

## GlyTouCanの更新および GlyCosmos Portalの公開

木下聖子 2019年12月3日

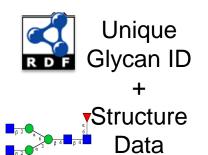
第42回日本分子生物学会年会

# Glycan Databases \*\*ClycomeDB\*\* \*\*C









Sharing

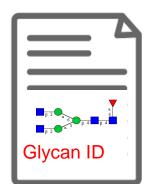


2

**4** Curation







Research Paper



Glycan ID



Knowledge-Sharing
of Glycan Knowledge

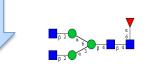
via Internet











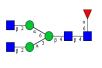


Glycan Research



## New GlyTouCan 3.0 (August, 2019)













Assign



#### Instant assignment of structures:

- Input data limited to GlycoCT & WURCS
- Only simple verification of accuracy
- Structures registered simultaneously could be duplicated



### **Batch Processing Phase:**

- Validates inputted data
- Generates images
- Assigns ID

### Advantages:

- Input data can be anything translatable to WURCS (GlycanFormatConverter)
- Validation status can be viewed on Profile Page
- Structure duplication can be avoided

### **User Profile Page:**

- Validation results
- Images
- Assigned ID





## GlyCosmos Overview



#### Repositories



The glycan structure repository GlyTouCan

assigns accession numbers to glycans



#### The glyco(proteo)mics repository GlycoPOST

stores mass spectrometry data obtained from glyco-(proteo)mics related experiments.

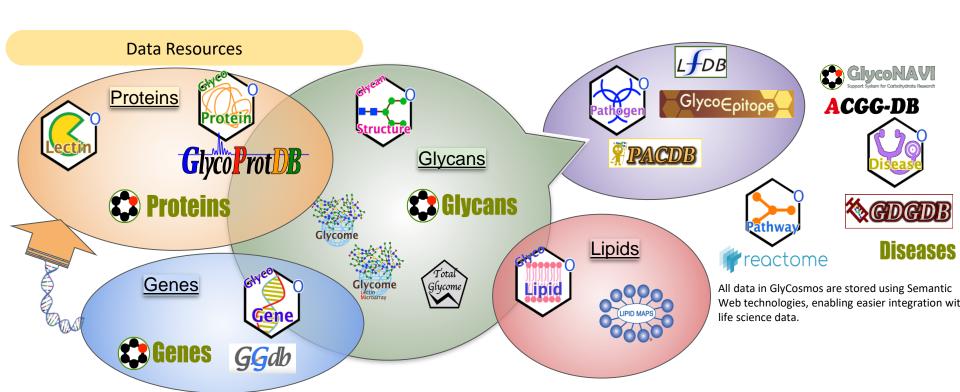
UniProt ID/Lipid MAPS ID + glycosylation site + GlyTouCan ID







### The Glycoconjugate repository GlyComb (TBA) will assign accession numbers to glycoconjugates such as glycoproteins, glycolipids



Submissions

Resources

Genes/Proteins/Lipids

(2) (G) GDGDB (glyco-disease genes)

(2) (a) LIPID MAPS Gene/Proteome DB

GlyCosmos Glycoproteins (glycoproteins)

GlycoNAVI-Proteins

GlyCosmos Glycolipids

Glycans/Glycoconjugates GlyCosmos Glycans

(Q) GlyCosmos Glycoproteins

GlycoProtDB (glycoproteins)

**©** GlyCosmos Lectins

(LfDB (lectins)

GlycoEpitope

M GlycomeAtlas

M-GlycomeAtlas

Pathways/Diseases

GlyCosmos Pathways

Glycomes Total Glycome Database

GlycoNAVI-Glycans

( GGDB (glycogenes)

@ GlycoNAVI-Genes

(2) FlyGlycoDB

## GlyCosmos

### 正式に日本糖質学会のオフィ シャルポータルとして承認 本年4月1日に公開

#### **Submissions:**

- GlyTouCan
- GlyComb (開発中)
- **GlycoPOST**

#### Resources:

- Genes/Proteins/Lipids
- Glycans/ Glycoconjugates
- Glycomes
- Pathways/Diseases
- **Ontologies**
- **Notations**

Release 2:

August 5, 2019

Release 3:

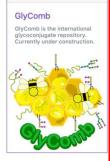
**December 12, 2019** 

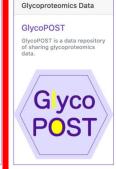


The GlyCosmos Portal is the official web portal of the Japanese Society for Carbohydrate Research (JSCR). It aims to provide a central location from which glycoscience-related web resources can be accessed, including glycan-related genes, proteins, glycoconjugates, diseases and pathways. GlyCosmos is also a member of the GlySpace Alliance, ensuring that all data is openly shared with the glycoscience community.

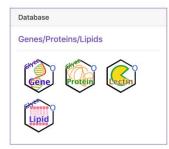
#### Submissions







#### Resources











#### Other Related Resources

Glycoinformatics Consortium (GLIC) provides and maintains a centralized source of software and databases for glycoscientists.

#### Glycomics@ExPASy

is the glycomics section of the SIB Bioinformatics Resource Portal which provides access to scientific databases and software tools in different areas of life sciences.

#### **GlyConnect**

is a platform integrating sources of information to help characterise the molecular components of protein alvcosylation.

is a data integration and dissemination project for carbohydrate and glycoconjugate related data. retrieving information from multiple international data sources, integrating and harmonizing this data via a user friendly Web interface

is a proteomic database to integrate proteome datasets generated from multiple projects and institutions.

#### MIRAGE

"Minimum Information Required for A Glycomics Experiment" guidelines for publishing glycomicsrelated research articles

is part of the Japanese National Project on Protein Structural and Functional Analyses.

is an open chemistry database at the National Institutes of Health (NIH)

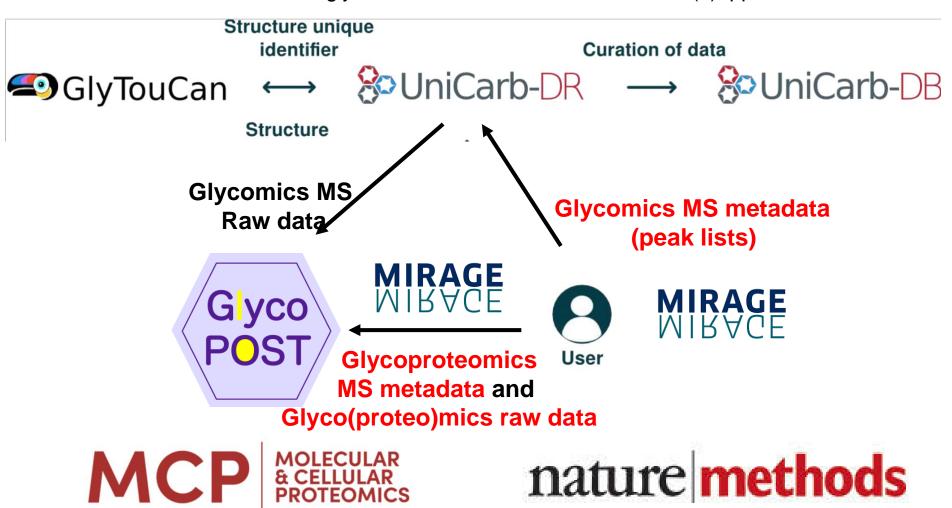
#### UniCarb-DB

is a repository of glycomics mass spectrometry



## **GlycoPOST**

Aoki-Kinoshita, K.F., Karlsson N. et al. Towards a standardized bioinformatics infrastructure for N-and O-glycomics. *Nature communications*, *10*(1), pp.1-10, 2019.













→ Login Login OKA University

#### **About GlycoPOST**

GlycoPOST is a mass spectrometry data repository for glycomics and glycoproteomics. It consists of a high-speed file upload process, flexible file management system and easy-to-use

#### **Statistics**

27 projects are registered. 7 s are opened.

#### **Data list**

ID	Project title	Description	Publication	Principal investigator	Announcement date	Detail
GPST000038	UniCarb-DR	Data from UniCarb-DR	31332201	Niclas G. Karlsson	2019/10/02	Detail page
GPST000027	GnT3 KO mouse brain	Bisecting GlcNAc is a general suppressor of terminal modification of N-glycan	31375533	Miyako Nakano	2019/09/21	Detail page
GPST000031	GnT3 KO mouse kidney	Bisecting GlcNAc is a general suppressor of terminal modification of N-glycan	31375533	Miyako Nakano	2019/09/21	Detail page
GPST000030	Reference glycan structure libraries of primary human cardiomyocytes and pluripotent stem cell-derived cardiomyocytes reveal cell-type and culture stage-specific glycan phenotypes	To generate glycan structure libraries, the current study used porous graphitized carbon (PGC) LC interfaced with MS (PGC-LC-MS), a technique that resolves glycan structures and enables characterizat		Rebekah L. Gundry	2019/08/31	Detail page
GPST000029	Standardization of PGC-LC-MS- based glycomics for sample specific glycotyping	Porous graphitized carbon (PGC) based chromatography achieves high-resolution separation of glycan structures released from glycoproteins. However, the implementation of PGC-based separations in glyco	31065629	Nicolle H Packer	2019/06/28	Detail page
GPST000024	Discrimination of Isomers of Released N- and O-Glycans Using Diagnostic Product Ions in Negative Ion PGC-LC-ESI-MS/MS	We used porous graphitized carbon-LC-ESI-MS/MS to separate and detect released N- and O-glycan isomers from mammalian model glycoproteins using negative mode resonance activation CID-MS/MS. By interro	29603058	Nicolle H. Packer	2019/06/28	Detail page
GPST000009	Atlantic Salmon mucus from skin, pyloric caeca and distal intestine	Diseases cause ethical concerns and economic losses in the Salmonid industry. The mucus layer comprised of highly O-glycosylated mucins is the first contact between pathogens and fish. Mucin glycans g	30923042	Sara Lindén	2019/04/10	Detail page

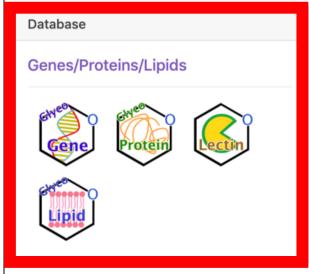
### Resources

#### **Submissions:**

- GlyTouCan
- **GlyComb** (under development)
- **GlycoPOST**

#### Resources:

- Genes/Proteins/Lipids
- Glycans/ Glycoconjugates
- **Glycomes**
- Pathways/Diseases
- **Ontologies**
- **Notations**



Database Glycans/Glycoconjugates





#### Release 2:

August 5, 2019

Release 3:

**December 12, 2019** 



Database **Glycomes** 



Pathways/Diseases







"Minimum Information Required for A Glycomics Experiment" guidelines for publishing glycomicsrelated research articles

is part of the Japanese National Project on Protein Structural and Functional Analyses.

is an open chemistry database at the National

UniCarb-DB is a repository of glycomics mass spectrometry







#### GlycoGene Database (GGDB)

GGDB is a database which includes genes associated with glycan synthesis such as glycosyltransferase, sugar nucleotide synthases, sugar-nucleotide transporters, and sulfotransferases.



#### **GG**db

#### **GlycoNAVI**



#### GlycoNAVI-Genes

GlycoNAVI-Genes is dataset of gene informtion. This is the content of GlycoNAVI. Currently under construction.

- GlycoNAVI

#### LIPID MAPS Gene/Proteome Database (LMPD)



LIPID MAPS Gene/Proteome Database

#### (LMPD)

Lipid-related genes and proteins entry from LIPID MAPS.



#### GlyCosmos Database





#### GlyCosmos Glycoproteins

Glycoprotein entries from UniProt. Glycosylation site information is also shown where available.

#### ACGG-DB





#### GlycoProtDB (GPDB)

GPDB is a glycoprotein database providing information of Asn (N)-glycosylated proteins and their glycosylated site(s), which were constructed by employing a bottom-up strategy using actual glycopeptide sequences identified by LC/MS-based glycoproteomic technologies.

- ACGG-DB

#### GlycoProtDB

#### GlycoNAVI





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#### **GlyCosmos Lectins**

Protein entries from PDB annotated as lectins in UniProt. Glycosylation site information is also shown where available.

#### ACGG-DB



#### Lectin Frontier DataBase (LfDB)

LfDB provides quantitative interaction data in terms of the affinity constants (Ka) of a series of lectins toward a panel of pyridylaminated (PA) glycans obtained by an automated frontal affinity chromatography with fluorescence detection (FAC-FD) system.

- ACGG-DB

LFDB

#### Lipids

#### GlyCosmos Database



#### GlyCosmos Glycolipids

Glycolipid entry from LIPID MAPS.



#### **Expression**

J. Biol. Chem. 1990 Jan 15;265(2):1139-45.

Isolation to homogeneity and partial characterization of a histo-blood group A defined Fuc alpha 1----2Gal alpha 1----3-N-acetylgalactosaminyltransferase from human lung tissue.

Clausen H. et al. PMID:2104827

Vox Sang. 1986 null;51(3):161-71.

Genetics of ABO, H, Lewis, X and related antigens.

Oriol R. et al. PMID: 2433836

Vox Sang. 1989 null;56(1):1-20.

ABH and related histo-blood group antigens; immunochemical differences in carrier isotypes and their distribution.

Clausen H. et al. PMID:2464874

Semin. Hematol. 1981 Jan; 18(1):39-62.

Blood group ABH and Ii antigens of human erythrocytes: chemistry, polymorphism, and their developmental change.

Hakomori S. PMID:6782678

kidney

lung

#### **Biological Resources**

GGENTRtr code	GGENTRtr-85
Official Symbol	ABO
Vector	pENTR/D-TOPO
Fusion Site	aaa aaa gca ggc tcc gcg gcc gcc ccc ttc acc AGT CTA ATG CCA GGA AGC CTG GAA CGG GGG TTC TGC ATG GCT GTT AGG GA CAG CAG TGC AAC CCC GAT GGG CCG CTG GG
Contract	一般寄託 <u>NBRC</u>



#### **Proteins**

#### ACGG-DB



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- ACGG-DB

#### GlycoProtDB

#### GlycoNAVI





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— GlycoNAVI

#### GlyCosmos Database



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- ACGG-DB

L+DB

#### Lipids

#### GlyCosmos Database



#### GlyCosmos Glycolipids

Glycolipid entry from LIPID MAPS.

### SOKA University

## GlyCosmos Glycoproteins



GlyCosmos Portal Submissions ▼ Resources ▼

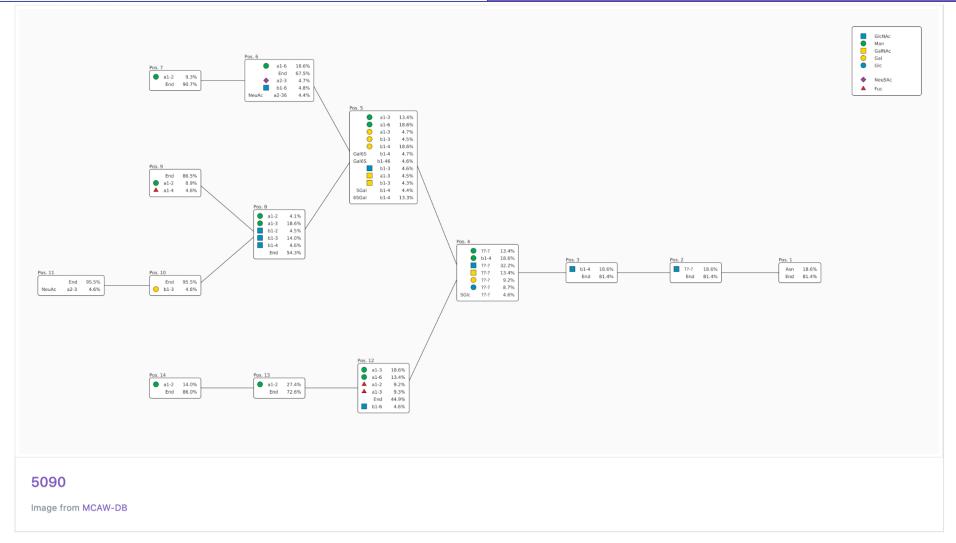
### **SUBMISSIONS** GlyTouCan GlyComb SST GlycoPOST **RESOURCES** Genes/Proteins/Lipids GGDB - glycogenes GDGDB - glycogene diseases GlycoNAVI-Genes GlycoProtDB - glycoproteins LfDB - lectins GlycoNAVI-Proteins GlycoProteins Glycans/Glycoconjugates GlyCosmos Glycans GlycoProtDB - glycoproteins GlycoNAVI-Glycans

### Glycoproteins list

Extracted glycoproteins list from UniProt

Protein	UniProt	Number of Glycoslationsites	Gene Symbol	Organism
Sodium channel subunit beta-1	A5A6L6	4	SCN1B	Pan troglodytes
Killer cell immunoglobulin-like receptor 2DS4	P43632	5	KIR2DS4	Homo sapiens
Matrix protein 2	A0A290YQ92	1	M2	Influenza A virus (A/Canada/32A/2015(H3N2
Matrix protein 2	F0TU71	1	M2	Influenza A virus (A/Puerto Rico/8-V24/1934
Matrix protein 2	C4LP44	1	M2	Influenza A virus (A/Managua/68.01/2007(H3
Germin-like protein subfamily 3 member 3	P94072	1	GER3	Arabidopsis thaliana
Type 2 lactosamine alpha-2,3- sialyltransferase	Q6KB54	6	ST3GAL6	Pan troglodytes
BTB/POZ domain-containing protein	Q9XWH8	6	btb-14	Caenorhabditis elegans

**Glycomes** 



#### **Human Protein Atlas**

Tissue with high expression from Human Protein Atlas

skin

Open LiteMol Viewer Open LiteMol Viewer Open LiteMol Viewer ation Site from UniProt ]



### **GlyCosmos Portal**

Portal Submissions • Resources

Heln



#### **Glycome Database**



#### **Total Glycome Database**

N-glycan, O-glycan, sphingolipids, glycosaminoglycans and free glycans as quantified from various types of cells.

#### **Glycome Database**



#### **GlycomeAtlas**

Visualization of glycome profiling data on human, mouse and zebrafish tissue samples.

#### **Glycome Database**

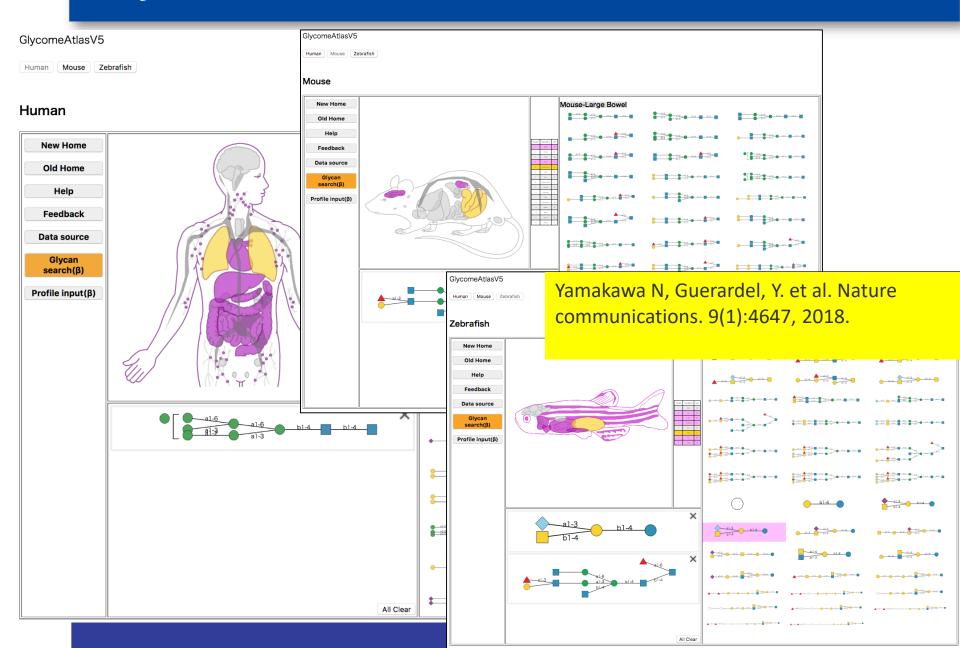


#### LM-GlycomeAtlas

LM-GlycomeAtlas is a web tool visualizing the data from Lectin Array analyses by the Kuno Laboratory at AIST.



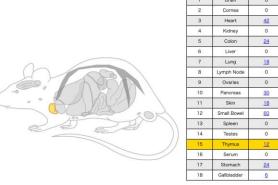
### **GlycomeAtlas**



### LM-GlycomeAtlas

- Glycome
- LM-GlycomeAtlas v.1.0 is a web tool visualizing the data from Lectin Microarray analyses using <u>45 lectins</u> by the Kuno Laboratory at AIST.

- Web tool to visualize laser microdissection-assisted lectin microarray analyses data using 45 lectins
  - high-throughput and in-depth glycomic profiling of formalinfixed paraffin-embedded tissue sections





Zoom In Zoom Out Rese

All Data	Averaged	Data

Molecules 2019, 24(16), 2962; https://doi.org/10.3390/molecules24162962

Open Access

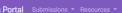
Article

### LM-GlycomeAtlas Ver. 1.0: A Novel Visualization Tool for Lectin Microarray-Based Glycomic Profiles of Mouse Tissue Sections

by Chiaki Nagai-Okatani <sup>1,\*</sup> □ □, Kiyoko F Aoki-Kinoshita <sup>2</sup> □, Shuichi Kakuda <sup>1</sup>, Misugi Nagai <sup>1</sup>, Kozue Hagiwara <sup>1</sup>, Katsue Kiyohara <sup>1</sup>, Noriaki Fujita <sup>1</sup>, Yoshinori Suzuki <sup>1</sup>, Takashi Sato <sup>1</sup>, Kiyohiko Angata <sup>1</sup> and Atsushi Kuno <sup>1,\*</sup> □ □

- <sup>1</sup> Glycoscience and Glycotechnology Research Group, Biotechnology Research Institute for Drug Discovery, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8568, Japan
- <sup>2</sup> Glycan & Life Science Integration Center (GaLSIC), Faculty of Science and Engineering, Soka University, Hachioji, Tokyo 192-8577, Japan
- \* Authors to whom correspondence should be addressed.

Received: 27 June 2019 / Accepted: 12 August 2019 / Published: 15 August 2019



#### Welcome to GlyCosmos!

As a foundation for integrating glycoscience research, we have started developing the Glycoscience Portal called GlyCosmos.

#### **♣** Submissions

GlyTouCan GlvTouCan is the international glycan structure repository.





glycoproteomics data.



#### Resources

Database











Database







GlvCosmos Pathway Database



✓ News

The heta version of the GlyCosmos Portal has her

Load more Tweets

Other Related

Resources

maintains a centralized source of software and databases for

Glycoinform atics Consortium

mics@ExPASy

is the alycomics section of the SIB formatics Resource Portal which

is a platform integrating sources of information to help characterise the molecular components of protein glycosylation.

A data integration and dissemination

data sources, integrating and harmonize this data via a user friendly Web interface

is a proteomic database to integrate

proteome datasets generated from multiple projects and institutions.

"Minimum Information Required for A

Glycomics Experiment" guidelines for

publishing glycomics-related research

**PDBi** 

project for carbohydrate and glycoconjugate related data, retrieving information from multiple international

privides access to scientific databases

d software tools in different areas of lif

provides an

glycoscie

Glyce

Tweets by @GlyCosmos

released! glycosmos.org

#### GlyCosmos Pathways

Pathways from Reactome containing glycoproteins as annotated in UniProt.

GlvCosmos link

#### Diseases

ACGG-DB



#### Glyco-Disease Genes Database(GDGDB)

GDGDB is a database of glycan-related diseases and their responsible genes.

- ACGG-DB in ACGG

ACGG-DB



### Pathogen Adherence to Carbohydrate Database

(PACDB)

PACDB provides the information on pathogens (e.g. bacteria, fungus, toxin and virus) adhering to carbohydrates expressed on the cell surface of host animals or plants.

- ACGG-DB in ACGG

https://acgg.asia/db/diseases/pacdb

#### GlycoNAVI



#### GlycoNAVI-Diseases

https://acgg.asia/db/diseases/gdgdb

GlycoNAVI-Diseases is dataset of glycanform for diseases. This is the content of GlycoNAVI. Currently under construction.

- GlycoBio in GlycoNAVI

GlycoNAVI link

Twitter GitHub





Supported by National Bioscience Database Center (NBDC) of Japan Science and Technology Agency (JST).

Funded by NIH Common Fund.

Grant # 1U01GM125267 - 01

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Powered by Ruby on Rails.

Based on Bootstrap, Icons from Font Awesome. Web fonts from Google.



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♠ Back To Top



## GlyCosmos Pathways

#### Pathway Names:

e.g. Metabolism

#### Click on a Pathway Name from the list below.

In the pathway map tree, click on circles to open/close subpathways, and click on pathways whose names are highlighted in light blue to view the detailed pathway map.

#### Keywords:

Homo sapiens 🛘 ragulator complex pro

#### Event Hierarchy:

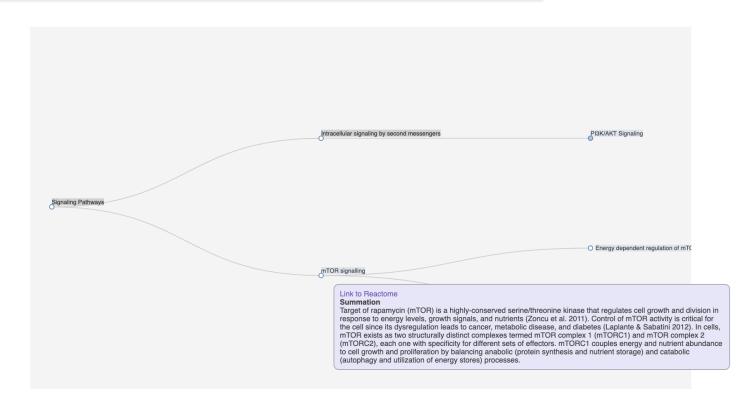
<u>Autophagy</u>

Cellular responses to external stimuli

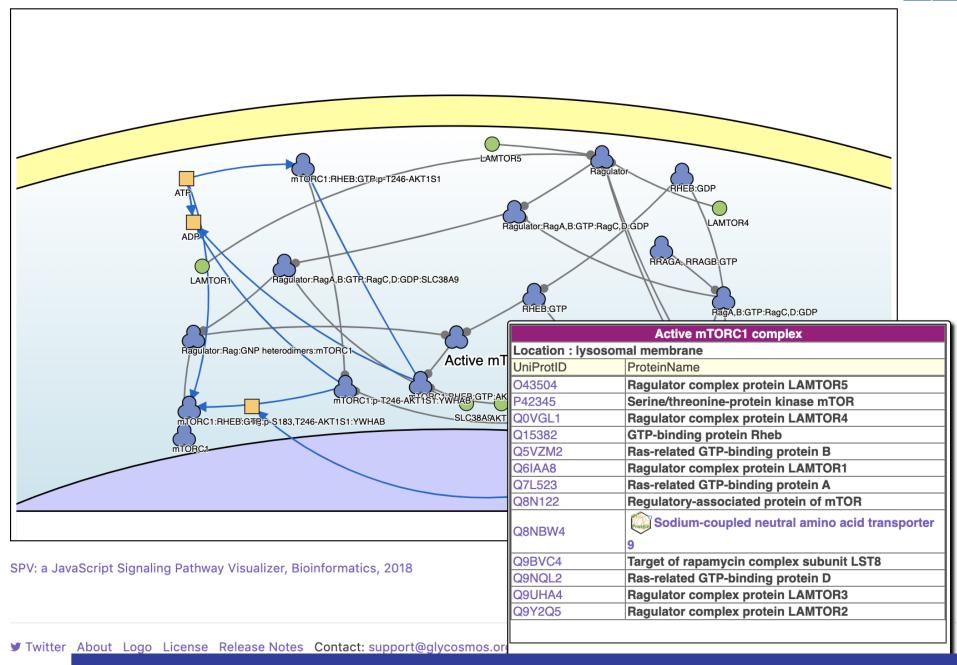
Gene expression (Transcription)

Immune System

Signaling Pathways

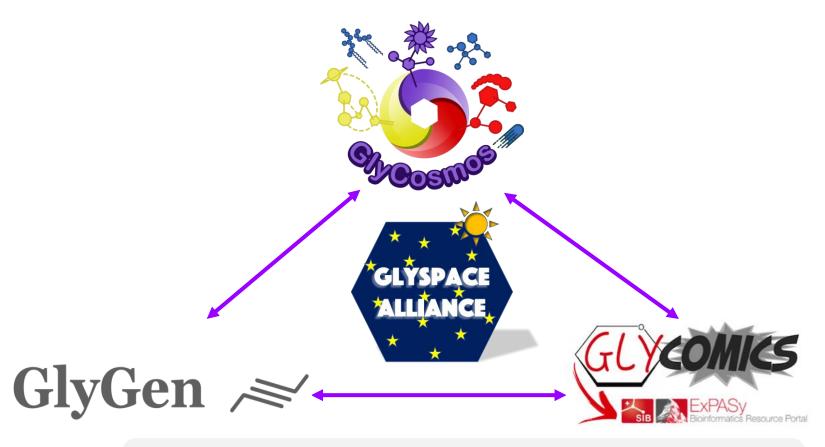


?nathway=mTOR signalling&species=48



### **SOKA University**

## GlySpace Alliance



Established August, 2018 @ Warren Workshop

http://glyspace.org

## GlySpace Alliance



目的: データの共有や連携についての合意を得ること

### 基本的な合意:

- データもソフトウェアも無料でオープンソースのライセンスで提供する
- 共通の標準を利用する(オントロジー、アクセッション番号など)
- 年1回の対面会議
  - 他のデータベースやソフトウェアのプロジェクトとの連携の議論など

### 現在の参加メンバー

- 糖鎖関連のマルチオミックス統合プロジェクト
- GlyConnect, GlyCosmos and GlyGen

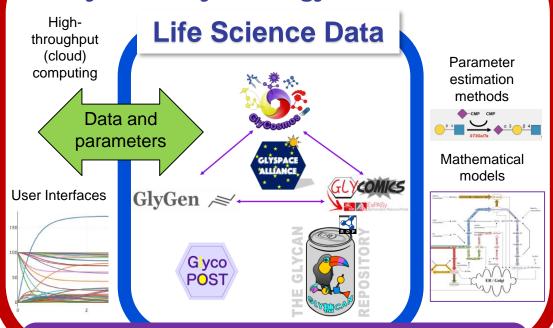
Established August, 2018 @ Warren Workshop

## Systems Glycobiology Consortium Soka University

Open Data

**Dynamic aspects of Glycobiology** 

**Systems Glycobiology Consortium** 



True understanding of glycan function and applications in medicine, agriculture, energy, etc.

#### 目的:

システム糖鎖生物学研究のため のオープンプラットフォーム の開発

- ・データベース
  - ・グライコミクス
  - ・トランスクリプトミクス
  - ・プロテオミクスなど
  - ・反応パラメーター
  - ・パスウェイモデル
- ・ソフトウェアモジュール
  - オンラインでシミュレーションを実施するツール

## まとめ

- GlyCosmos が糖鎖関連データの基盤を提供している
  - 4ヶ月おきのリリースを通して継続的にデータの更新を実施している
- GlySpace Allianceと共同に信頼できるデータを共有している
- 今後の発展として、ダイナミクスを含む糖鎖の機能解析を可能にする
- 日本糖質学会のオフィシャルポータルとして、コミュニティーからのコメント、提案、改良を歓迎

support@glycosmos.org



## Acknowledgements

#### **Soka University**

Masaaki Shiota

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Shinichiro Tsuchiya

Akihiro Fujita

Haruko Kitakaze

#### **AIST**

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Kiyohiko Angata

Hisashi Narimatsu

Atsushi Kuno

Chiaki Nagai-Okatani





#### **Niigata University**

Shujiro Okuda

Yu Watanabe

#### The Noguchi Institute

Issaku Yamada

#### **SPARQLite, LLC**

Nobuyuki P. Aoki Daisuke Shinmachi

#### GlyTouCan Users

### Funding agencies:

Integrated Database Project (Japan Science and Technology Agency (JST) and National Bioscience Database Center and NIH

#### **Collaborators**

Miguel Rojas
Niclas Karlsson
Julien Mariethoz
Frederique Lisacek

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Toshisuke Kawasaki

Shoko Nishihara

Nicki Packer

Carsten Kettner

Stuart Haslam

William S. York

