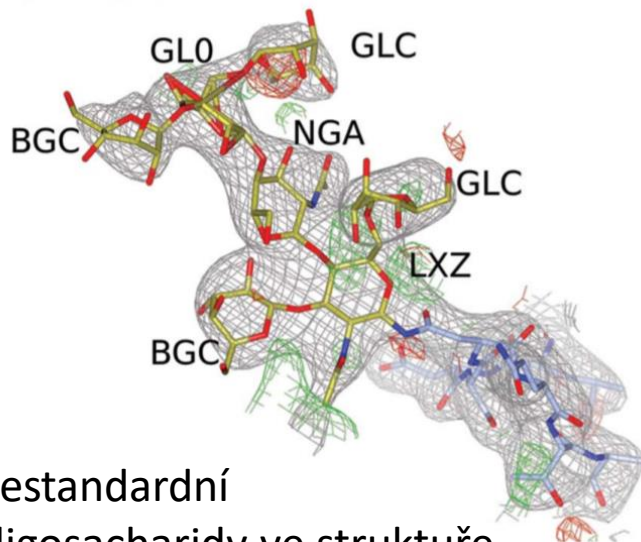
Predicted lectins in fungal genomes

<https://www.unilectin.eu/mycolec/>

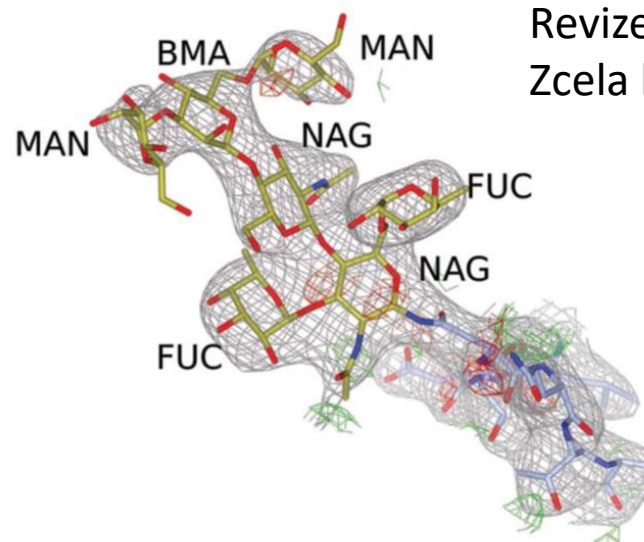
# Cukry – 3D struktura

- Co nás zajímá – struktury **glykoproteinů**, struktury sacharidů v **komplexu** s proteiny (**lektiny, enzymy, protilátky**).
- **RTG** krystalografie. Problém: **velká flexibilita sacharidů** (ve struktuře je viditelná jen část glykanu).

Problém: Kvalita 3D struktur sacharidů v PDB může být **nízká**...



Nestandardní oligosacharidy ve struktuře, 2008.



Revize struktury, 2019.  
Zcela běžné oligosacharidy

Host cell recognition by the henipaviruses: Crystal structures of the Nipah G attachment glycoprotein and its complex with ephrin-B3

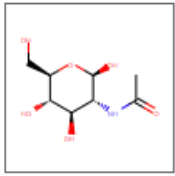
Kai Xu\*, Kanagalaghatta R. Rajashankar<sup>1</sup>, Yee-Peng Chan<sup>2</sup>, Juha P. Himanen<sup>3</sup>, Christopher C. Broder<sup>2</sup>, and Dimitar B. Nikolov<sup>4,5</sup>

\*Structural Biology Program, Memorial Sloan-Kettering Cancer Center, 1275 York Avenue, New York, NY 10021; <sup>1</sup>Northeastern Collaborative Access 1

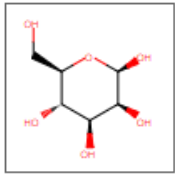


# Cukry – 3D struktura

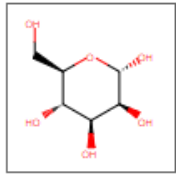
12 bound ligands:



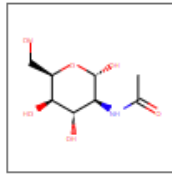
10 x NAG



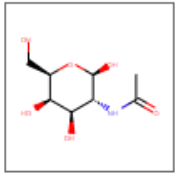
3 x BMA



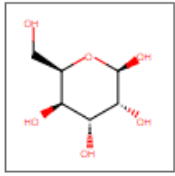
2 x MAN



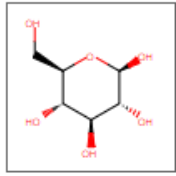
1 x LXZ



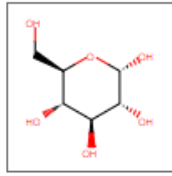
1 x NGA



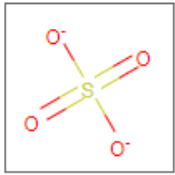
2 x GLO



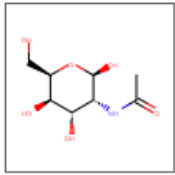
5 x BGC



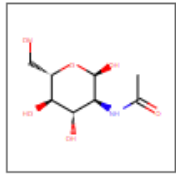
3 x GLC



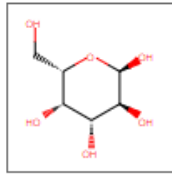
22 x SO4



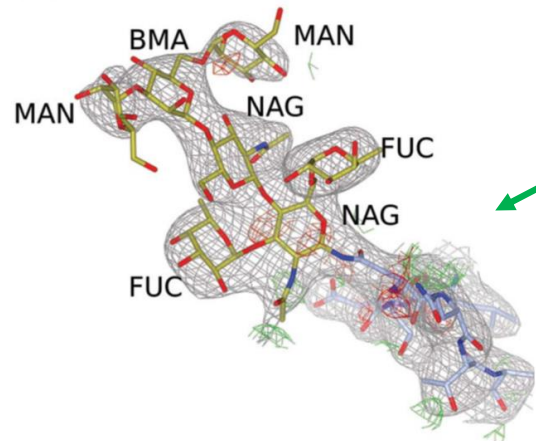
1 x LXB



1 x NGZ



1 x GXL



## Building and rebuilding N-glycans in protein structure models

Bart van Beusekom,<sup>a</sup> Natasja Wezel,<sup>a</sup> Maarten L. Hekkelman,<sup>a</sup> Anastassis Perrakis,<sup>a</sup> Paul Emsley<sup>b</sup> and Robbie P. Joosten<sup>a\*</sup>

<sup>a</sup>Department of Biochemistry, The Netherlands Cancer Institute, Plesmanlaan 121, 1066 CX Amsterdam, The Netherlands, and <sup>b</sup>MRC Laboratory for Molecular Biology, Francis Crick Avenue, Cambridge Biomedical Campus, Cambridge CB2 0QH, England. \*Correspondence e-mail: r.joosten@nki.nl

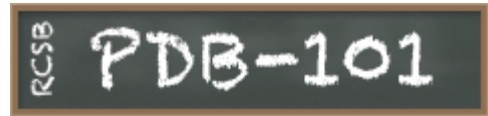
N-Glycosylation is one of the most common post-translational modifications and is implicated in, for example, protein folding and interaction with ligands and receptors. N-Glycosylation trees are complex structures of linked carbohydrate residues attached to asparagine residues. While carbohydrates are typically modeled in protein structures, they are often incomplete or have the wrong chemistry. Here, new tools are presented to automatically rebuild existing glycosylation trees, to extend them where possible, and to add new glycosylation trees if they are missing from the model. The method has been incorporated in the *PDB-REDO* pipeline and has been applied to build or rebuild 16 452 carbohydrate residues in 11 651 glycosylation trees in 4498 structure models, and is also available from the *PDB-REDO* web server. With better modeling of N-glycosylation, the biological function of this important modification can be better and more easily understood.

# Cukry – 3D struktura

## How Carbohydrates are Specified in PDB Entries

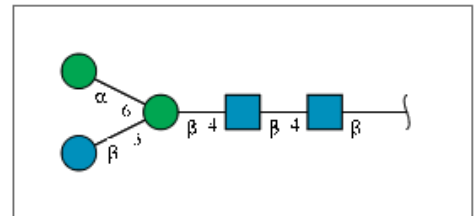
In 2020, members of the wwPDB worked together to ensure that carbohydrates in PDB structures are represented in a consistent way, improving methods for finding carbohydrate-related entries. All carbohydrate-containing entries in the PDB archive were remediated. This project incorporated standards used by the glycoscience community to enable easy translation of PDB data to other representations commonly used by glycobiologists.

[Detailed information about this remediation is described at wwPDB.org.](https://www.wwpdb.org)



Please note, it is not uncommon for portions of a biological macromolecule to be unresolved in experimental data. Segments of carbohydrates may be fully or partially missing from the atomic coordinates (i.e., they could not be modeled from available experimental data). In glycosylated proteins, often only the first sugar of the chain is resolved and included in the coordinates for the PDB entry. In these cases (where only a single sugar is resolved), the sugar will be presented as a ligand. Other sites of glycosylation, if they contain two or more resolved sugars, will be treated as separate branched entities.

**Carbohydrate polymer :** NEW  
**Components:** [NAG](#), [BMA](#), [MAN](#), [BGC](#)





# Cukry – 3D struktura

- Určení struktury **komplexních** sacharidů je obecně problém.

**RTG** – velká flexibilita, problémy s krystalizací.

**NMR** – tradiční metoda pro určení struktury oligosacharidů (práce v roztoku), problémy s přiřazením signálů a vyhodnocením dat (malé rozdíly mezi jednotlivými jádry).

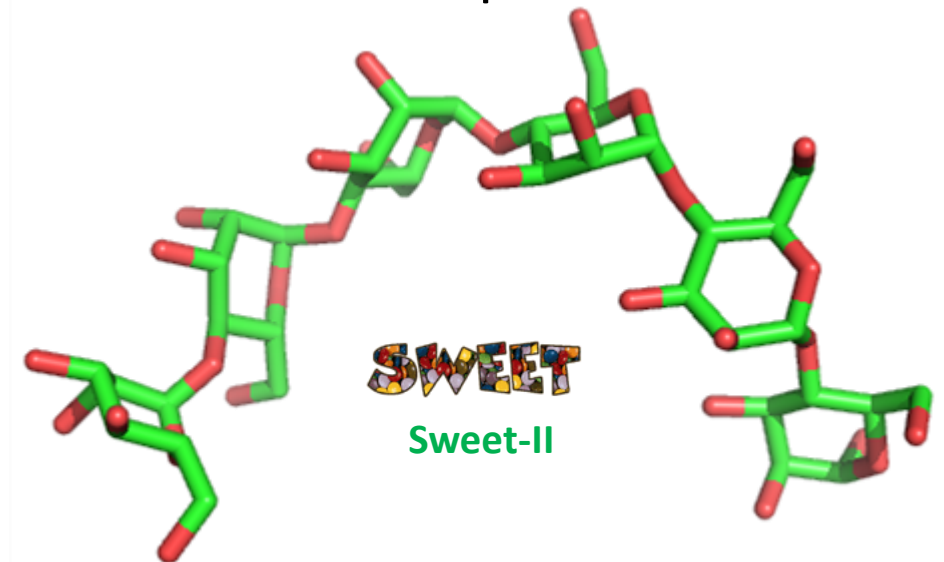
- **Molekulové modelování** sacharidů je často **nezbytnou** součástí interpretace experimentálních dat.

Please select the desired monosaccharides and glycosidic linkages.

If you are not sure how to do please look at the [example page](#).

An example for branches structures are [here](#).  
Remember - not all constructions are reasonable.

Input for the web-interface:



# Cukry – 3D struktura

- Určení struktury **komplexních** sacharidů je obecně problém.

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- **Molekulové modelování** sacharidů je často **nezbytnou** součástí interpretace experimentálních dat.

It should be noted that under physiological conditions oligosaccharides are frequently highly flexible, and a single static structure is an incomplete model. For this reason, the user is encouraged to employ molecular dynamics simulations to develop a more complete understanding of the spatial and dynamic properties of their system.

All builders at GLYCAM-Web generate molecular structure files that can be used in visualization programs or as input for simulations. For the builders that generate 3D structures from a primary sequence (e.g., DManpb1-6DGlcNacp1-OH), we offer the interfaces listed below for setting the primary sequence.



<http://glycam.org/>

**Carbohydrate Builder**

Step 1: Set Glycan Sequence

Step 2: Options

Step 3: Download

Isomer

Ring Type

Configuration

Select a ring type or select a configuration and the default ring type will be chosen.

							Monosaccharide	
Man	Gal	Glc	Ido	All	Alt	Gul	Tal	
Xyl	Lyx	Rib	Ara	Fru	Psi	Sor	Tag	
					Fuc	Rha	Qui	
					GalNAc	GlcNAc	ManNAc	
					GalA	GlcA	IdoA	
				Neu5Ac	KDN	KDO	Neu5Gc	

The tools below help you to assemble or select a glycan, which is then automatically energy minimized with the GLYCAM force field [1] to generate one or more 3D models. The file formats available for download include PDB (coordinates), as well as AMBER (topology and coordinates). The beta-test Carbohydrate Builder does not currently provide files for MD simulation.

**Requirements**

- A familiarity with carbohydrate nomenclature.

Linkage

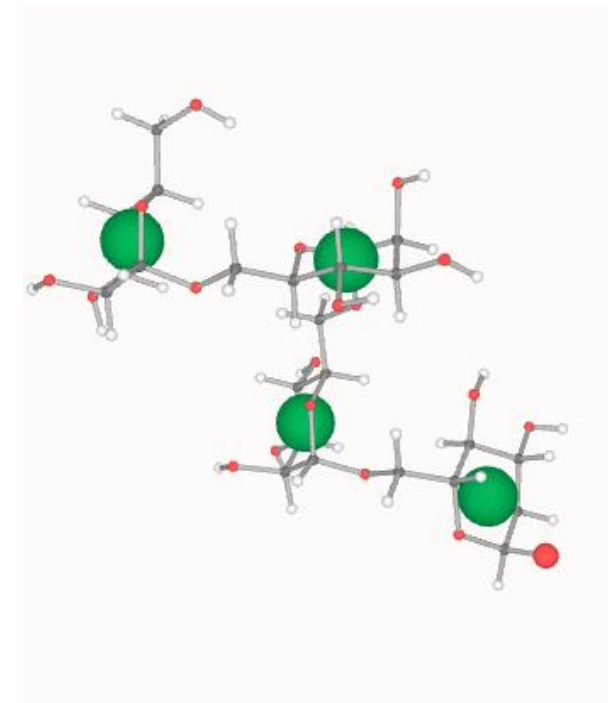
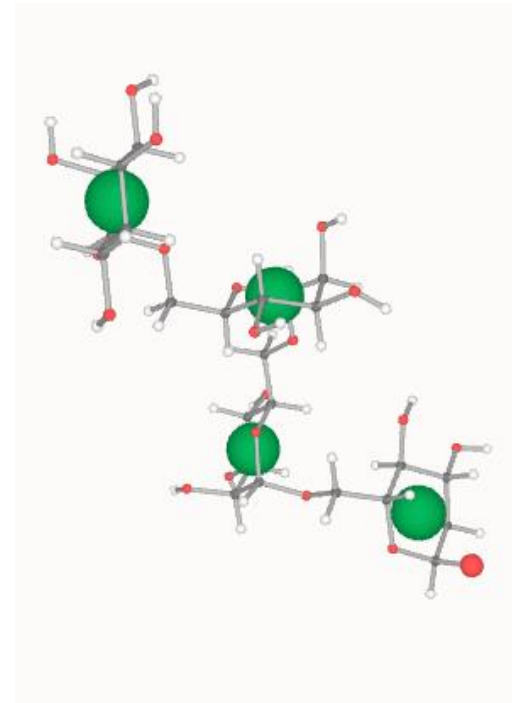
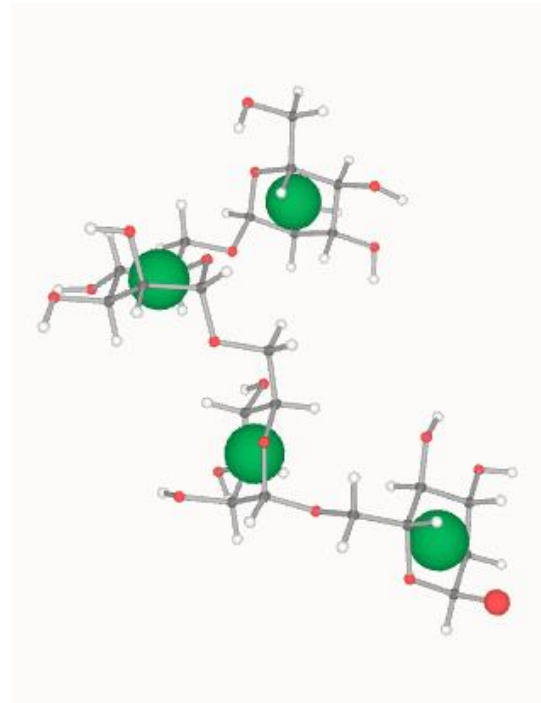
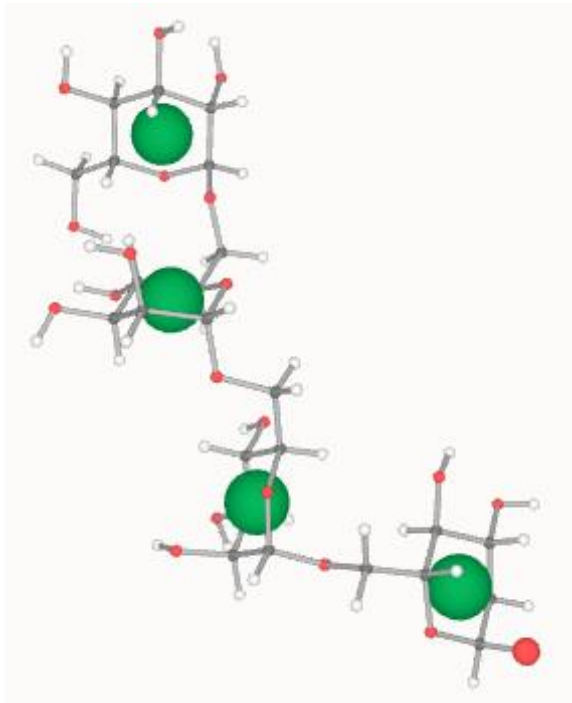
<input type="button" value="1-5"/>	<input type="button" value="1-6"/>	<input type="button" value="1-7"/>	<input type="button" value="1-8"/>	<input type="button" value="1-9"/>
<input type="button" value="2-5"/>	<input type="button" value="2-6"/>	<input type="button" value="2-7"/>	<input type="button" value="2-8"/>	<input type="button" value="2-9"/>

Aglycon

DManpa1-6DManpa1-6DManpa1-6DMan

Click the buttons in the table to download the files you need. Counterions are automatically added to the charged, solvated systems.






















DManpa1-6DManpa1-6DManpa1-6DManpa1-OH



It should be noted that under physiological conditions oligosaccharides are frequently highly flexible, and a single static structure is an incomplete model. For this reason, the user is encouraged to employ molecular dynamics simulations to develop a more complete understanding of the spatial and dynamic properties of their system.

Prefer the legacy Carbohydrate Builder Interface? [Build sequence from non-reducing terminal to anomer.](#)

**Monosaccharide** ● Standard/Mammalian  
● Alphabetical

 Man	 Gal	 Glc	 Ido	 All	 Alt	 Gul	 Tal
 Xyl	 Lyx	 Rib	 Ara	 Fru	 Psi	 Sor	 Tag
					 Fuc	 Rha	 Qui
					 GalNAc	 GlcNAc	 ManNAc
					 GalA	 GlcA	 IdoA
				 Neu5Ac	 KDN	 KDO	 Neu5Gc

**Sequence**

DManpa1-6DManpa1-6DManpa1-6DManpa1-OH

**Linkage**

α 1-? ▾ β 1-? ▾

**Residue**

Residue:

Isomer:

Ringtype:

**Beta-test Carbohydrate Builder (New!)**

Assemble a glycan by connecting monosaccharides. This new tool is still in development.

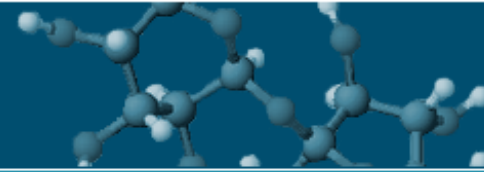


# Glykobioinformatika – databáze

- Databáze obsahující informace o **proteinech** (sacharidy jsou součástí glykoproteinů, lektiny).
- Vlastní databáze **sacharidů** (struktury).
- Databáze **enzymů** a **drah** účastníků se syntéz a odbourávání glykanů (sacharidů).
- Informace o **interakcích** protein-sacharid
- **„Glykocentra“ – sdružené databáze, vlastní specializované databáze, analytické nástroje**

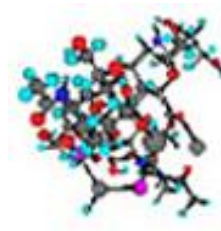
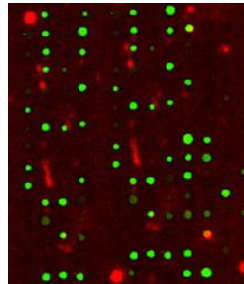
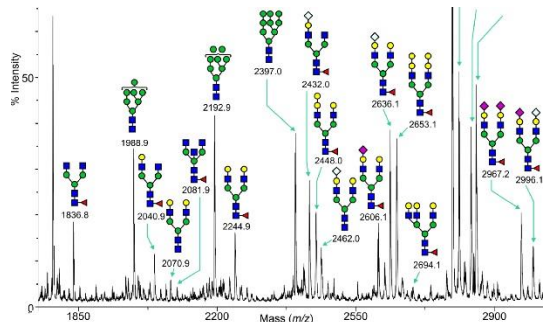
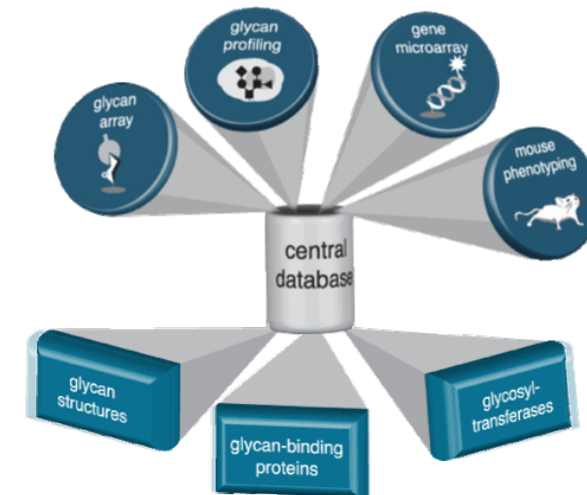
# „Glykocentra“

**CFG** functionalglycomicsgateway



The Consortium for Functional Glycomics (CFG) is a large research initiative funded by [NIGMS](#) to define the paradigms by which protein-carbohydrate interactions mediate cell communication. The CFG works with the scientific community to create unique [resources and services](#) that Participating Investigators can use in their own research. These resources and services, which are provided free of charge by the CFG's [Scientific Cores](#), include glycan array screening, gene microarray screening, mouse phenotyping, glycan profiling, a reagent bank, and data analysis tools. Resulting data sets are integrated and made accessible to the community via the CFG's [central database](#). The CFG also has publicly accessible [specialty databases](#) that offer detailed information on glycan-binding proteins, glycan structures, and glycosyltransferases. The number of investigators using CFG resources in their work continues to grow, as reflected by the rate of [new publications involving CFG resources](#). Our vision is to harness the combined research power of our Participating Investigators and our Scientific Cores to achieve our goals.

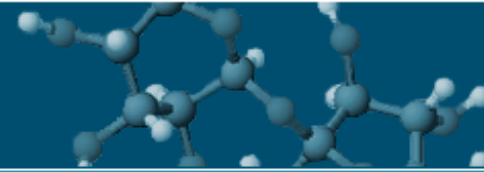
## CONSORTIUM FOR FUNCTIONAL GLYCOMICS



<http://glycan-dev.mit.edu/static/consortium/consortium.shtml>

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## CONSORTIUM FOR FUNCTIONAL GLYCOMICS

### SEARCH FOR GLYCANS

Select the type of search you wish to perform from the list below. Once obtained, search results can be further refined.

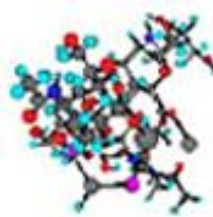
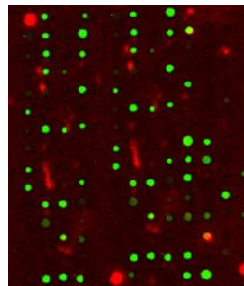
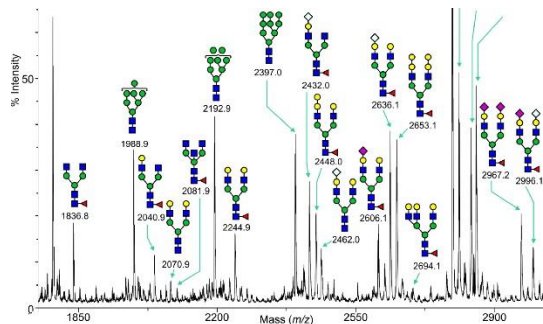
**Sub-structure** Search for all glycans containing specific sub-structural motifs, which can be built using our interactive templates.

**Molecular weight** Search for all glycans that fall within or outside a specified molecular weight range.

**Composition** Search for all glycans that contain a specified number and type of monosaccharide constituents.

**Linear nomenclature** Search for glycans using the IUPAC or linear codes for their monosaccharide constituents.

**Multiple search criteria** Search for glycans using one or more of these criteria: name, family, ID, source (i.e., species, organ, tissue, cell type, and disease), molecular weight, composition, and nomenclature.



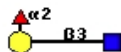
<http://glycan-dev.mit.edu/static/consortium/consortium.shtml>

# CONSORTIUM FOR FUNCTIONAL GLYCOMICS

„Glykocentra“

Glycan : carbSynthe\_0085\_D000

## Cartoon Representation



## IUPAC 2D Representation



## IUPAC Code

**Fuc** a1-2 **Gal** b1-3 **GlcNAc** b#Sp2.BT

## Linear Code

Fa2Ab3GNb#Sp2.BT

## Link to 3D Model (GLYCAM - Web)

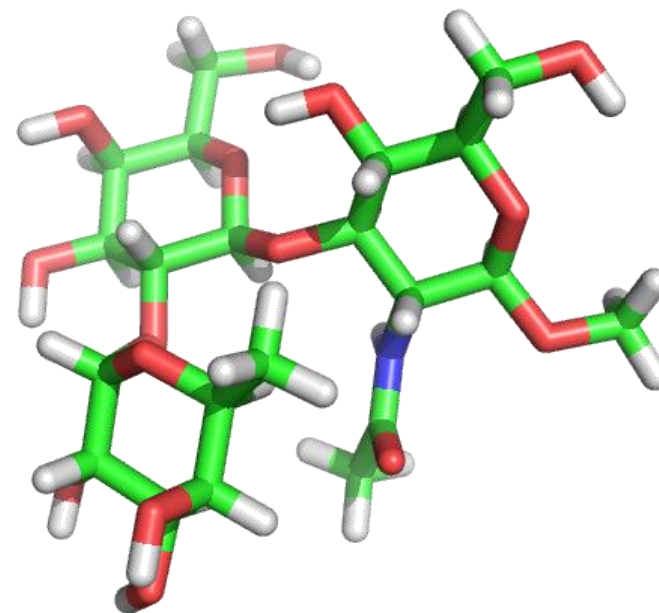
[Link to GLYCAM for Fa2Ab3GNb](#)

## Sub Structure Search Interface

[Load this structure for sub structure search](#)

## General Information

Glycan Family:	Synthetic
Sub. Family:	Synthetic
Scientific Name:	Fuca2Galb3GlcNAcb#SP2.BT
Common Name:	Led (H type 1)
Last Updated:	04/28/2003
Oligosaccharide Molecular Wt.:	529.479
Calculated Oligosaccharide Molecular Wt.:	529.479
Permethylated MW.:	692
Composition:	Hex <sub>1</sub> dHex <sub>1</sub> HexNAc <sub>1</sub>
Status:	Public



Customize the below sub-structure by clicking on monosaccharides or linkages that you wish to modify.

- Clicking on a monosaccharide allows you to add extensions, replace it with a different monosaccharide, or add modifiers (phosphate groups, sulfate groups, etc.) Extensions can only be added towards the non-reducing end.
- Clicking on a monosaccharide and selecting "Trim" removes it, along with all associated monosaccharides toward the non-reducing end.
- Clicking on a linkage allows you to replace it with other linkages, including "wild cards." Click "Run Query" to search for glycans that contain the finished structure.

Build from other templates



Match the motif at non-reducing end only:

Run Query

# CONSORTIUM FOR FUNCTIONAL GLYCOMICS

# „Glykocentra“

Glycan Binding Protein : cbp\_1499

## General Information

Name:	Aspergillus fumigatus lectin (AFL)
Complete Name:	Fucose-specific lectin FleA
Family:	Other
Sub Family:	Plant/fungal lectin
Spec. Sci. Name:	Aspergillus fumigatus
Entry Date [mm/dd/yyyy]:	07/08/2009
Status:	Public

## Primary Sequence

STPGAQQVLF RTGIAAVNLT NHLRVYFQDV YGSIRESLYE GSWANGTEKN VIGNAKLGSP  
VAATSKELKH IRVYTLTEGN TLQEFAYDSG TGWYNGGLGG AKFQVAPYSR IAAVFLAGTD  
ALQLRIYAQK PDNTIQEYMW NGDGWKEGTN LGGALPGTGI GATSFRTYDY NGPSIRIWFQ  
TDDLKLVQRA YDPHKGWYYPD LVTIFDRAPP RTAIAATSFG AGNSSIYMRI YFVNSDNTIW  
QVCWDHGGKY HDKGTITPVI QGSEVAIISW GSFANNGPDL RLYFQNGTYI SAVSEWWNR  
AHGSQLGRSA LPPA

## Known Sites of Expression

- Recombinant from E. coli

## Other Public Databases

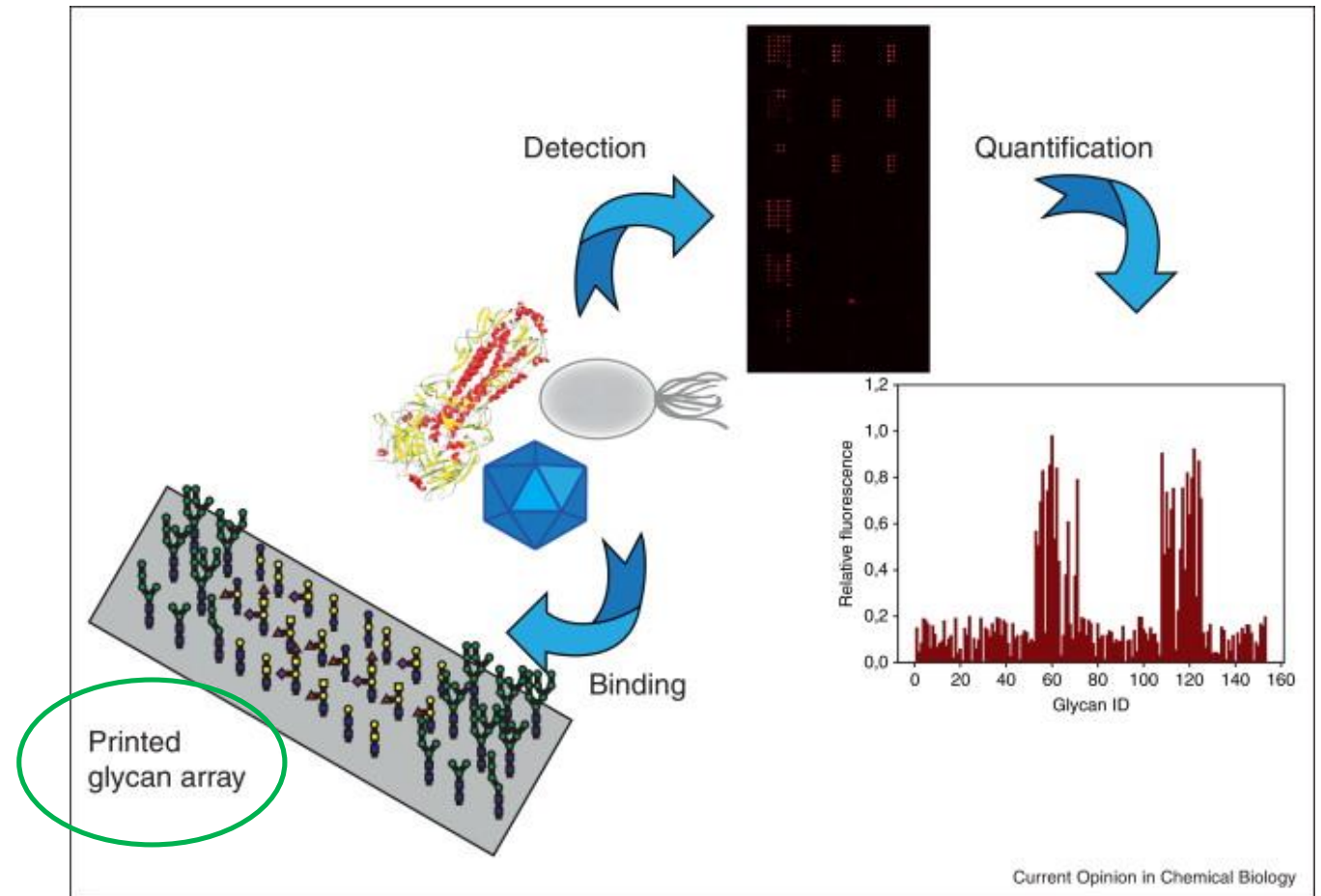
Gen. Bank.:	GenBank:3511258
Swiss. Prot.:	Swiss Prot:Q4WW81

## Associated Resource Requests

[cfg\\_rRequest\\_2058](#)

## Primary Screen Information

Glycan Array Version:	PA_v41
Protocol Id:	Protocol Direct Binding
Replicate Number:	1
Result Nature:	Data
Protein/Sample Concentration:	1 micrograms/ml
Experiment Date [mm/dd/yyyy]:	06/01/2010
Supplying Investigator:	Anne Imberty
Assay Information:	Samples were directly labeled with AlexaFluor 488.
Annotation:	Aspergillus fumigatus lectin (AFL)-1





# CONSORTIUM FOR FUNCTIONAL GLYCOMICS

# „Glykocentra“

Glycan Binding Protein : cbp\_1499

## General Information

Name:	Aspergillus fumigatus lectin (AFL)
Complete Name:	Fucose-specific lectin FleA
Family:	Other
Sub Family:	Plant/fungal lectin
Spec. Sci. Name:	Aspergillus fumigatus
Entry Date [mm/dd/yyyy]:	07/08/2009
Status:	Public

## Primary Sequence

STPGAQQVLF RTGIAAVNLT NHLRVYFQDV YGSIRESLYE GSWANGTEKN VIGNAKLGSP  
VAATSKELKH IRVYTLTEGN TLQEFAYDSG TGWYNGGLGG AKFQVAPYSR IAAVFLAGTD  
ALQLRIYAQK PDNTIQEYMW NGDGWKEGTN LGGALPGTGI GATSFRTYDY NGPSIRIWFQ  
TDDLKLVQRA YDPHKGWYYPD LVTIFDRAPP RTAIAATSFG AGNSSIYMRI YFVNSDNTIW  
QVCWDHGGY HDKGTITPVI QGSEVAIISW GSFANNGPDL RLYFQNGTYI SAVSEWWNR  
AHGSQLGRSA LPPA

## Known Sites of Expression

- Recombinant from E. coli

## Other Public Databases

Gen. Bank.:	GenBank:3511258
Swiss. Prot.:	Swiss Prot:Q4WW81

## Associated Resource Requests

[cfg\\_rRequest\\_2058](#)

## Primary Screen Information

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Supplying Investigator:	Anne Imberty
Assay Information:	Samples were directly labeled with AlexaFluor 488.
Annotation:	Aspergillus fumigatus lectin (AFL)-1

## Analyte Information

Protein Sample Analyzed: : Aspergillus fumigatus lectin (AFL)

## Raw Files for this Primary Screen

[Download](#)

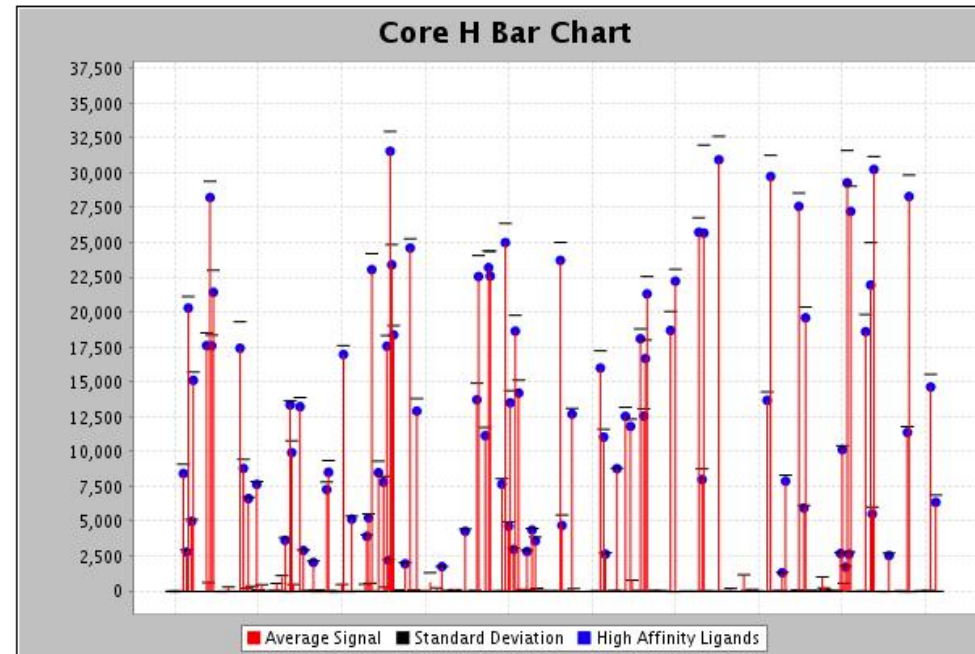
## Readout for this primary screen

[Search Readout](#)

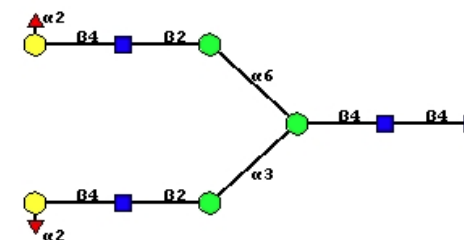
## Enhanced Glycan Array Data Browser (New Feature)

[Click This Link to Launch the New Flex-based Glycan Array Data Browser Tool](#)

## Bar Chart For 100 MicroMolar Concentration



## Glycan Being Browsed



# CONSORTIUM FOR FUNCTIONAL GLYCOMICS

# „Glykocentra“

Eur J Biochem. 1998 Dec 1;258(2):623-56.

## Identification of highly fucosylated N-linked oligosaccharides from the human parotid gland.

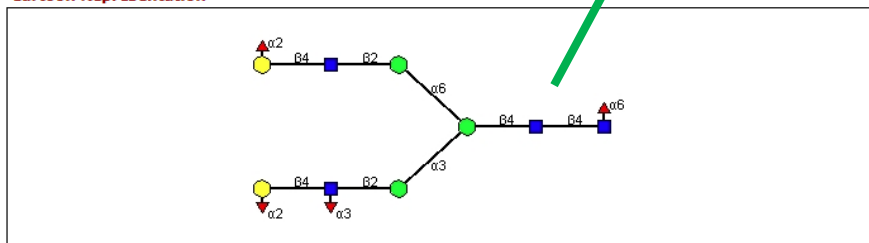
Guile GR<sup>1</sup>, Harvey DJ, O'Donnell N, Powell AK, Hunter AP, Zamze S, Fernandes DL, Dwek RA, Wing DR.

### Author information

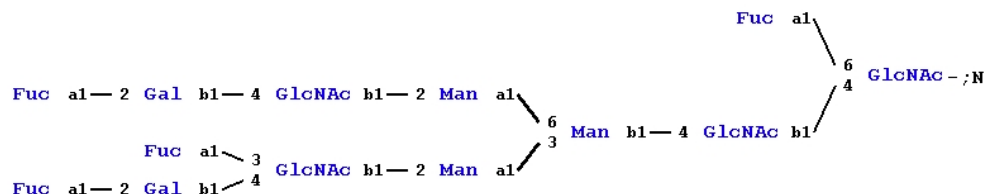
1 Oxford Glycobiology Institute, Department of Biochemistry, UK.

Glycan : carbNlink\_20325\_D000

#### Cartoon Representation



#### IUPAC 2D Representation



### Sub Structure Search Interface

Load this structure for sub structure search

### Analyte Information

Protein Sample Analyzed: : Aspergillus fumigatus lectin (AFL)

### Raw Files for this Primary Screen

[Download](#)

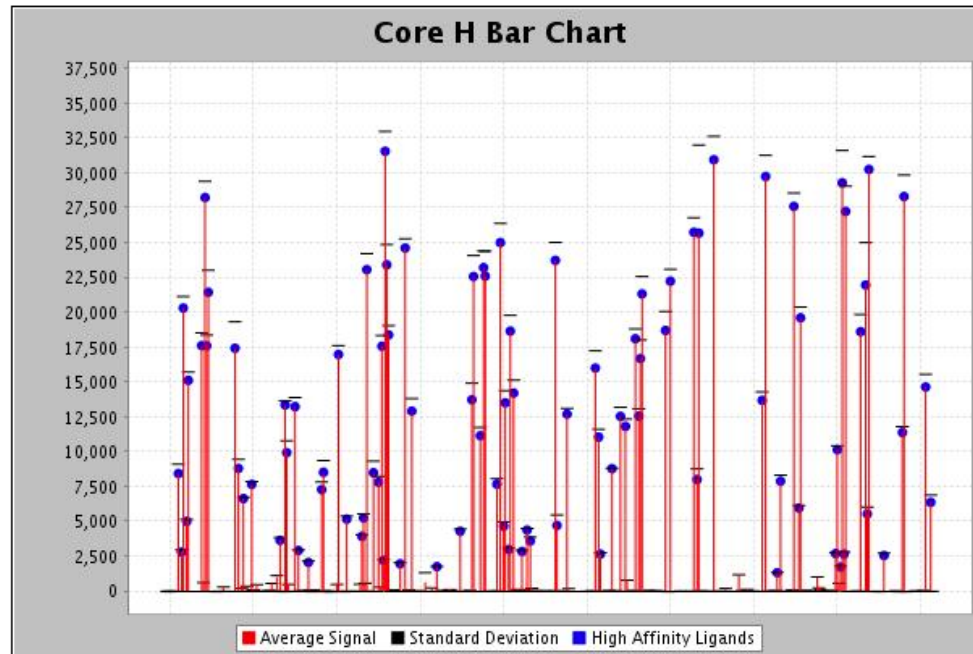
### Readout for this primary screen

[Search Readout](#)

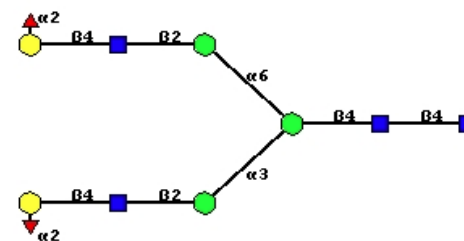
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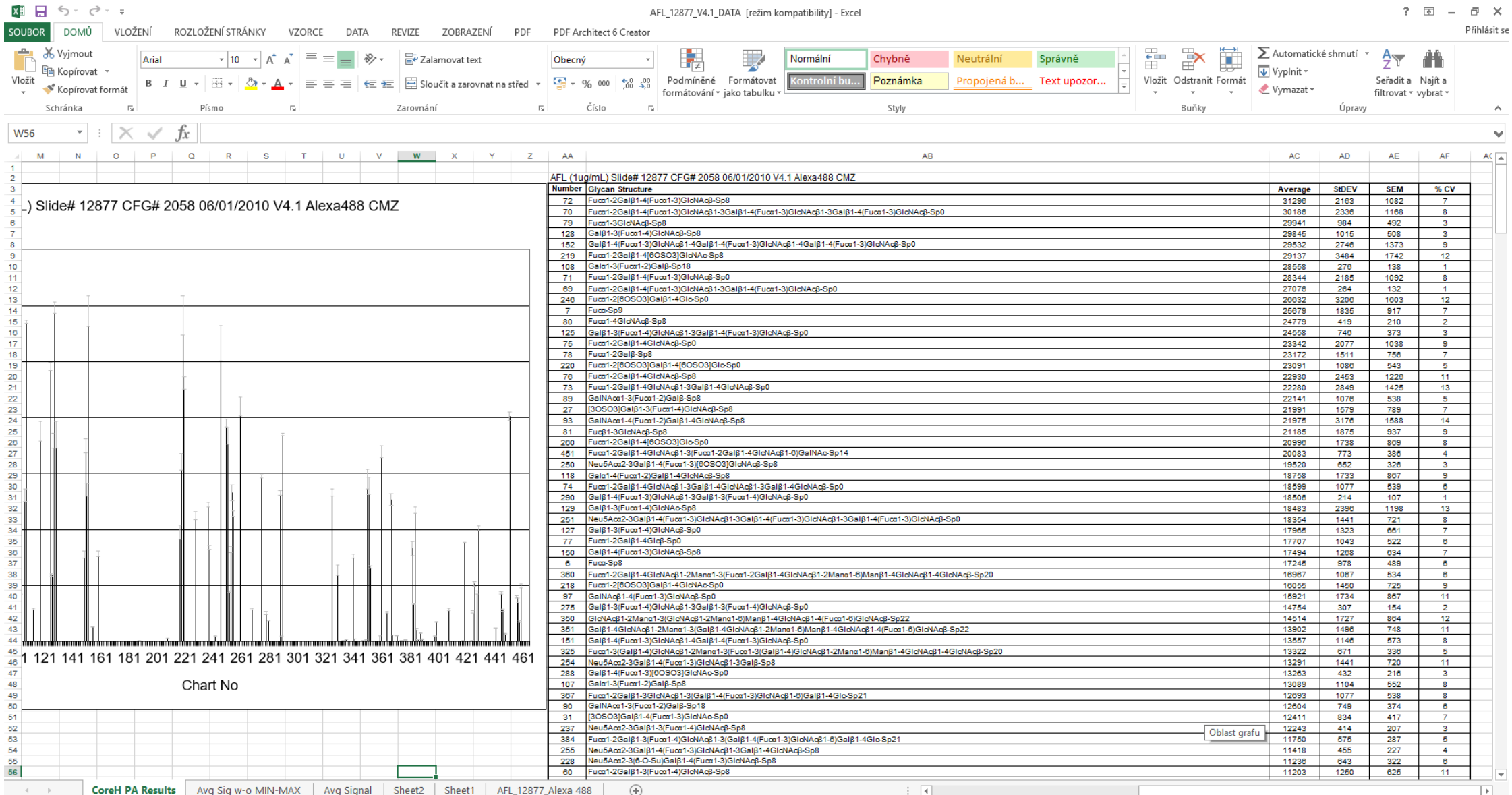


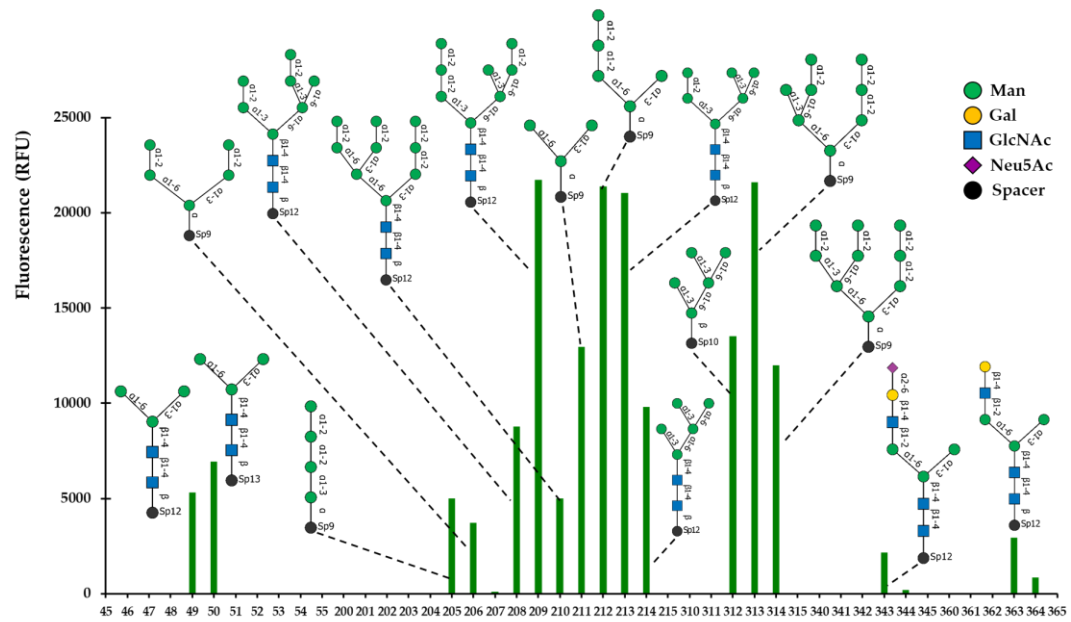
### Glycan Being Browsed



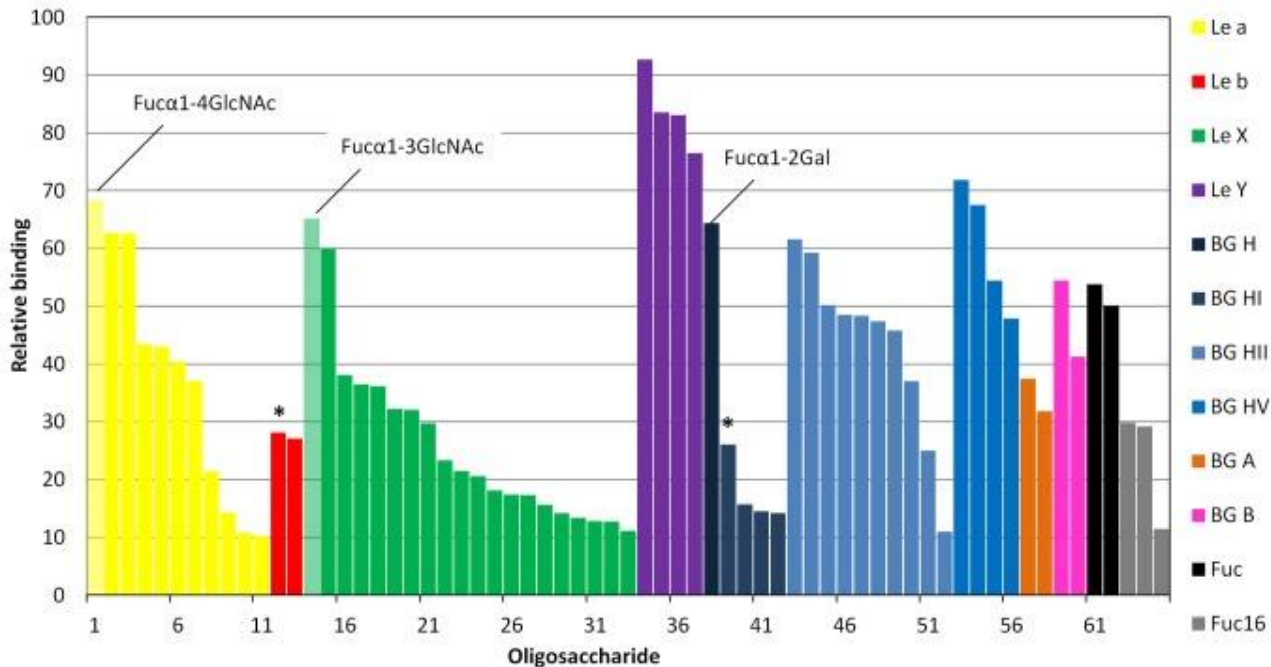
# CONSORTIUM FOR FUNCTIONAL GLYCOMICS

# „Glykocentra“

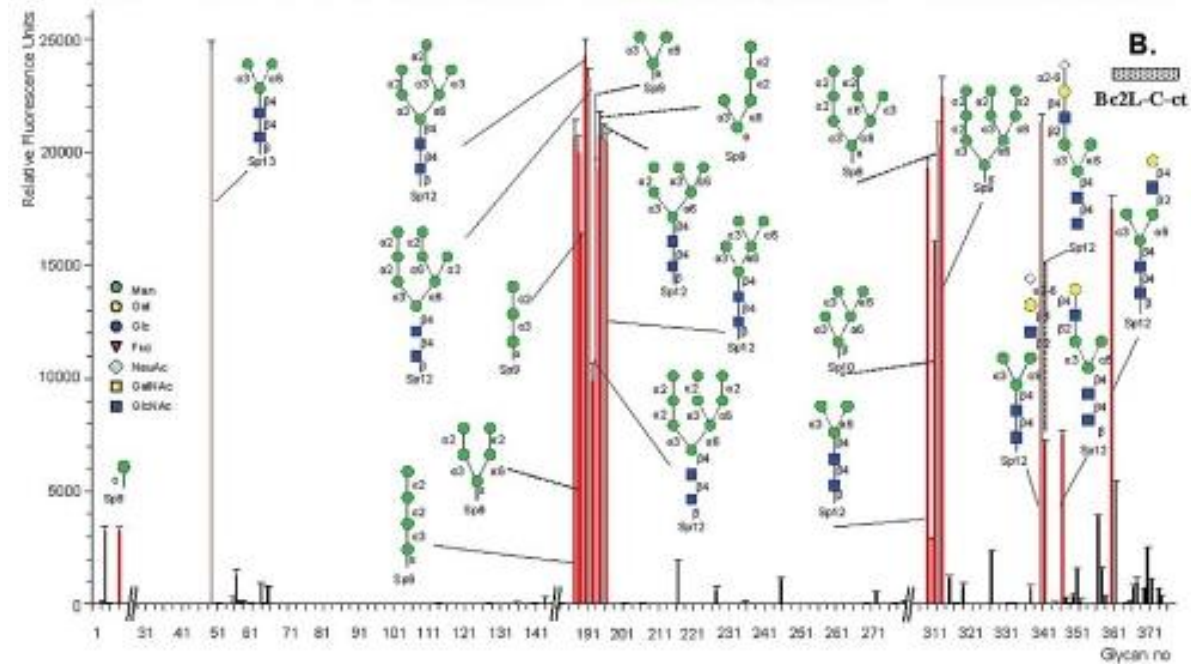
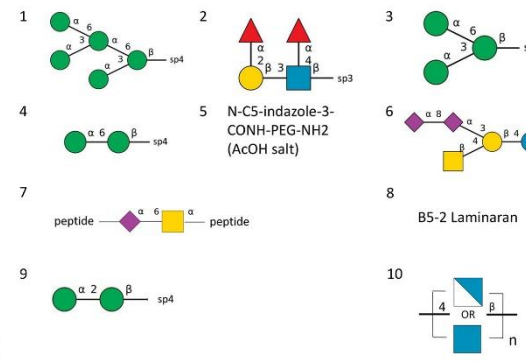
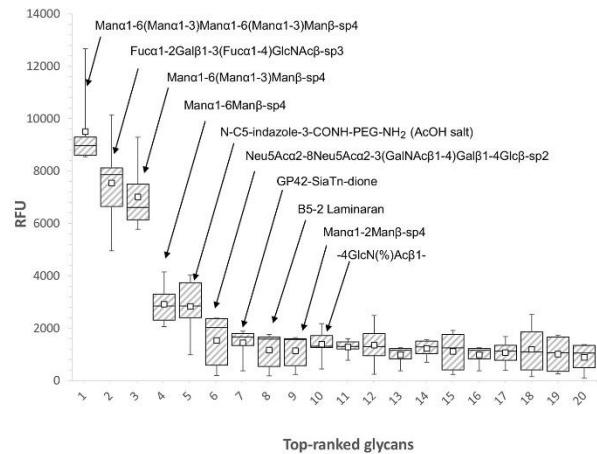




Carbohydrate number



A





# „Glykocentra“

<http://glyco3d.cermav.cnrs.fr/home.php>

GLYCO3D 2.0

Glyko struktury

Disac3-DB

BioOligo-DB

Polysac3-DB

NMR oligo

EPS-DB

GAG-DB

CBMcarb-DB

Unilectin

mAbscarb-DB

Polys-Glycan Builder

Monosac-DB

Click Display

Other tools





GlycoPedia

„Glyko drbna“

<https://www.glycopedia.eu/>

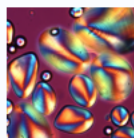
# Glyko stránky

news

e-chapters

resources

search



## Starch : Structure and Morphology

Serge Perez - Anne Imberty



3S6S  
opyranose  
1,8-S 0-D



Glucopyran  
2,3,6-S 0

## Library of Bio-active Monosaccharides. 1D,...

Serge Perez

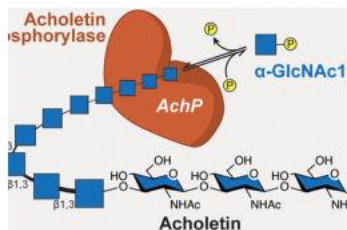
18

mars  
2022

news

## Acholetin : A newly discovered Poly 1-3 $\beta$ -D GlcNAc bacterial polysaccharide

Using genomic data and activity-based screening, the researchers identified a glycoside phosphorylase enzyme...



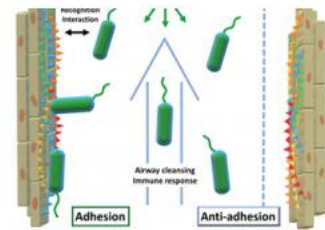
11

mars  
2022

news

## Glycomimetics against Multi-Drug Resistant Pathogens

The collection of glycopedia virtual chapters has been extended with a new contribution Multi-drug resistant...



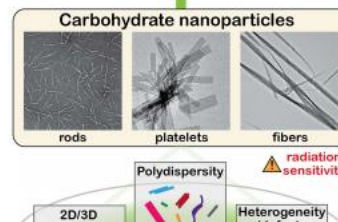
22

février  
2022

news

## Recent Advances in Electron Microscopy of Carbohydrate Nanoparticles

Carbohydrate nanoparticles, both naturally derived and synthetic ones, have attracted scientific and...

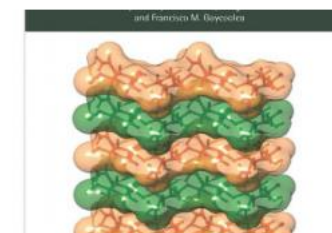


2 janvier  
2022

news

## Chitin and Chitosan in the Bioeconomy

Chitin is the second most abundant natural polymer in the world after cellulose, mainly derived from the food...



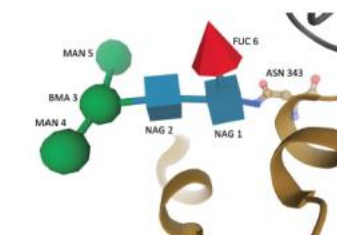
20

décembre  
2021

news

## Modernized uniform representation of carbohydrate molecules in the Protein Data Bank

Carbohydrate molecules present in more than 14,000 Protein Data Bank (PDB) structures have recently been...



# Lipidy

Lipidy jsou heterogenní skupina biomolekul nerozpuštěných ve vodě a rozpustných v organických rozpouštědlech. Jsou to deriváty vyšších monokarboxylových kyselin a alifatických či alicyklických hydroxyderivátů nebo aminoderivátů. Patří do ní následující látky:

1. Tuky a oleje ([acylglyceroly](#))
2. Glycerolipidy ([glycerofosfolipidy](#), [plasmalogeny](#), kardiolipin)
3. [Sfingolipidy](#)
4. [Steroidy](#) ([cholesterol](#), [žlučové kyseliny](#), [steroidní hormony](#))
5. Izoprenoidy ([ubichinon](#), [plastochinon](#), [dolichol](#))
6. [Vitaminy](#) rozpustné v tucích
7. Deriváty mastných kyselin ([leukotrieny](#), [prostaglandiny](#), prostacykliny, [tromboxany](#))

Lipidy hrají v organismu roli jako zásobní látky, strukturální složky membrán, hormony a vitaminy.

## 4.8.16 lipids

Small, biologically active molecules of variable structure, commonly defined by their solubility in non-polar solvents. Hydrophobic or amphipathic small molecules that may originate, entirely or in part, by the carbanion-based condensations of thioesters (fatty acyls, glycerolipids, glycerophospholipids, sphingolipids, saccharolipids, and polyketides) and/or by carbocation-based condensations of isoprene units (prenol lipids and sterol lipids).

**Základní pojmy z biochemie, V. Mikeš, Katedra biochemie  
PřF Masarykovy Univerzity v Brně, 2. doplněné vydání 2001**



## Terminology of bioanalytical methods (IUPAC Recommendations 2018)

<https://doi.org/10.1515/pac-2016-1120>  
Received November 21, 2016; accepted February 1, 2018



# Lipidy a lipidomika

- **Zásobní látky (zdroj energie), mechanická ochrana, tepelná izolace, hormony, složky membrán, vitaminy**

## Lipidomika

Lipidomika je vědní obor, který se zabývá studiem biochemických drah lipidů v biologických systémech. Slovo lipidom označuje veškeré lipidy v buňce, tkáni nebo organismu v daném čase a je podmnožinou metabolomu. Lipidomika je relativně mladý obor, který se rozvíjí v souvislosti s rychlými pokroky v lékařství, analytické chemii a informačních technologiích. Lipidy hrají velmi důležité role při vzniku a průběhu mnoha metabolických chorob jako je například obezita, ateroskleróza, cévní mozková příhoda, hypertenze nebo diabetes. V lipidomickém výzkumu se pracuje s velkými soubory dat, které kvantitativně popisují změny v obsahu a složení jednotlivých druhů lipidů. Analýza lipidomu znamená identifikaci a kvantifikaci tisíců molekulárních druhů lipidů, zkoumá se struktura a interakce s dalšími sloučeninami, jejich dynamika a změny, které nastanou v průběhu vzniku choroby. Informace získané z těchto studií hrají důležitou roli při objasňování vzniku a průběhu nemocí na molekulární úrovni.

## Lipidy

Lipidy jsou strukturně různorodé chemické sloučeniny, které plní řadu klíčových biologických funkcí, například jako stavební složky buněčných membrán, zdroje a zásobárny energie, nebo jako signální molekuly. Lipidy mohou být obecně definovány jako hydrofobní nebo amphipatické molekuly, které alespoň částečně vznikají kondenzací thioesterů (mastné kyseliny, polyketidy, atd.) nebo isoprenových jednotek (prenoly, steroly, atd.). Lipidy se obecně dělí na "jednoduché" a "složené" lipidy, přičemž jednoduchými lipidy rozumíme ty, které při hydrolýze poskytují nanejvýš dva typy produktů, kdežto složené lipidy dávají při hydrolýze tři nebo více produktů.



<http://lipidomics.uochb.cas.cz/lipidomika.html>

Lipidomics: a global approach to lipid analysis in biological systems

Andrew D. Watson<sup>1</sup>

Department of Medicine, Division of Cardiology, David Geffen School of Medicine, University of California at Los Angeles, Los Angeles, CA 90095

1. How to preserve and extract lipids?
2. What amount of lipids is present in the sample ?
3. How to fractionate a natural lipid extract?
4. What are the components present within each fraction?
5. What amounts of each component are present in the lipid extract?

- [General organizations](#)
- [Companies involved in Scientific Research](#)
- [Sites devoted to sciences and techniques](#)
- [Databases and encyclopedia](#)
- [Browsing on the net](#)
- [Discussion Groups](#)

- [Food and Nutrition journals on-line](#)
- [Scientific journals](#)
- [Scientific Societies and organizations](#)
- [Scientific Libraries](#)
- [Publishers](#)

## Analýza lipidů

## Odkazy

# CYBERLIPID CENTER

<http://cyberlipid.gerli.com/>

1. This site for cyberlipid studies is an online, non-profit scientific organization whose purpose is to collect, study and diffuse information on all aspects of lipidology.
2. The site seeks to establish contacts between students, teachers, scientists and technicians and expose various models in all fields, forgotten studies of the past, work in progress and hot fields.
3. The site will try to feature an extensive, always upgraded, annotated bibliography devoted to the main presented topics.

[Lipid suppliers](#)

[Sites directly involved in fat and lipids](#)

[Journals devoted to lipids](#)

## Historie

## Kalendář

**1758**

First study by Poulletier de la Salle FP of a lipid (cholesterol) isolated from bile stones.

**1779**

Discovery by the Swedish scientist Scheele CW of glycerol obtained by heating several oils and fats with lead oxide.

**1783**

Fourcroy AF introduced alcohol to extract brain lipids.

**2022**

8-10 March 2022 – 10th International Singapore Lipid Symposium (iSLS10) – Themes of Precision health and medicine, nutritional science, healthy longevity, cardiometabolic diseases, infection biology, microbiome and more.

For information contact : [web site](#)

10-15 July 2022 – 25th International Symposium on Plant Lipids (ISPL meeting), Grenoble, France

For information contact: [web site](#)

6-9 November 2022 – The 17th GERLI Lipidomics Meeting "Lipids: from membrane dynamics to signaling" will be held in Saint-Jean-Cap-Ferrat, France (on the French Riviera, near Nice).

For information contact : [web site](#)





## Lipid classification, structures and tools\*

Eoin Fahy\*, Dawn Cotter, Manish Sud, and Shankar Subramaniam

University of California, San Diego, 9500 Gilman Dr., La Jolla, CA 92093-0411, USA

### Abstract

The study of lipids has developed into a research field of increasing importance as their multiple biological roles in cell biology, physiology and pathology are becoming better understood. The Lipid Metabolites and Pathways Strategy (LIPID MAPS) consortium is actively involved in an integrated approach for the detection, quantitation and pathway reconstruction of lipids and related genes and proteins at a systems-biology level. A key component of this approach is a bioinformatics infrastructure involving a clearly defined classification of lipids, a state-of-the-art database system for molecular species and experimental data and a suite of user-friendly tools to assist lipidomics researchers. Herein, we discuss a number of recent developments by the LIPID MAPS bioinformatics core in pursuit of these objectives. This article is part of a Special Issue entitled Lipidomics and Imaging Mass Spectrometry.

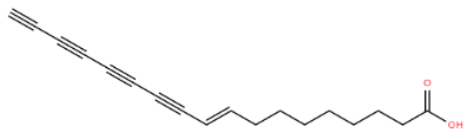
## Lipidy a lipidomika

### International Lipid Classification and Nomenclature Committee (2005):

Klasifikační systém zahrnující 8 hlavních kategorií, každá je dále členěná (třídy, podtřídy a někdy podpodtřídy)

#### Lipid of the Month

April, 2022



Protegenin A

### Lipid Classification System

The LIPID MAPS Lipid Classification System is comprised of eight lipid categories, each with its own subclassification hierarchy. All lipids in the LIPID MAPS Structure Database (LMSD) have been classified using this system and have been assigned LIPID MAPS ID's (LM\_ID) which reflects their position in the classification hierarchy. LMSD can be searched by lipid class, common name, systematic name or synonym, mass, InChIKey or LIPID MAPS ID with the search box in the banner, or alternatively, by LIPID MAPS ID, systematic or common name, mass, formula, category, main class, subclass data, or structure or sub-structure with one of the search interfaces in the [LMSD database](#) section. Each LMSD record contains an image of the molecular structure, common and systematic names, links to external databases, Wikipedia pages (where available), other annotations and links to structure viewing tools. In addition to LMSD search interfaces, you can drill down through the classification hierarchy below to the LMSD record for an individual lipid.



# Lipidy – strukturní databáze

- Třídění lipidů a informatika lipidů obecně je, ve srovnání s proteiny a nukleovými kyselinami, poměrně nový obor.
- **LIPID MAPS Structure Database (LMSD)**

The LIPID MAPS® Structure Database (LMSD) is a relational database encompassing structures and annotations of biologically relevant lipids. As of 05/01/2021, LMSD contains **45684** unique lipid structures, making it the largest public lipid-only database in the world.

The LIPID MAPS® Structure Database (LMSD) is a relational database encompassing structures and annotations of biologically relevant lipids. As of today, LMSD contains **47433** unique lipid structures, making it the largest public lipid-only database in the world.

<https://www.lipidmaps.org/data/structure/index.php>

Lipid Category	Curated	Computationally-generated	All
Fatty Acyls [FA]	8551	1875	10426
Glycerolipids [GL]	347	7379	7726
Glycerophospholipids [GP]	1725	8312	10037
Sphingolipids [SP]	1784	3168	4952
Sterol Lipids [ST]	3483	0	3483
Prenol Lipids [PR]	2344	0	2344
Saccharolipids [SL]	51	1294	1345
Polyketides [PK]	7120	0	7120
<b>TOTAL</b>	<b>25405</b>	<b>22028</b>	<b>47433</b>

Structures of lipids in the database come from several sources: (i) LIPID MAPS Consortium's core laboratories and partners; (ii) lipids identified by LIPID MAPS experiments; (iii) biologically relevant lipids manually curated from LIPID BANK, LIPIDAT, Lipid Library, Cyberlipids, ChEBI and other public sources; (iv) novel lipids submitted to peer-reviewed journals; (v) computationally generated structures for appropriate classes.

→ **Klasifikace podle LIPID MAPS systému**

→ **Přidělení ID**

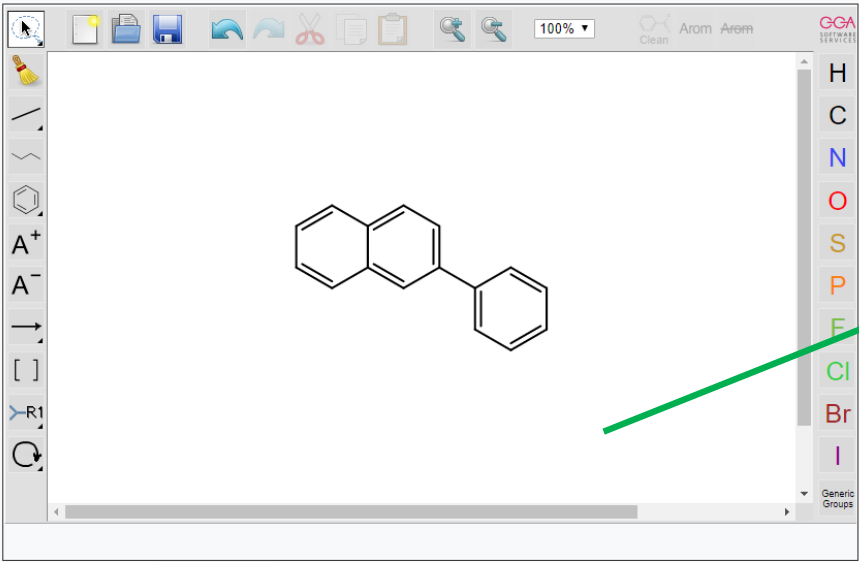
LIPID ID (LM ID) format

Characters	Position	Description
LMFA01030001	1–2	Database designation
LMFA01030001	3–4	Two-letter category code
LMFA01030001	5–6	Two-digit class code
LMFA01030001	7–8	Two-digit subclass code
LMFA01030001	9–12	Unique four character identified with in a subclass

# Lipidy – strukturní databáze

- Třídění lipidů a informatika lipidů obecně je, ve srovnání s proteiny a nukleovými kyselinami, poměrně nový obor.
- **LIPID MAPS Structure Database (LMSD)**

Structure-based search using GGA Ketcher



Search type: Substructure

LM ID:

Name(Common, Systematic, or Synonym):

Include:  All records  Curated records only  Computationally generated records only

Records per page: 50

Sort by: LM\_ID

Submit Reset

## LMSD: Structure-based search results

Modify Search

LM_ID	Common Name	Systematic Name	Formula	Mass	Main Class	Sub Class
<a href="#">LMPR0103330002</a>	Gossypol ( <a href="#">W</a> <a href="#">E</a> )	-	C <sub>30</sub> H <sub>30</sub> O <sub>8</sub>	518.1941	Isoprenoids [PR01]	C15 isoprenoids (sesquiterpenes) [PR0103]

LIPID MAPS does not verify the accuracy of this Wikipedia entry

Download results CSV

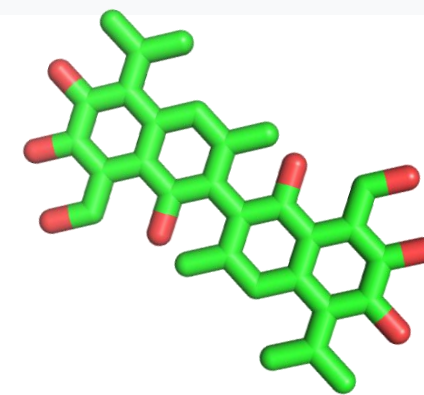
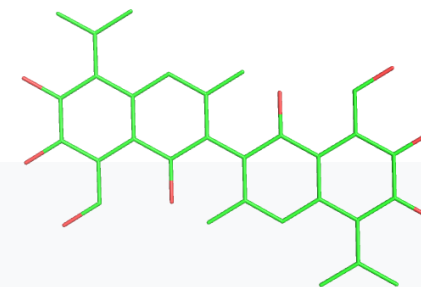
## Gossypol

From Wikipedia, the free encyclopedia

*Not to be confused with Gossypetin.*

**Gossypol** is a natural phenol derived from the cotton plant (genus *Gossypium*). Gossypol is a phenolic aldehyde that permeates cells and acts as an inhibitor for several dehydrogenase enzymes. It is a yellow pigment.

Among other things, it has been tested as a male oral contraceptive in China. In addition to its putative contraceptive properties, gossypol has also long been known to possess antimalarial properties.<sup>[1]</sup>



# (Bio)informatické nástroje

Nástroje pro grafické znázornění lipidů

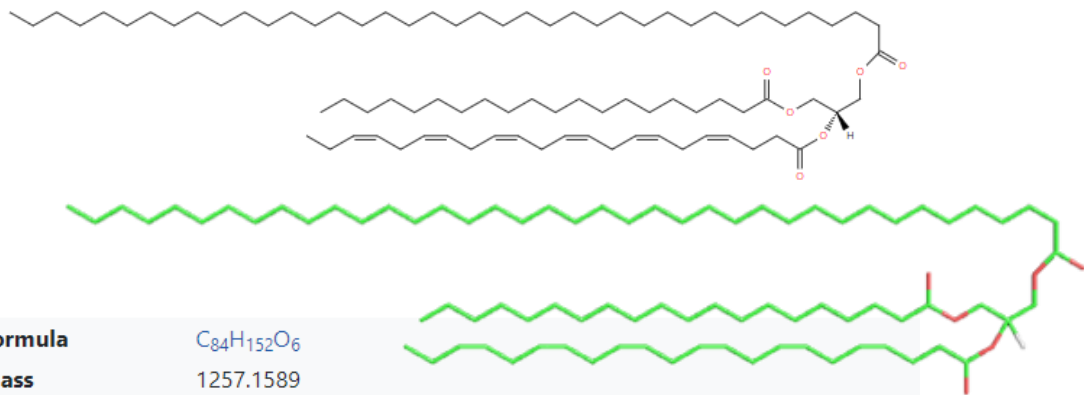
Lipid Structure Drawing Tools

sn1-Acyl group  
20:0

sn2-Acyl group  
22:6(4Z,7Z,10Z,13Z,16Z,19Z)

sn3-Acyl group  
39:0

Submit Reset



Nástroje pro MS analýzu lipidů

Mass Spectrometry Tools

Product ion calculation tool for Glycerolipids (+ ion mode)

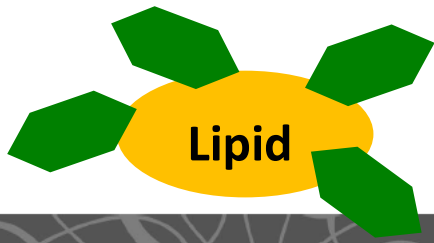
Ion  $[M+NH_4]^+$  sn1 20:0 sn2 22:6(4Z,7Z,10Z,13Z,16Z,19Z) sn3 26:0

Submit Reset

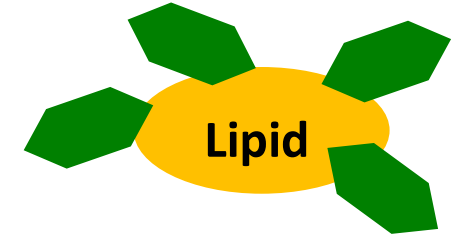
Commonly occurring product ions for TG(20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/26:0)

m/z	Ion Description
1092.9893	Precursor ion $[M+NH_4]^+$
1075.9627	Precursor ion $[M+H]^+$
1057.9521	Precursor ion $[M+H]^+$ with loss of H <sub>2</sub> O
763.6599	Neutral loss of sn1 RCOOH + NH <sub>3</sub> from $[M+NH_4]^+$
747.7225	Neutral loss of sn2 RCOOH + NH <sub>3</sub> from $[M+NH_4]^+$
679.5660	Neutral loss of sn3 RCOOH + NH <sub>3</sub> from $[M+NH_4]^+$
453.4302	sn3 acyl chain $[(RC=O)+74]^+$
435.4196	sn3 acyl chain $[(RC=O)+74]^+$ with loss of H <sub>2</sub> O
385.2737	sn2 acyl chain $[(RC=O)+74]^+$
379.3934	sn3 acyl chain $[(RC=O)^+]$
369.3363	sn1 acyl chain $[(RC=O)+74]^+$
367.2631	sn2 acyl chain $[(RC=O)+74]^+$ with loss of H <sub>2</sub> O
361.3829	sn3 acyl chain $[(RC=O)^+]$ with loss of H <sub>2</sub> O
351.3257	sn1 acyl chain $[(RC=O)+74]^+$ with loss of H <sub>2</sub> O
311.2369	sn2 acyl chain $[(RC=O)^+]$
295.2995	sn1 acyl chain $[(RC=O)^+]$
293.2264	sn2 acyl chain $[(RC=O)^+]$ with loss of H <sub>2</sub> O
277.2890	sn1 acyl chain $[(RC=O)^+]$ with loss of H <sub>2</sub> O





# Lipidy + sacharidy



- Antigeny
- Receptory
- Adheze

- Lipidová část slouží k ukotvení v membráně

## Glycolipids: Animal

Hakomori Sen-iron, Pacific Northwest Research Institute and University of Washington, Seattle, Washington, USA

Ishizuka Ineo, Teikyo University School of Medicine, Tokyo, Japan

Glycolipids are carbohydrates linked to lipid (either ceramide or glyceride). They are found in animal cells and tissues.

### Introduction

Glycolipids are ubiquitous components of all animal cell membranes and are particularly abundant at the cell surface membrane. The majority of glycolipids belong to the class 'glycosphingolipids' (GSLs; also called sphingoglycolipids), which have a backbone lipid (termed 'ceramide') consisting of fatty acids and a long-chain aliphatic amino alcohol, discovered and named 'sphingosine' by JLW Thudichum in 1876. Sphingosine has the structure 1,3-dihydroxy-2-amino-octadecene, exhibiting the D-erythro stereoconfiguration with regard to the asymmetric carbon 1 (C1), C2 and C3 (Figure 1a). Fatty acids with various chain lengths are linked to the 2-amino group of sphingosine to form ceramide (Figure 1b). Various sugar residues are linked to the C1 primary hydroxyl group of the sphingosine moiety in ceramide to form galactosylceramide (GalCer) (Figure 1c), glucosylceramide (GlcCer) (Figure 1d), or a variety of more complex oligosaccharides, resulting in a wide variety of GSLs. One example of such a structure, 'GM3', which has sialic acid, galactose and glucose, is shown in Figure 1e. The sugar linkage to the C1 hydroxyl group of ceramide is always  $\beta$ , with only a single known exception –  $\alpha$ -Gal ceramide, which is found in sea anemones.

GSLs are also found in plants, including yeast, although the ceramide and carbohydrate structures are distinctively different from those of animal GSLs. The ceramide of plant GSLs has a sphingosine analogue, termed 'phytosphingosine', which has an additional hydroxyl group at the C4 position. The carbohydrate moiety of plant GSLs has a novel glycan, termed 'phytoglycosphingolipid', consisting of phosphoinositol, glucosamine and mannose. GSLs are rarely found in bacteria, except for a novel group of 'sphingobacteria' that includes *Sphingomonas paucimobilis*.

A further class of glycolipids, termed 'glycoglycerolipids', has been found and characterized. They have 1,2-diacyl-sn-glycerol or 1-alkyl-2-acyl-sn-glycerol as a backbone lipid, to which a monosaccharide or relatively short oligosaccharide is linked through the primary hydroxyl group (Figure 2). Only two glycoglycerolipids have been well characterized as animal tissue components. Their distribution is limited to the nervous system (brain, spinal cord, peripheral nerves) and testis. In contrast to animal tissues, glycoglycerolipids are the major component in plants and bacteria.



doi: 10.1002/9780470015902.a0000706.pub.2

Another class of glyceroglycolipids is the 'glycosylphosphatidylinositol anchor' (GPI anchor). A large number of functionally important cell-surface proteins are anchored through this class of glycolipids (see below).  
**See also:** Glycolipids: distribution and biological function

### Structure

The most extensive studies on the structure and function of animal cell glycolipids have been focused on GSLs. GSLs consist of two distinct moieties: ceramide, which is hydrophobic, and carbohydrate, which is hydrophilic. A molecular model of GSL based on X-ray crystallography indicates that the axis of the ceramide is perpendicular to the axis of the carbohydrate chain. GSLs have a strong tendency to aggregate to form micelles in aqueous media, or to form microdomains in the cell membrane bilayer.

GSLs from animal tissues are classified according to two criteria: (1) the presence or absence of strongly acidic group (sialic acid or sulfate), or cationic amino group (very rarely present); and (2) differences in core carbohydrate structure. Four subclasses based on criterion (1) are neutral GSLs, gangliosides (GSLs containing sialic acid), sulfatide (sulfated GSL) and a few cationic GSLs having free amino group. Three subclasses based on criterion (2) are: ganglio-series, lacto-series and globo-series GSLs. In the current literature, approximately 50 ganglio-series, 80 lacto-series and 10 globo-series GSLs are known. For ganglio-series GSLs, 2 neutral, 7 sulfated and ~40 sialylated species are known. For lacto-series, 14 neutral, 2 sulfated, ~30 sialylated and ~32 fucosylated species are known. In some cases, hybrid types between the lacto- and ganglio-series or between the globo- and lacto-series have been observed. In certain protozoa, parasites and marine invertebrates, novel GSL structures have been observed that cannot be assigned to any of the three subclasses described above.

### Neutral glycosphingolipids

The most abundant GSL in animal tissues is galactosylceramide (GalCer; cerebroside) in brain, discovered by

## Create a Sphingolipid Glycan Structure

Core:

Core chain style:

Glycan:

Glycan chain orientation:

### Usage

Sugar residues allowed:

**Glc, Gal, Man, GlcNAc, GalNAc, Xyl, Fuc, NeuAc, NeuGc, KDN**

Glycan sequence must be in the format:

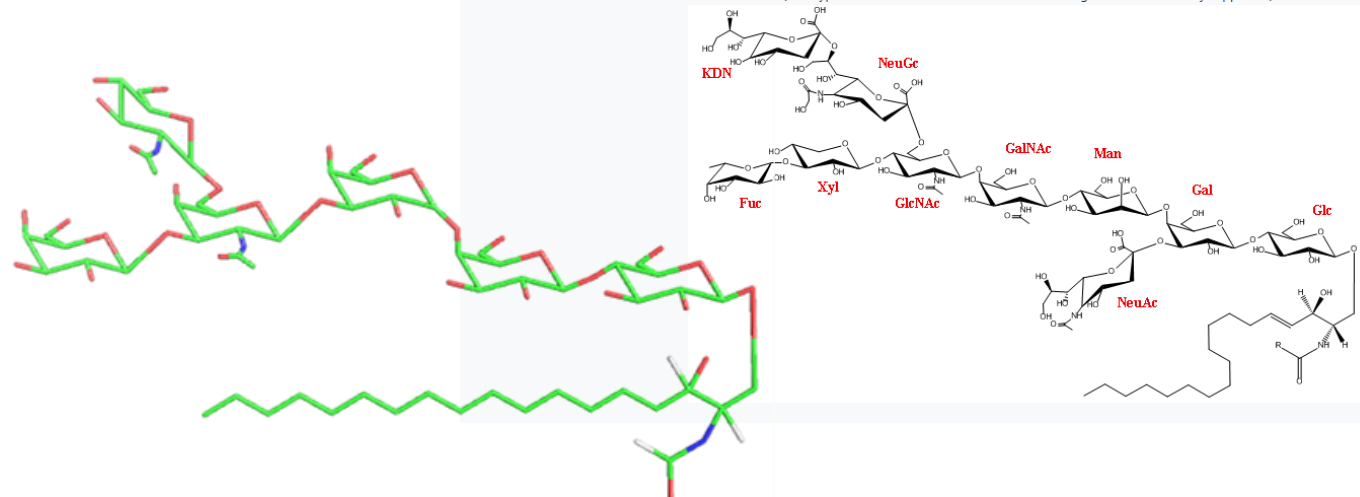
**[sugar (as an abbreviation)][anomer (either a or b)][linkage in (x-y form)]**

Examples:

Galb1-4Glc, Fucal-2Galb1-3GalNAcb1-4Galb1-4Glc, NeuAca2-3Galb1-3GalNAcb1-3Gala1-4Galb1-4Glc

Branched glycans are designated by parentheses: GalNAca1-3GalNAcb1-3(Galb1-3GalNAcb1-4)Gala1-4Galb1-4Glc

(The hypothetical structure below contains all 10 sugar residues currently supported)







# Lipidy + proteiny

## MINIREVIEWS

### Lipoproteins of Bacterial Pathogens<sup>∇</sup>

A. Kovacs-Simon, R. W. Titball, and S. L. Michell\*

## LipoP - 1.0

### Signal peptidase I & II cleavage sites in gram- bacteria

The LipoP 1.0 server produces predictions of lipoproteins and discriminates between lipoprotein signal peptides, other signal peptides and n-terminal membrane helices in Gram-negative bacteria.

**Note:** Although LipoP 1.0 has been trained on sequences from Gram-negative bacteria only, the following paper reports that it has a good performance on sequences from Gram-positive bacteria also:

[Methods for the bioinformatic identification of bacterial lipoproteins encoded in the genomes of Gram-positive bacteria](#)

O. Rahman, S. P. Cummings, D. J. Harrington and I. C. Sutcliffe

*World Journal of Microbiology and Biotechnology* **24**(11):2377-2382 (2008)

<https://services.healthtech.dtu.dk/service.php?LipoP-1.0>



We present a Hidden Markov Model method for the prediction of lipoprotein signal peptides of Gram-positive bacteria, trained on a set of 67 experimentally verified lipoproteins.

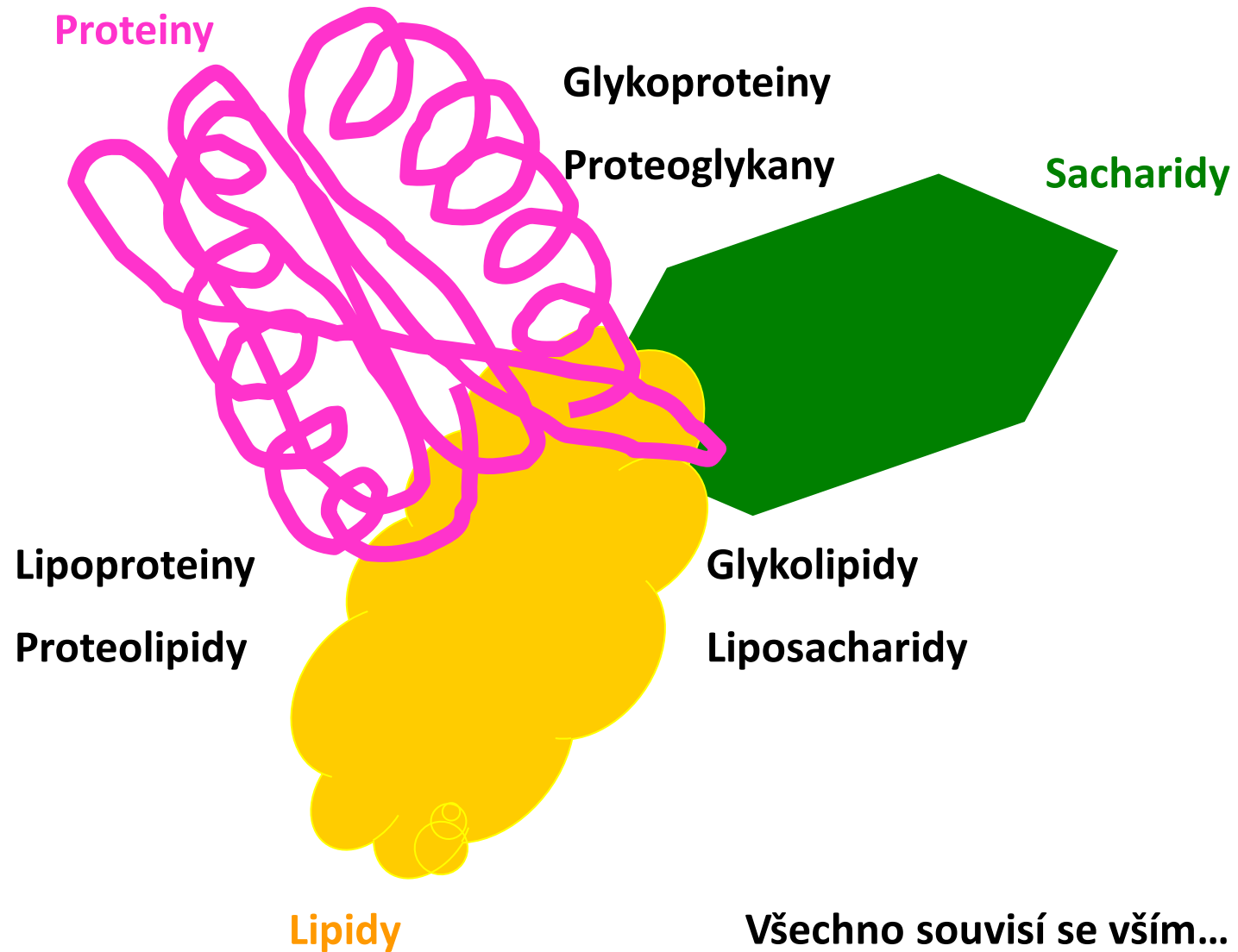
The method outperforms LipoP and the methods based on regular expression patterns, in various data sets containing experimentally characterized lipoproteins, secretory proteins, proteins with an N-terminal TM segment and cytoplasmic proteins.

The method is also very sensitive and specific in the detection of secretory signal peptides and in terms of overall accuracy outperforms even SignalP, which is the top-scoring method for the prediction of signal peptides.

**Abstract** Bacterial lipoproteins are a diverse and functionally important group of proteins that are amenable to bioinformatic analyses because of their unique signal peptide features. Here we have used a dataset of sequences of experimentally verified lipoproteins of Gram-positive bacteria to refine our previously described lipoprotein recognition pattern (G+LPP). Sequenced bacterial genomes can be screened for putative lipoproteins using the G+LPP pattern. The sequences identified can then be validated using online tools for lipoprotein sequence identification. We have used our protein sequence datasets to evaluate six online tools for efficacy of lipoprotein sequence identification. Our analyses demonstrate that LipoP (<http://www.cbs.dtu.dk/services/LipoP/>) performs best individually but that a consensus approach, incorporating outputs from predictors of general signal peptide properties, is most informative.

<http://bioinformatics.biol.uoa.gr/PRED-LIPO/>





# Použitá a doporučená literatura

## Terminology of bioanalytical methods (IUPAC Recommendations 2018)

<https://doi.org/10.1515/pac-2016-1120>

Received November 21, 2016; accepted February 1, 2018

## Evolutionary aspects of ABO blood group in humans

Massimo Franchini\*, Carlo Bonfanti

Department of Hematology and Transfusion Medicine, Azienda Ospedaliera Carlo Poma, Mantova, Italy

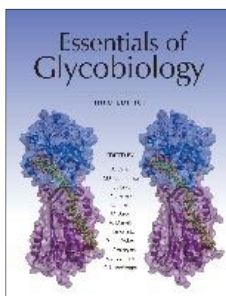
### ABSTRACT

The antigens of the ABO blood group system (A, B and H determinants) are complex carbohydrate molecules expressed on red blood cells and on a variety of other cell lines and tissues. Growing evidence is accumulating that ABO antigens, beyond their key role in transfusion medicine, may interplay with the pathogenesis of many human disorders, including infectious, cardiovascular and neoplastic diseases. In this narrative review, after succinct description of the current knowledge on the association between ABO blood groups and the most severe diseases, we aim to elucidate the particularly intriguing issue of the possible role of ABO system in successful aging. In particular, focus will be placed on studies evaluating the ABO phenotype in centenarians, the best human model of longevity.

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## New insights into influenza A specificity: an evolution of paradigms

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### Technical Note

## SugarSketcher: Quick and Intuitive Online Glycan Drawing

Davide Alocci<sup>1,2</sup>, Pavla Suchánková<sup>3,4</sup>, Renaud Costa<sup>5</sup>, Nicolas Hory<sup>5</sup>, Julien Mariethoz<sup>1,2</sup>, Radka Svobodová Vařeková<sup>3,4</sup>, Philip Toukach<sup>6</sup> and Frédérique Lisacek<sup>1,2,7,\*</sup>



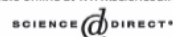
## Lectins

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Based in large part on the previous version of this *Encyclopedia of Life Sciences (ELS)* article, *Lectins* by Nathan Sharon and Holina Lk.



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## Lectin-mediated drug targeting: history and applications

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## Multivalent glycoconjugates as anti-pathogenic agents†

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*Glycoconj J* (2013) 30:41–50  
DOI 10.1007/s10719-012-9397-y

## Genomics and epigenomics of the human glycome

Vlatka Zokloš · Mislav Novokmet · Ivona Bečeheli · Gordan Lauc

Feng Li<sup>1,2</sup>, Olga V. Glinskii<sup>1,3</sup> and Vladislav V. Glinsky<sup>1,2</sup>

*Proteomics* 2013, **13**, 341–354

DOI 10.1002/pmic.201200149

## Host cell recognition by the henipaviruses: Crystal structures of the Nipah G attachment glycoprotein and its complex with ephrin-B3

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# Použitá a doporučená literatura

## Glycoproteins

Tony Merry, *University of Manchester, Manchester, UK*

Sviatlana Astrautsova, *Grodno State Medical University, Grodno, Belarus*

Based in part on the previous version of this *Encyclopedia of Life Sciences (ELS)* article, "Glycoproteins" by "Terry D Butters".

## Glycolipids: Animal

Hakomori Sen-itiroh, *Pacific Northwest Research Institute and University of Washington, Seattle, Washington, USA*

Ishizuka Ineo, *Teikyo University School of Medicine, Tokyo, Japan*

Glycolipids are carbohydrates linked to lipid (either ceramide or glyceride). They are found in animal cells and tissues.

Advanced article

Article Contents

- Introduction
- Structure
- Synthesis and Degradation
- Function
- Conformational Structure, Distribution and Organization of Glycosphingolipids in Membrane

## Lipid classification, structures and tools\*

Eoin Fahy\*, Dawn Cotter, Manish Sud, and Shankar Subramaniam

University of California, San Diego, 9500 Gilman Dr., La Jolla, CA 92093-0411, USA

## MINIREVIEWS

Lipoproteins of Bacterial Pathogens<sup>∇</sup>

A. Kovacs-Simon, R. W. Titball, and S. L. Michell\*

## Kazuistika dívky s dědičnou poruchou glykosylace

MUDr. Martin Magner, Ing. Kateřina Veselá, RNDr. Hana Hansíková, CSc.,

prof. MUDr. Jiří Zeman, DrSc., MUDr. Tomáš Honzík, Ph.D.

Klinika dětského a dorostového lékařství, 1. LF UK a VFN Praha

Identification of novel N-glycosylation sites at non-canonical protein consensus motifs

Mark S. Lowenthal<sup>1</sup>, Kiersta S. Davis, Trina Formolo, Lisa E. Kilpatrick, and Karen W. Phinney

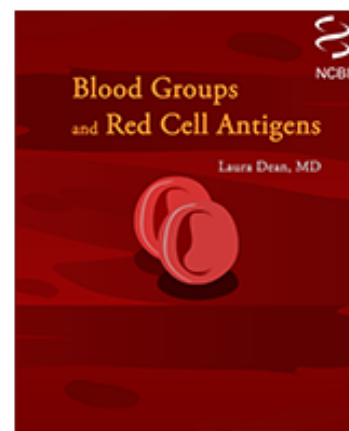
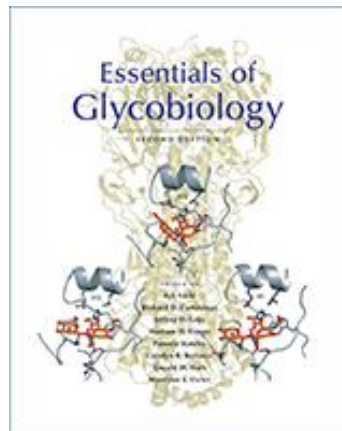
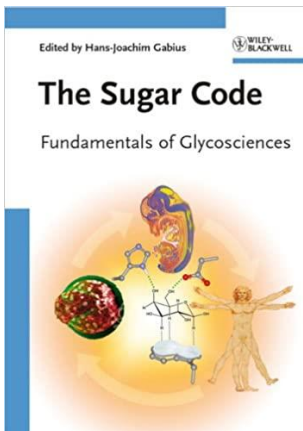
## Building and rebuilding N-glycans in protein structure models

Bart van Beusekom,<sup>a</sup> Natasja Wezel,<sup>a</sup> Maarten L. Hekkelman,<sup>a</sup> Anastassis Perrakis,<sup>a</sup> Paul Emsley<sup>b</sup> and Robbie P. Joosten<sup>\*\*</sup>

## Lipidomics: a global approach to lipid analysis in biological systems

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## Sweet new world: glycoproteins in bacterial pathogens

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