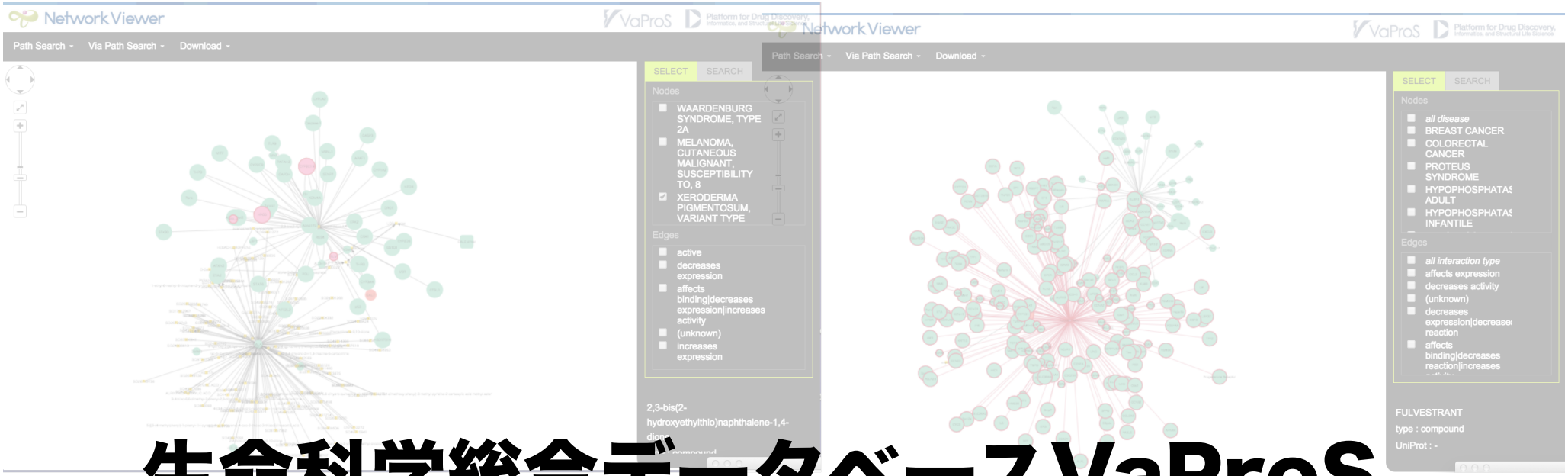
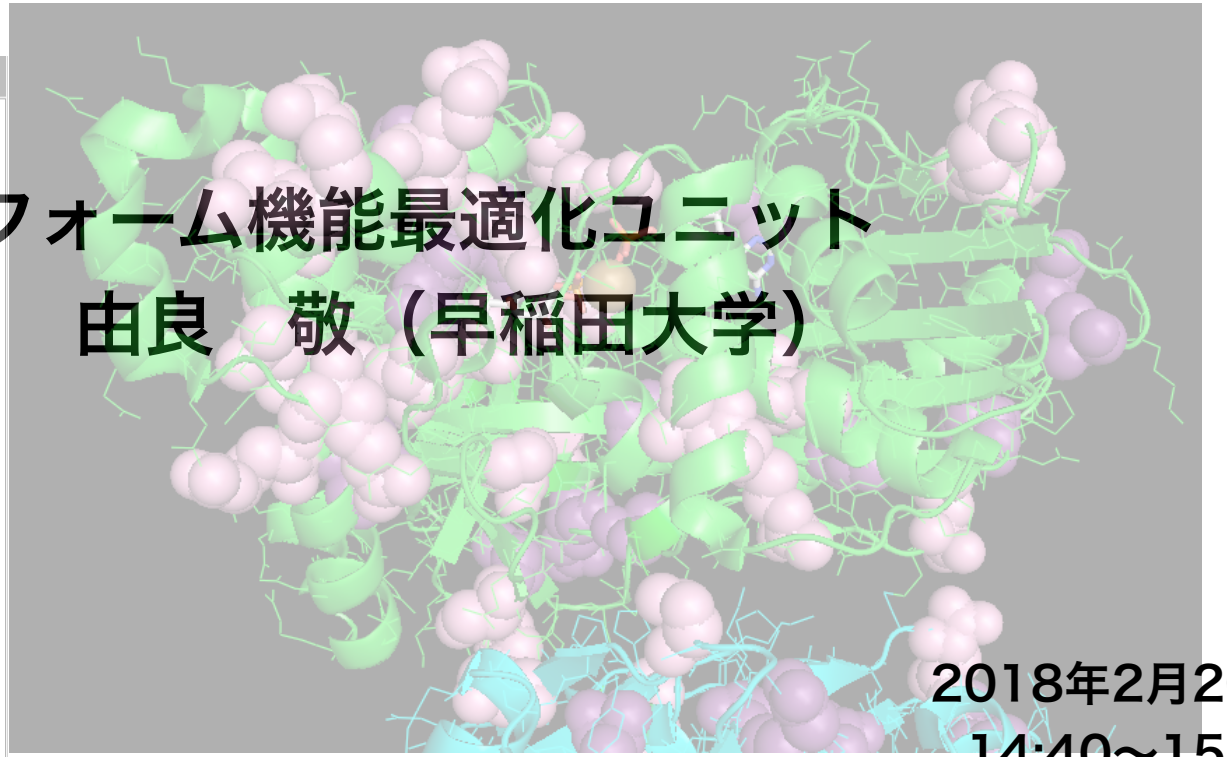


生命科学総合データベースVaProS



プラットフォーム機能最適化ユニット
代表　由良　敬（早稲田大学）

2018年2月20日
14:40〜15:20
大阪大学

VAriation effect on PROtein Structure and function
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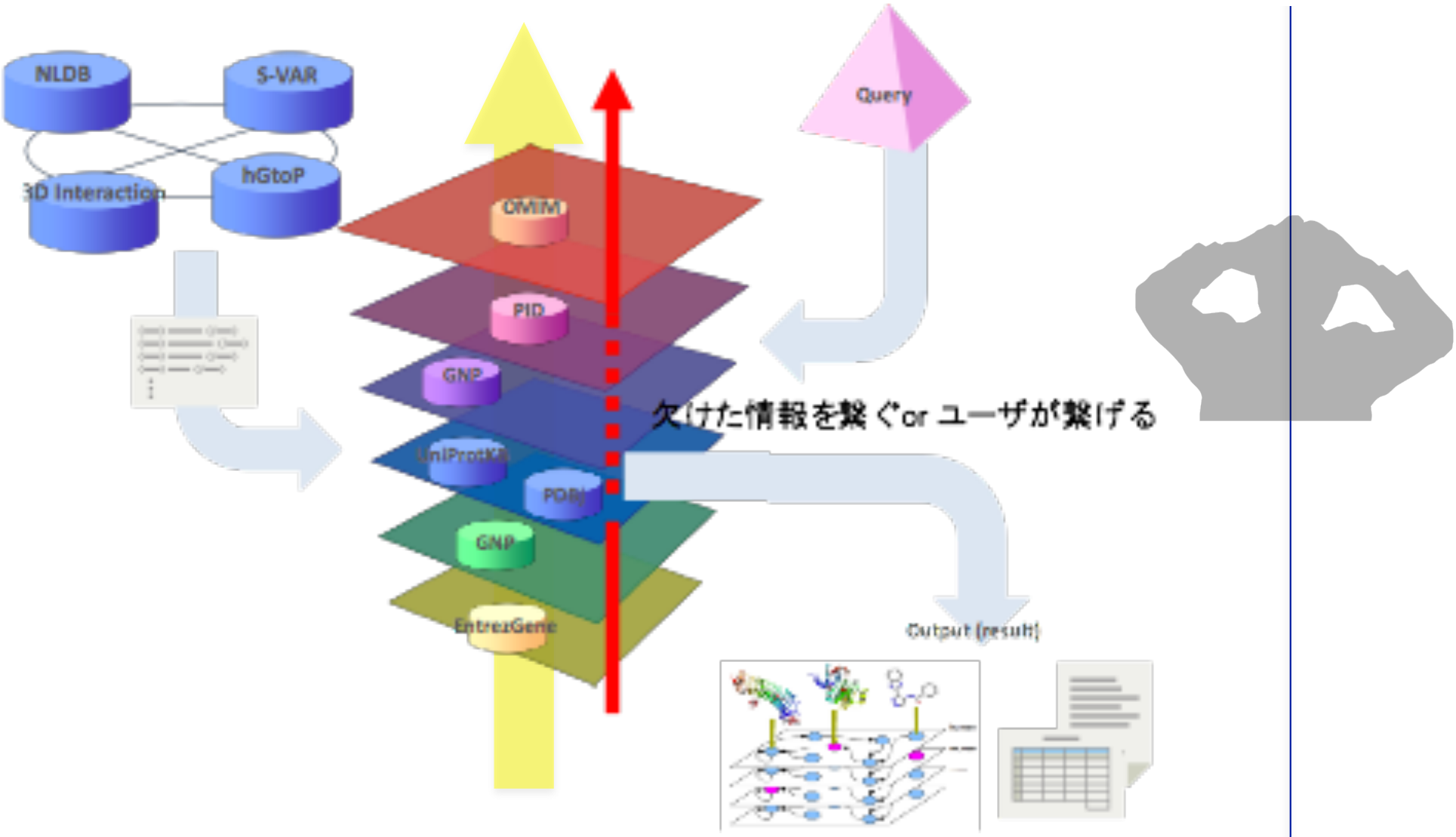
データクラウドVaProSによる知識の発見

データの取得方法、データの読み方、データの解析方法などの困難から、
ユーザを解放し、知識（データの関係）を発見するアプリケーションを構築する。



プロのインフォマティッシャンが、脳の中で行っている（でもできない）多元解析を実現できるアプリケーションにする。

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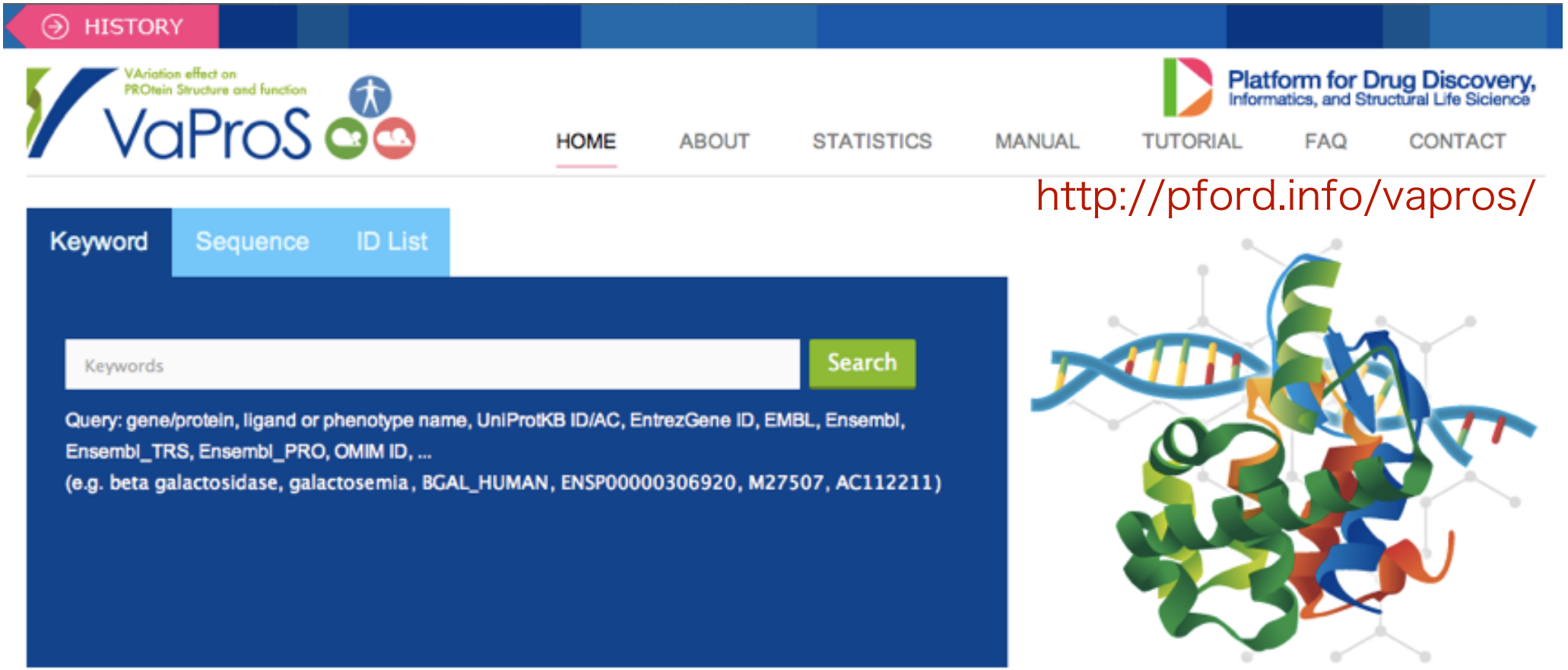
VaProSがめざしていること



http://pford.info/vapros/

学習する（考える）のは、あくまでも人間

VaProS: VAriation effect on PROtein Structure and function

VaProS, VAriation eff
the collaboration betwe
VaProS has been deve
the selected outcomes
more...

core technology to lead
stitute of Genetics,
University, together with
l Innovation Project.

ビッグデータを検索し、その関連から
新しい知見（仮説）を見出すこと

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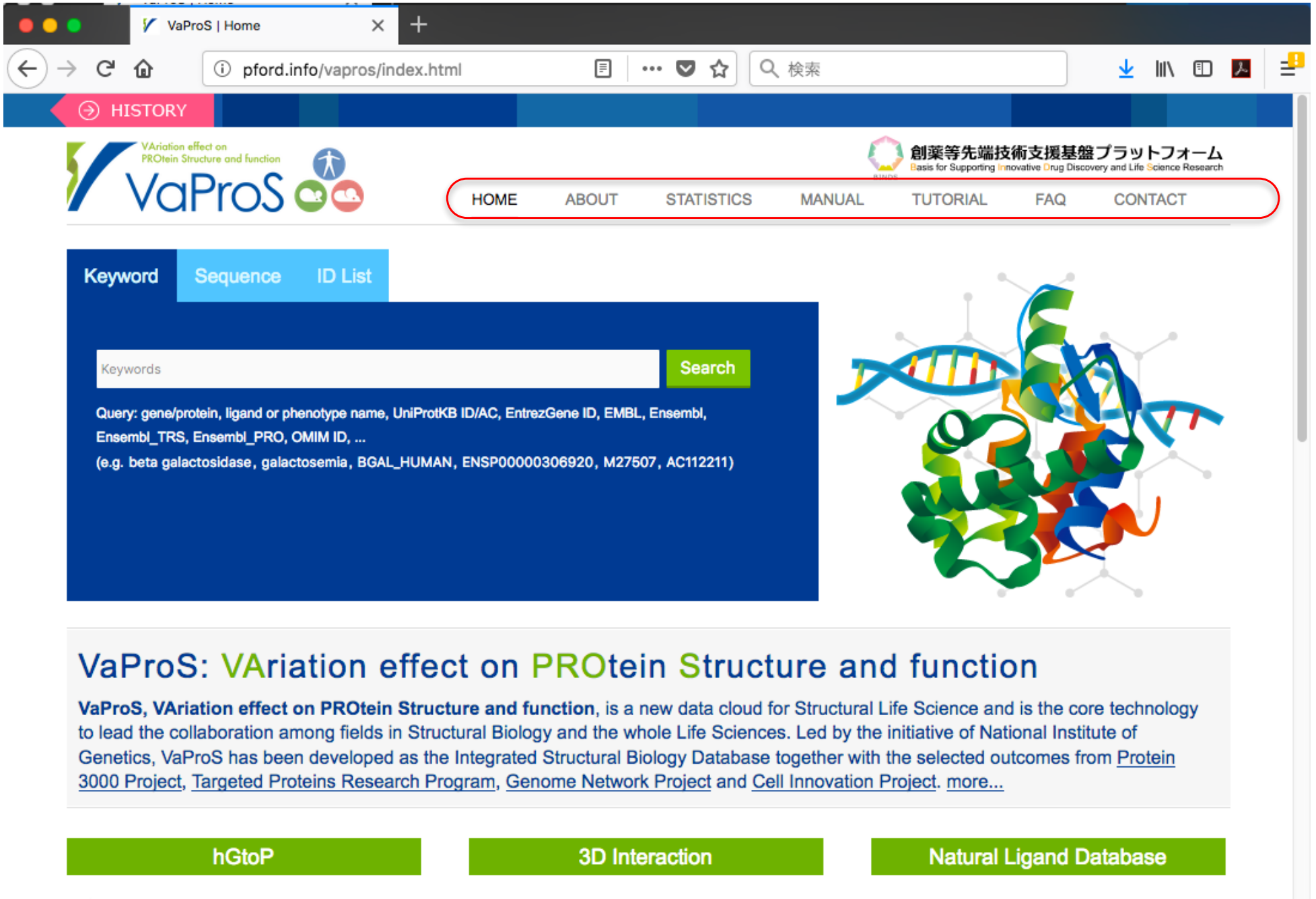
VaProSのトップページ



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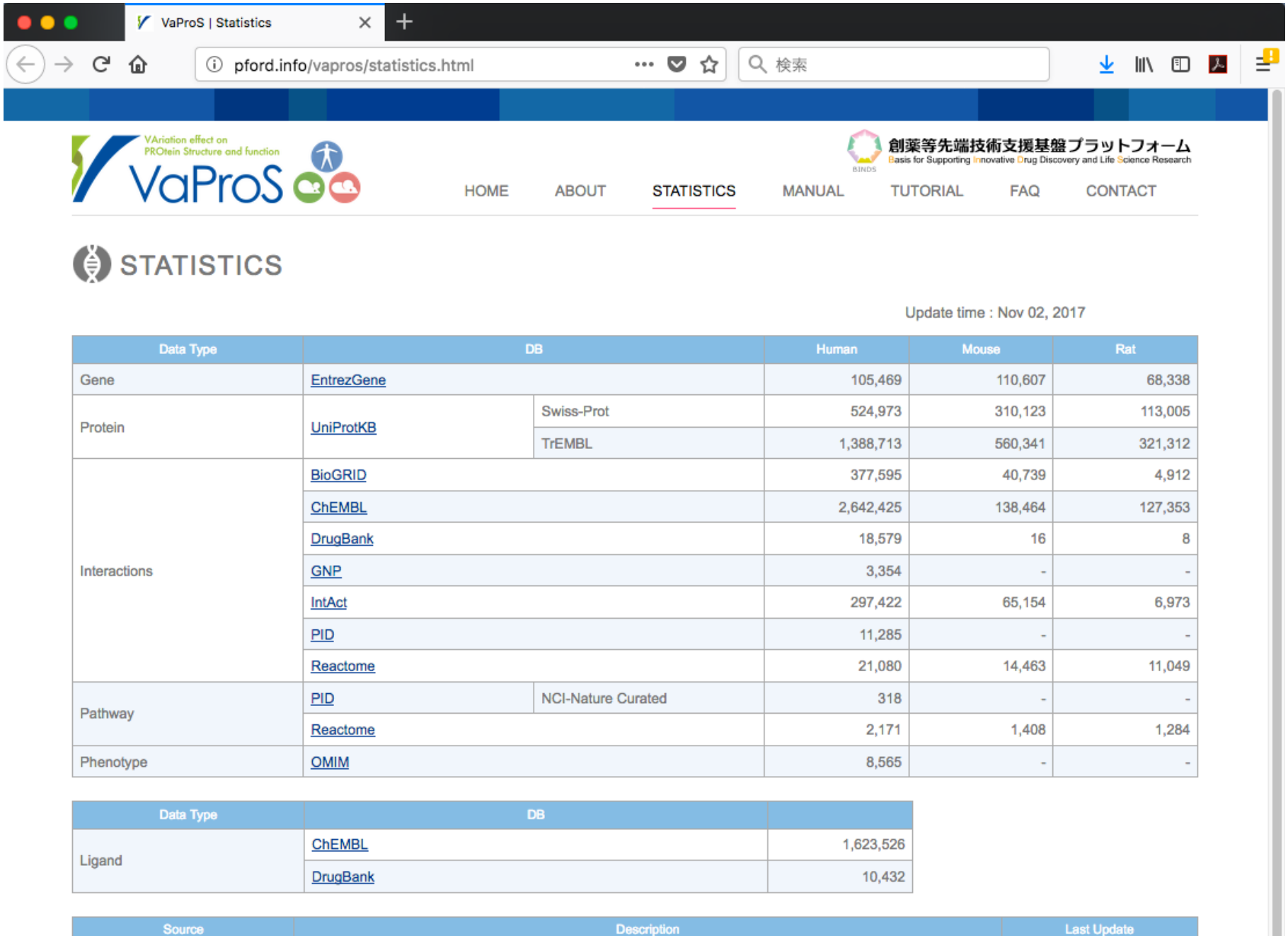
接続されているデータベース http://pford.info/vapros/statistics.html



VaProS | Statistics

pford.info/vapros/statistics.html

検索

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STATISTICS

Update time : Nov 02, 2017

Data Type	DB		Human	Mouse	Rat
Gene	EntrezGene		105,469	110,607	68,338
Protein	UniProtKB	Swiss-Prot	524,973	310,123	113,005
		TrEMBL	1,388,713	560,341	321,312
Interactions	BioGRID		377,595	40,739	4,912
	ChEMBL		2,642,425	138,464	127,353
	DrugBank		18,579	16	8
	GNP		3,354	-	-
	IntAct		297,422	65,154	6,973
	PID		11,285	-	-
	Reactome		21,080	14,463	11,049
Pathway	PID	NCI-Nature Curated	318	-	-
	Reactome		2,171	1,408	1,284
Phenotype	OMIM		8,565	-	-

Data Type	DB	
Ligand	ChEMBL	1,623,526
	DrugBank	10,432

Source	Description	Last Update

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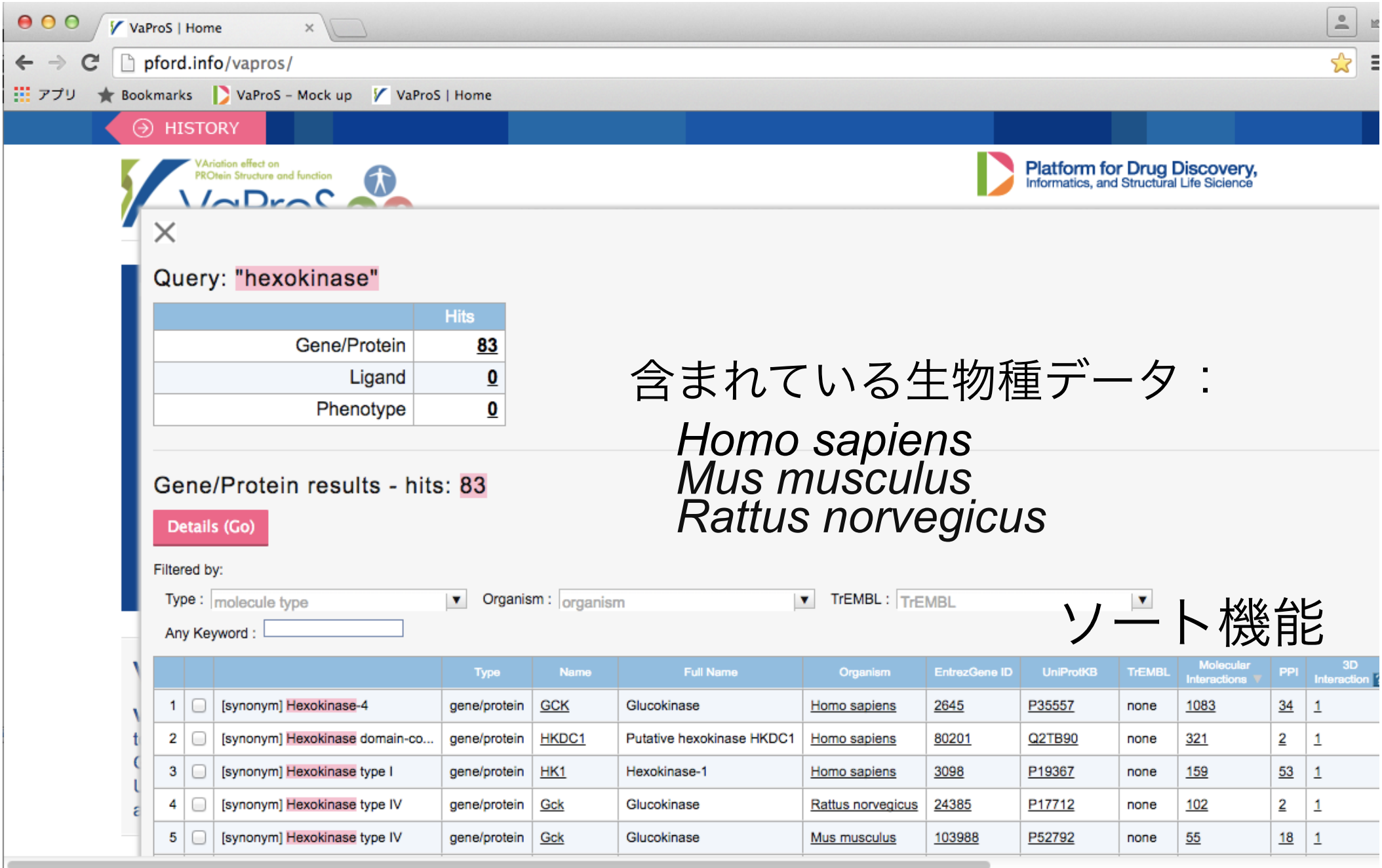
接続されているツール類

http://pford.info/vapros/statistics.html

Source		Description	Last Update
	3D Interaction	A database of human proteins with molecular interaction information. Interactions between a human protein and a protein, nucleic acid, or ligand can be obtained which is derived from a homology search against PDB.	Last Update of PDB:20151007, Release of UniProt:2015_09
	Natural Ligand Database	A database of protein-ligand interactions in three-dimension. The ligand in the database is a "natural ligand" generated by the knowledge of enzymatic reactions appeared in KEGG combined with a three-dimensional data of protein-analog interactions in PDB.	Oct 5, 2015
	hGtoP	A database of human proteins identified in the genome. This database focuses on a structural annotation of each protein.	Mar 13, 2015
	GNP	The National Institute of Genetics has developed "Genome Network Platform Viewer" to make use of the integrated database of the Genome Network Project. This system integrates experimental data generated from the project in association with the public databases.	May 11, 2012
	COXPRESdb	A database of gene coexpression. DNA microarray or RNA-seq analyses produce information on relative expression levels for thousands of genes simultaneously. In addition, large collections of expression data contain information about concerted changes in transcript levels in these datasets beyond the original purpose of each dataset.	Aug 19, 2014
	S-VAR	A tool to assess functional impact of missense and multiple mutations on a protein. The assessment enables one to prioritize the mutations for further studies.	May 19, 2015
	Mutation@A Glance	A web-based integrated viewer for genetic variants observed in human individuals/populations. It enables users to analyze their functional impacts through a visual inspection of the variants displayed on the protein 3D structure, along with both DNA and protein sequences.	Mar.14, 2016

格納されているデータの種類



含まれている生物種データ：

Homo sapiens
Mus musculus
Rattus norvegicus

ソート機能

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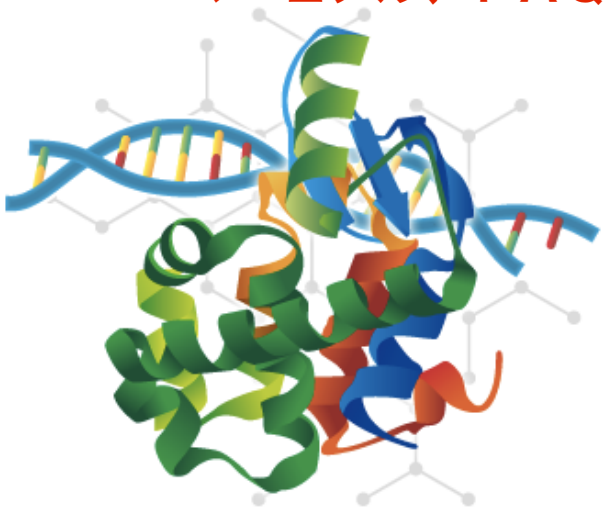
マニュアル、ＦＡＱなど

Keyword Sequence ID List

hexokinase [gene/protein] Search

Query: gene/protein, ligand or phenotype name, UniProtKB ID/AC, EntrezGene ID, EMBL, Ensembl, Ensembl_TRS, Ensembl_PRO, OMIM ID, ...
(e.g. beta galactosidase, galactosemia, BGAL_HUMAN, ENSP00000306920, M27507, AC112211)



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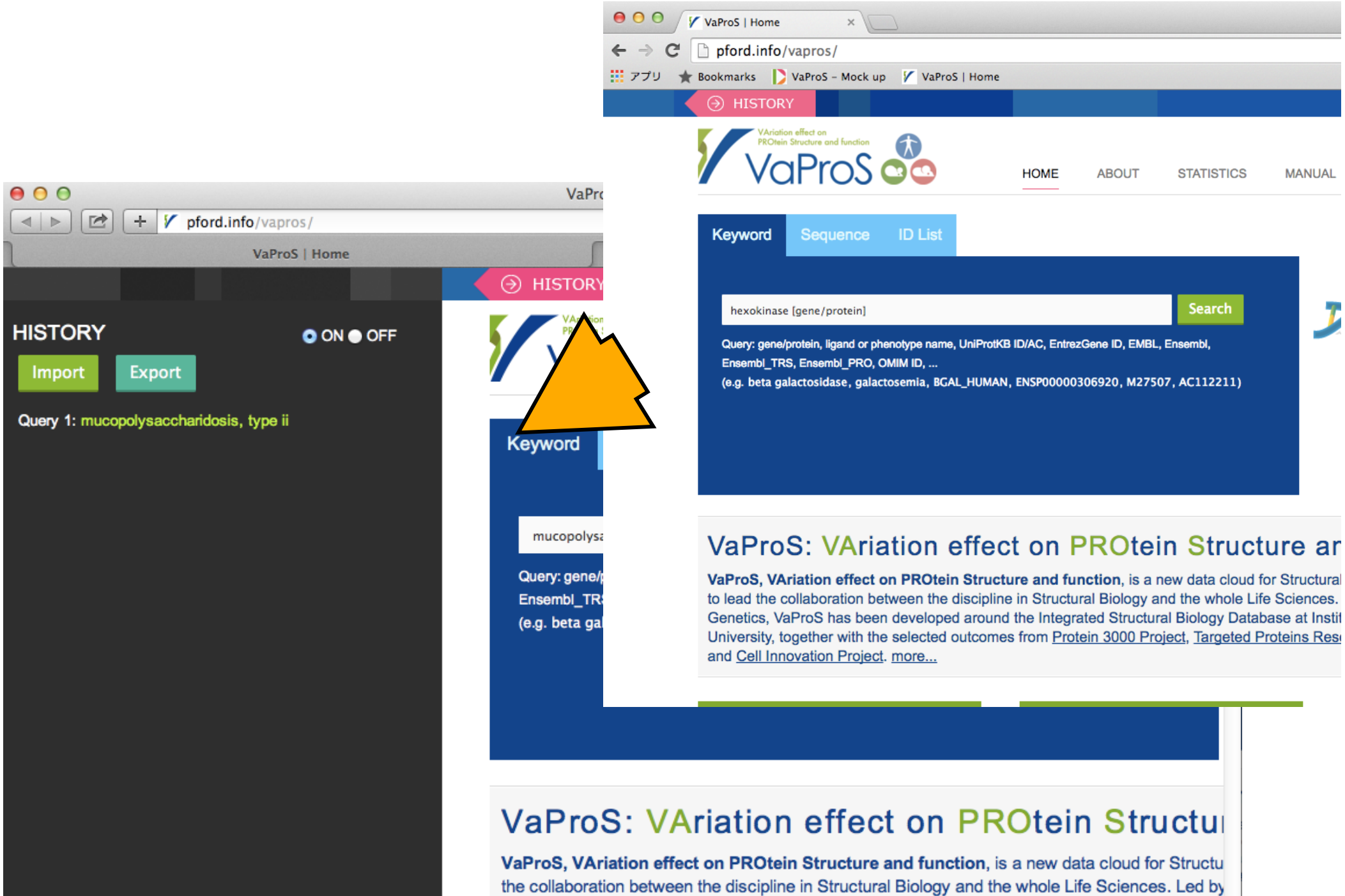
VaProS, VAriation effect on PROtein Structure and function, is a new data cloud for Structural Life Science and is the core technology to lead the collaboration between the discipline in Structural Biology and the whole Life Sciences. Led by the initiative of National Institute of Genetics, VaProS has been developed around the Integrated Structural Biology Database at Institute for Protein Research in Osaka University, together with the selected outcomes from Protein 3000 Project, Targeted Proteins Research Program, Genome Network Project and Cell Innovation Project. more...

履歴機能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ID List
hexokinase [gene/protein]
Search
Query: gene/protein, ligand or phenotype name, UniProtKB ID/AC, EntrezGene ID, EMBL, Ensembl, Ensembl_TRS, Ensembl_PRO, OMIM ID, ...
(e.g. beta galactosidase, galactosemia, BGAL_HUMAN, ENSP00000306920, M27507, AC112211)
HISTORY
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Import
Export
Query 1: mucopolysaccharidosis, type ii
VaProS: VAriation effect on PROtein Structure ar
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to lead the collaboration between the discipline in Structural Biology and the whole Life Sciences.
Genetics, VaProS has been developed around the Integrated Structural Biology Database at Instit
University, together with the selected outcomes from Protein 3000 Project, Targeted Proteins Res
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VaProS: VAriation effect on PROtein Structu
VaProS, VAriation effect on PROtein Structure and function, is a new data cloud for Structu
the collaboration between the discipline in Structural Biology and the whole Life Sciences. Led by

まずは検索

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Sequence
mucopolysaccharidosis
Search
Query: gene/protein, compound or disease name, UniProtKB ID/AC, EntrezGene ID, EMBL, Ensembl, Ensembl_TRS, Ensembl_PRO, OMIM ID, ...
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Keyword Sequence ID List

配列による検索

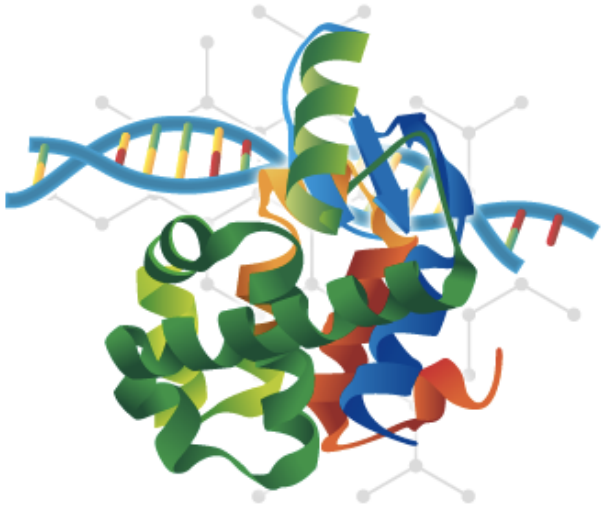
複数のIDで検索

hexokinase [gene/protein]

Search

Query: gene/protein, ligand or phenotype name, UniProtKB ID/AC, EntrezGene ID, EMBL, Ensembl, Ensembl_TRS, Ensembl_PRO, OMIM ID, ...

(e.g. beta galactosidase, galactosemia, BGAL_HUMAN, ENSP00000306920, M27507, AC112211)



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Keyword Sequence ID List
Query: DNA/protein sequence (FASTA format). example
Space and numerical/control characters are automatically neglected.
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hGtoP
3D In

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VaProS
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Keyword Sequence ID List
ID: EntrezGene ID, UniProtKB AC. example (UniProtKB AC)
EntrezGene ID UniProtKB AC
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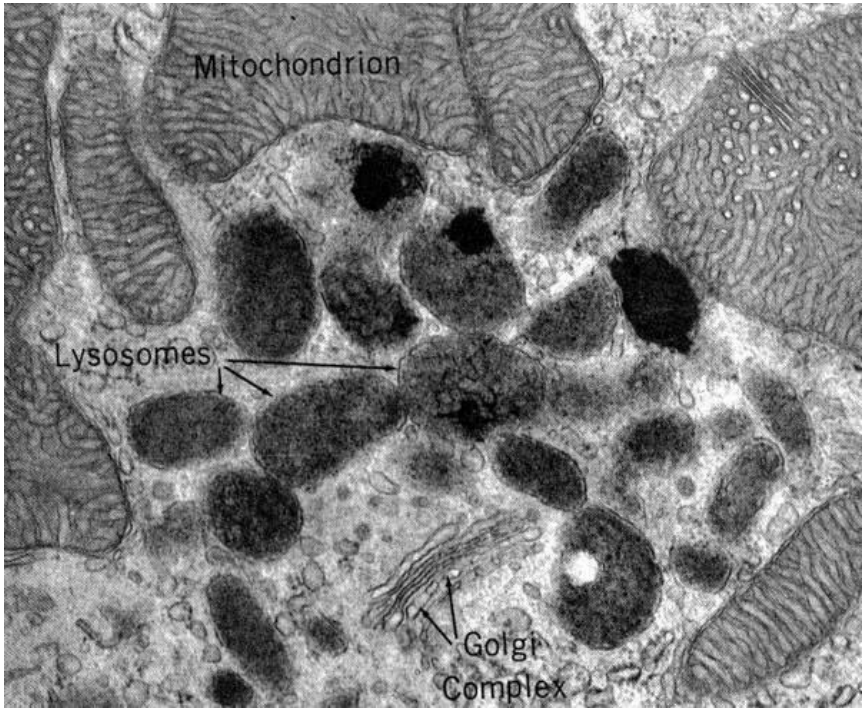
the selected outcomes from Protein 3000 Project, Targeted Proteins Research Program, Genome Network Project and Cell Innov
more...
hGtoP
3D Interaction
Natural Ligand D

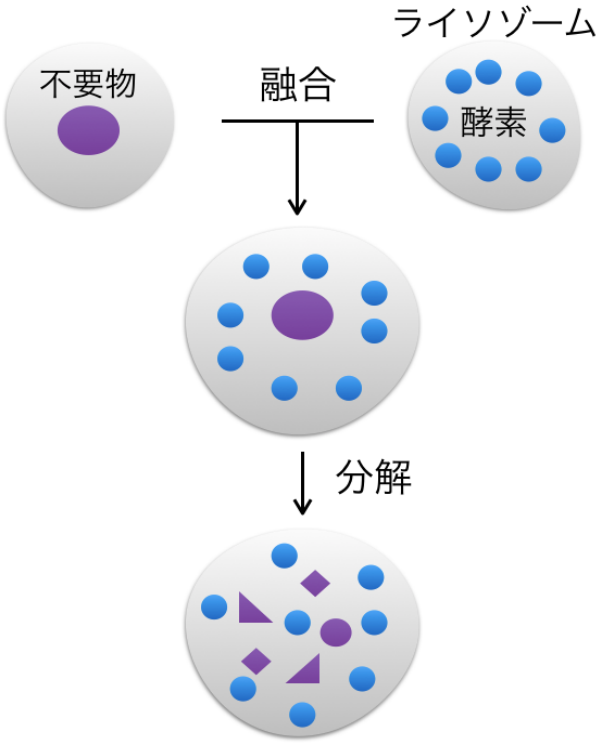
ライソゾームとは

ライソゾーム(リソソーム)

細胞内外で不要になった生体高分子の分解と再利用をおこなう細胞小器官
直径は0.1～1.2 μm程度
6～10 nmの一重の生体膜に囲まれている
1955年にド・デューブが発見（1974年ノーベル生理医学賞）



Source: dematice.org

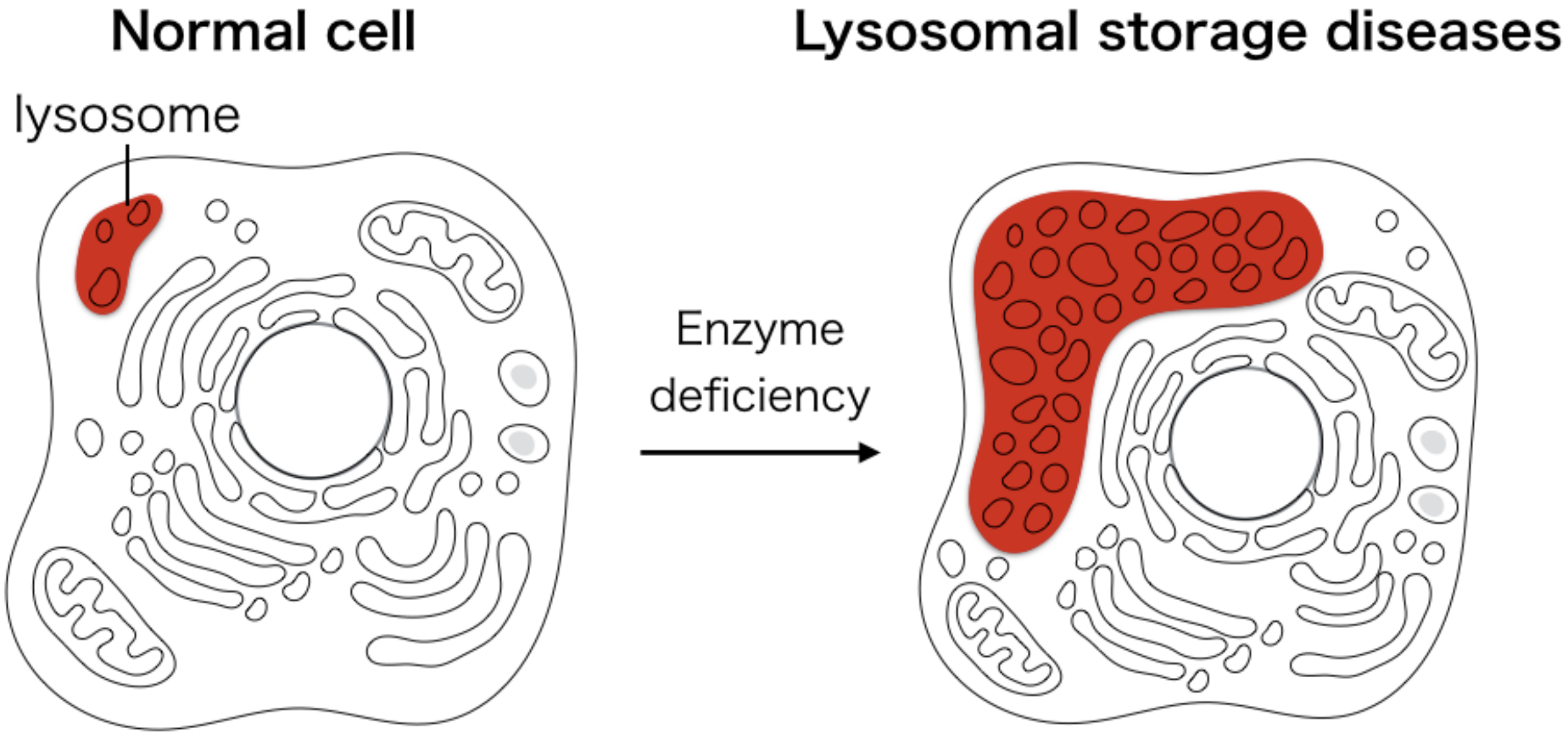


参考：C. De Duve, et al., Biochem. J., 1955

ライソゾーム病とは

- ライソゾーム酵素の欠損や輸送障害によって発症する遺伝性疾患（特定疾患）
- ライソゾームによって分解されなければならない物質が蓄積することによる疾患
- 約60種類のライソゾーム病が知られている
- 1963年にHersによってライソゾーム病の概念が確立

(H. G. Hers, *Gastroenterology*, 1965)



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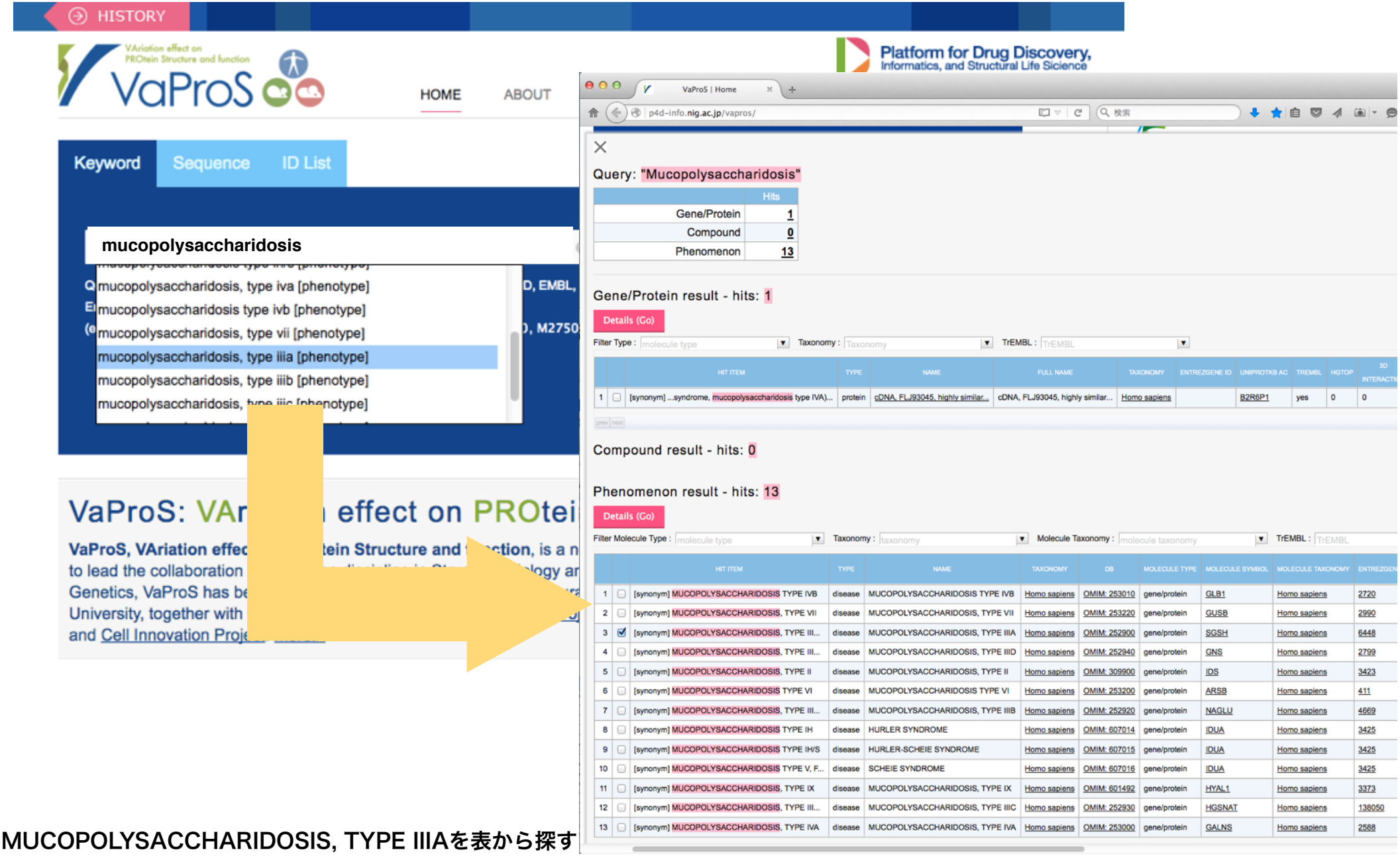
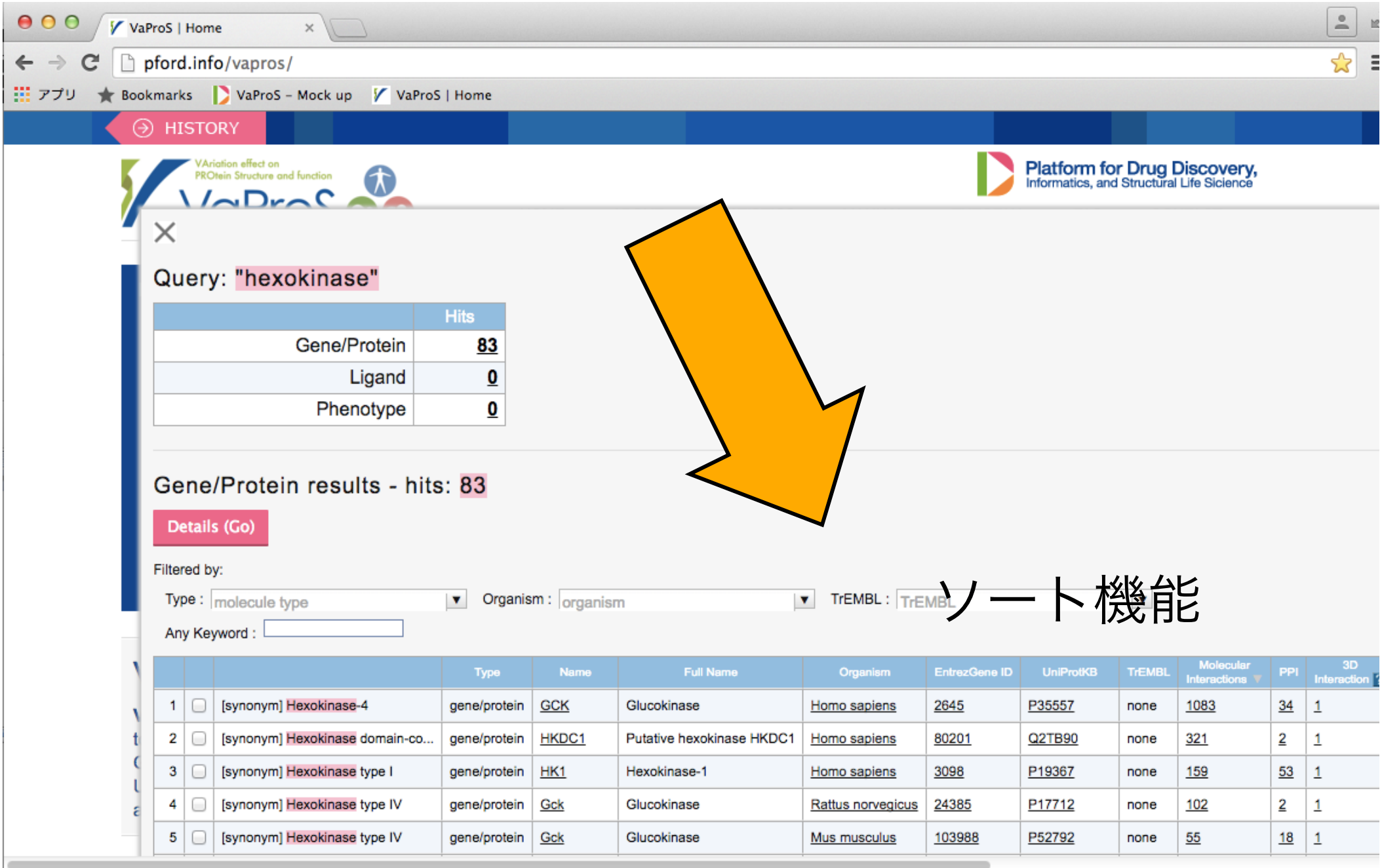
ムコ多糖症を調べる



MUCOPOLYSACCHARIDOSIS, TYPE IIIAを表から探す

最初の検索結果をソートする



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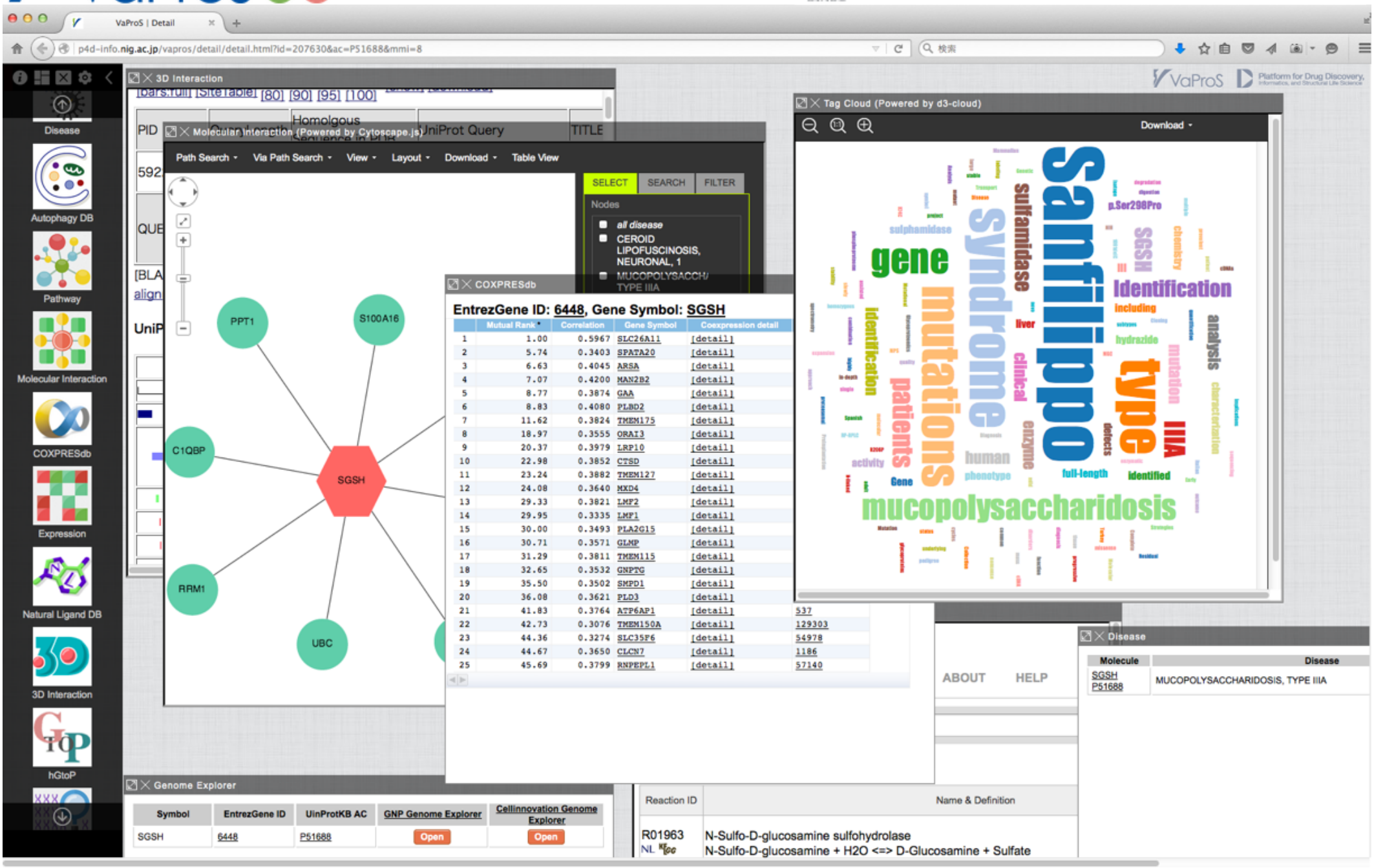
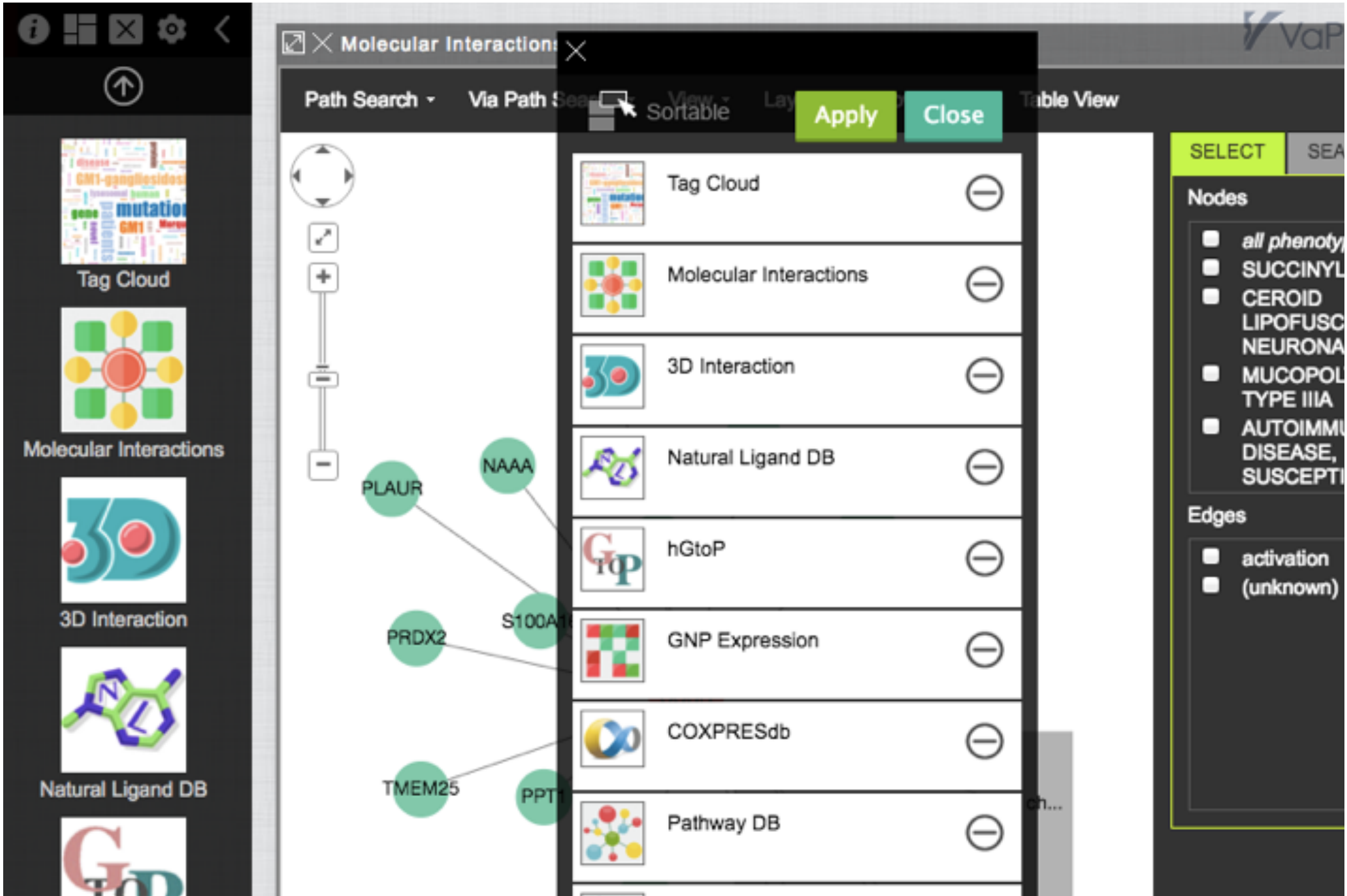
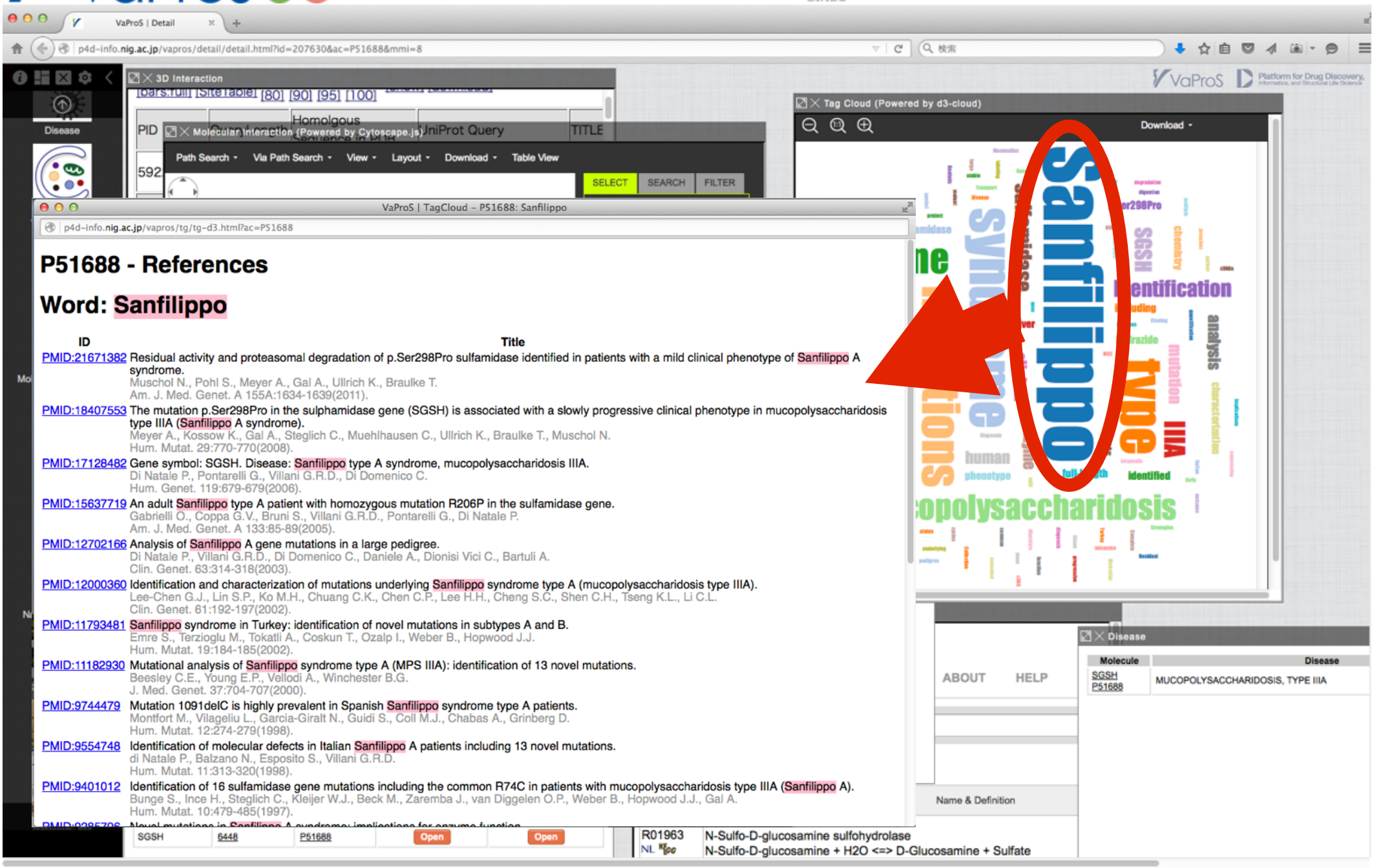


検索結果初期画面

ムコ多糖症


Molecular Interaction
Path Search
Via Path
Sortable
Apply
Close
Table View
Tag Cloud
Molecular Interactions
3D Interaction
Natural Ligand DB
hGtoP
GNP Expression
COXPRESdb
Pathway DB
SELECT
Nodes
Edges
activation
(unknown)
PLAUR
NAAA
PRDX2
TMEM25
PPT1

ムコ多糖症



mucopolysaccharodosis type IIIA は、Sanfilippo type A syndromeともよばれている。

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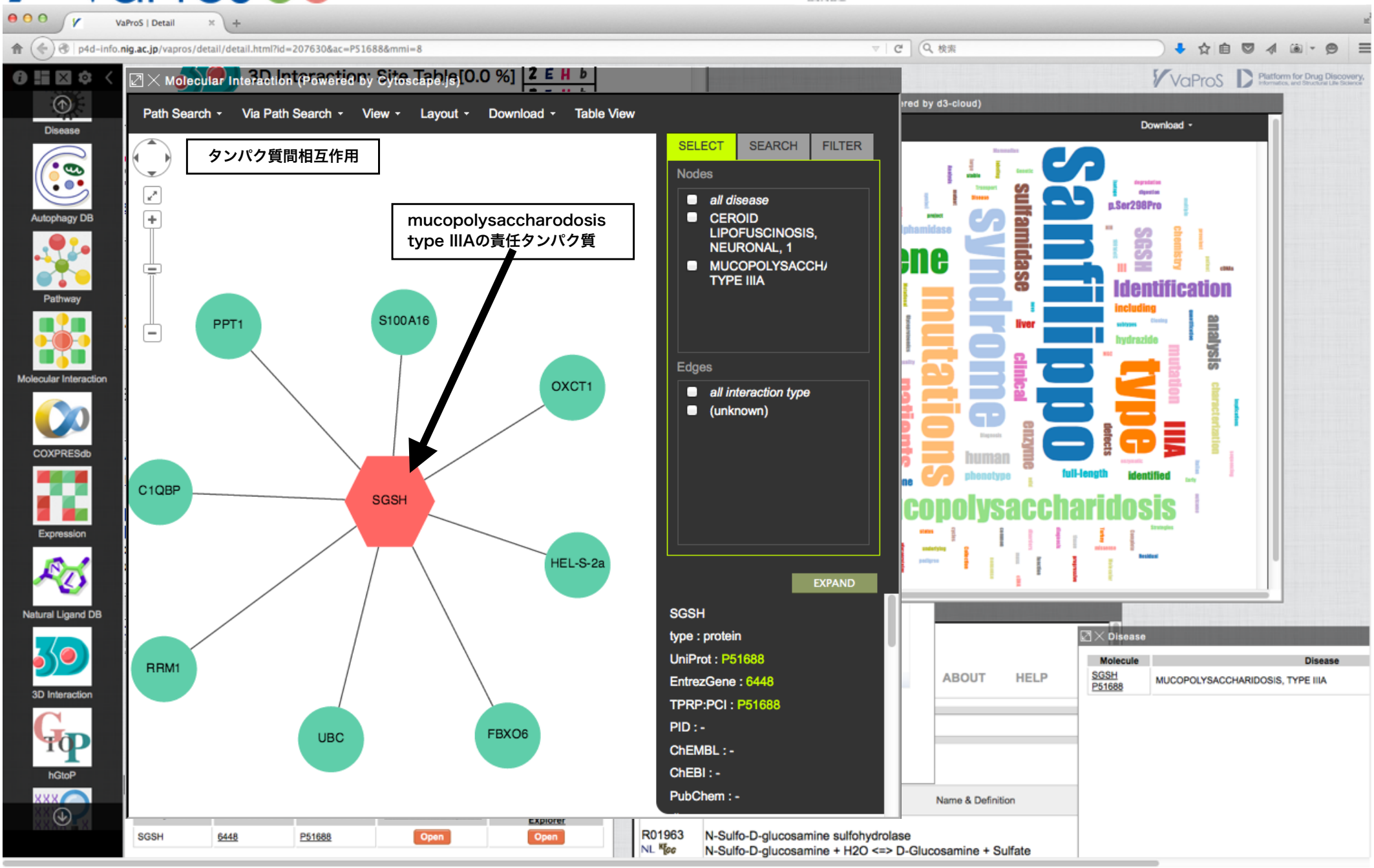
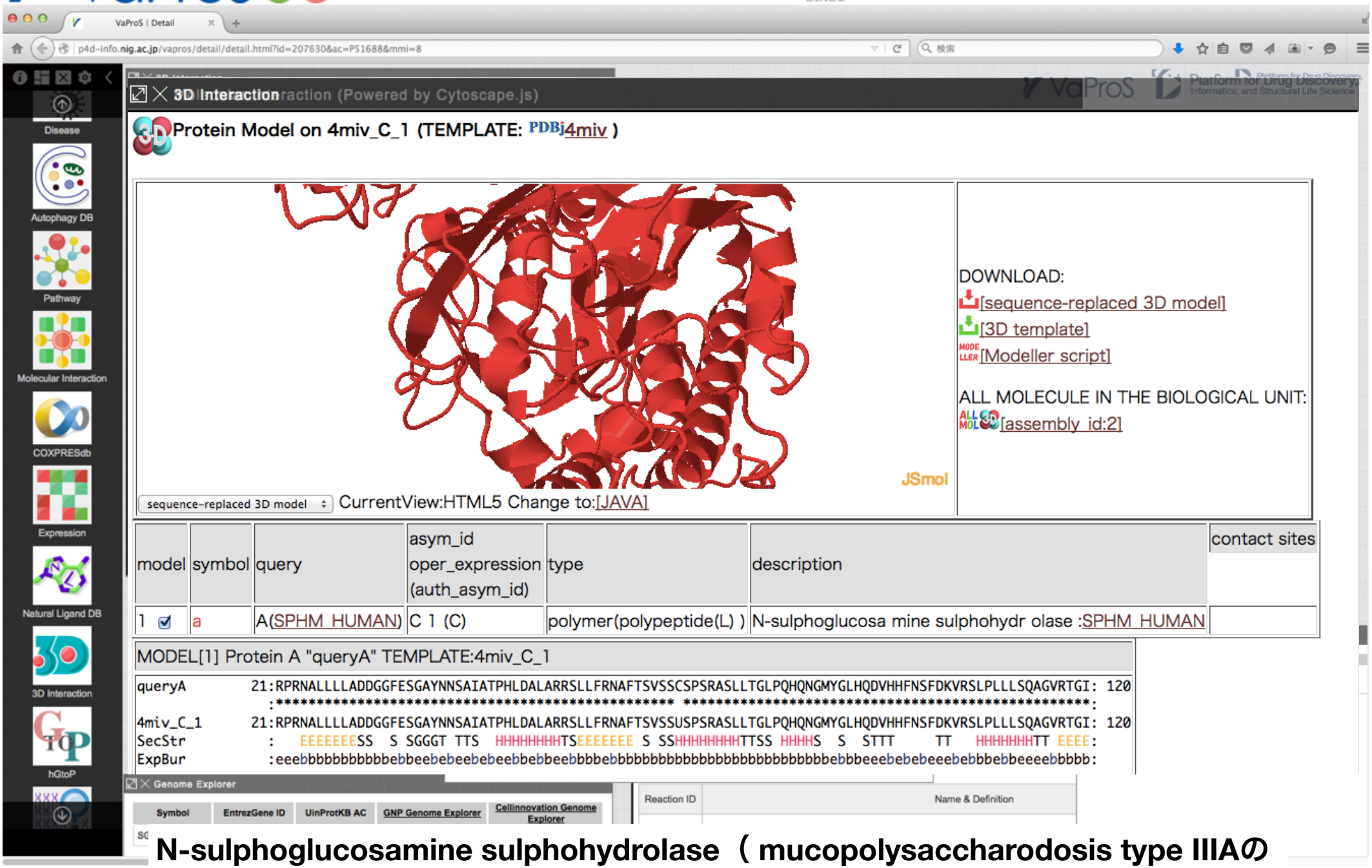


実験的に相互作用が明らかになっているタンパク質群

ムコ多糖症



N-sulphoglucosamine sulphohydrolase（ mucopolysaccharodosis type IIIAの責任タンパク質）は、立体構造が明らかになっている

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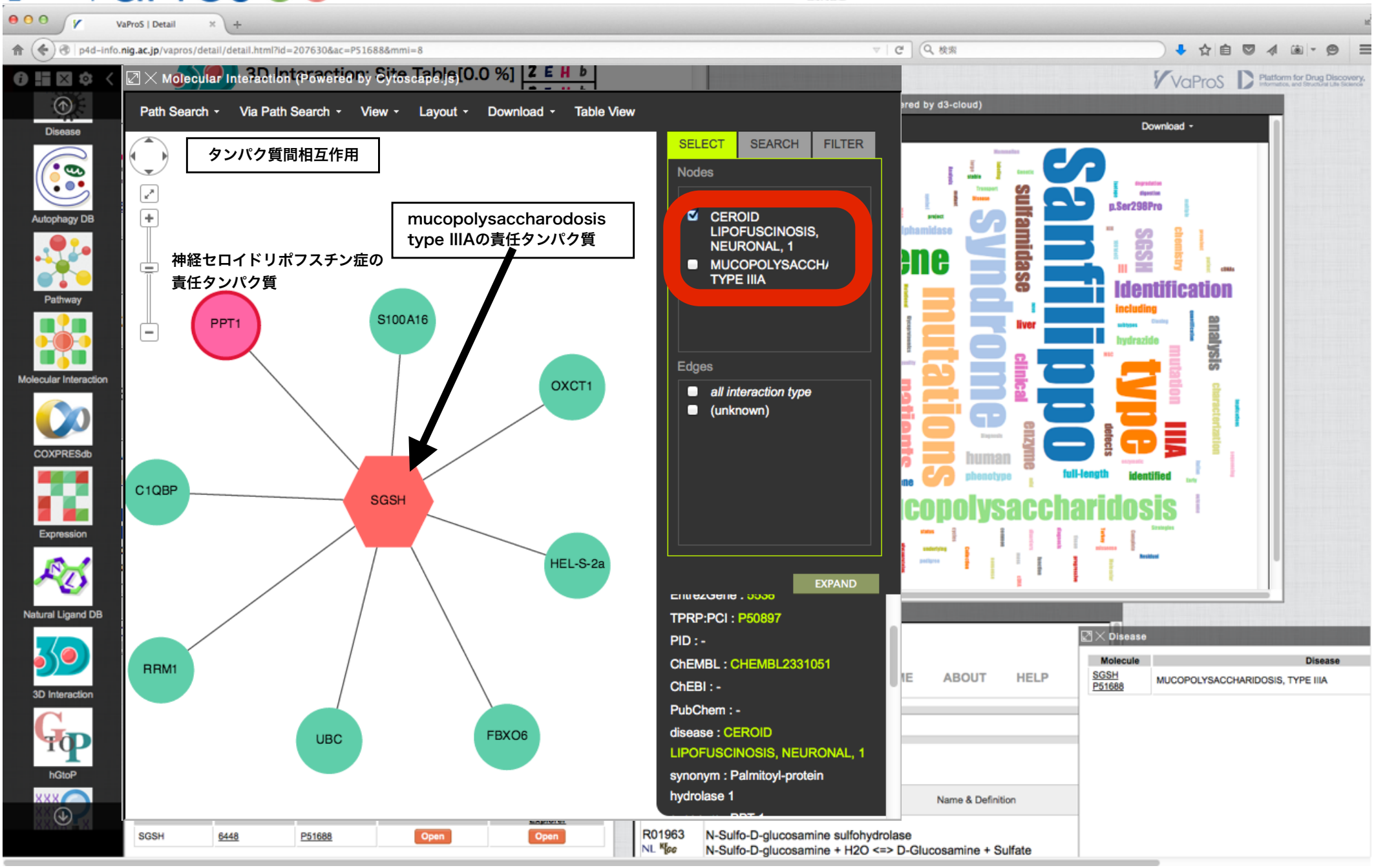

実験的に相互作用が明らかになっているタンパク質群

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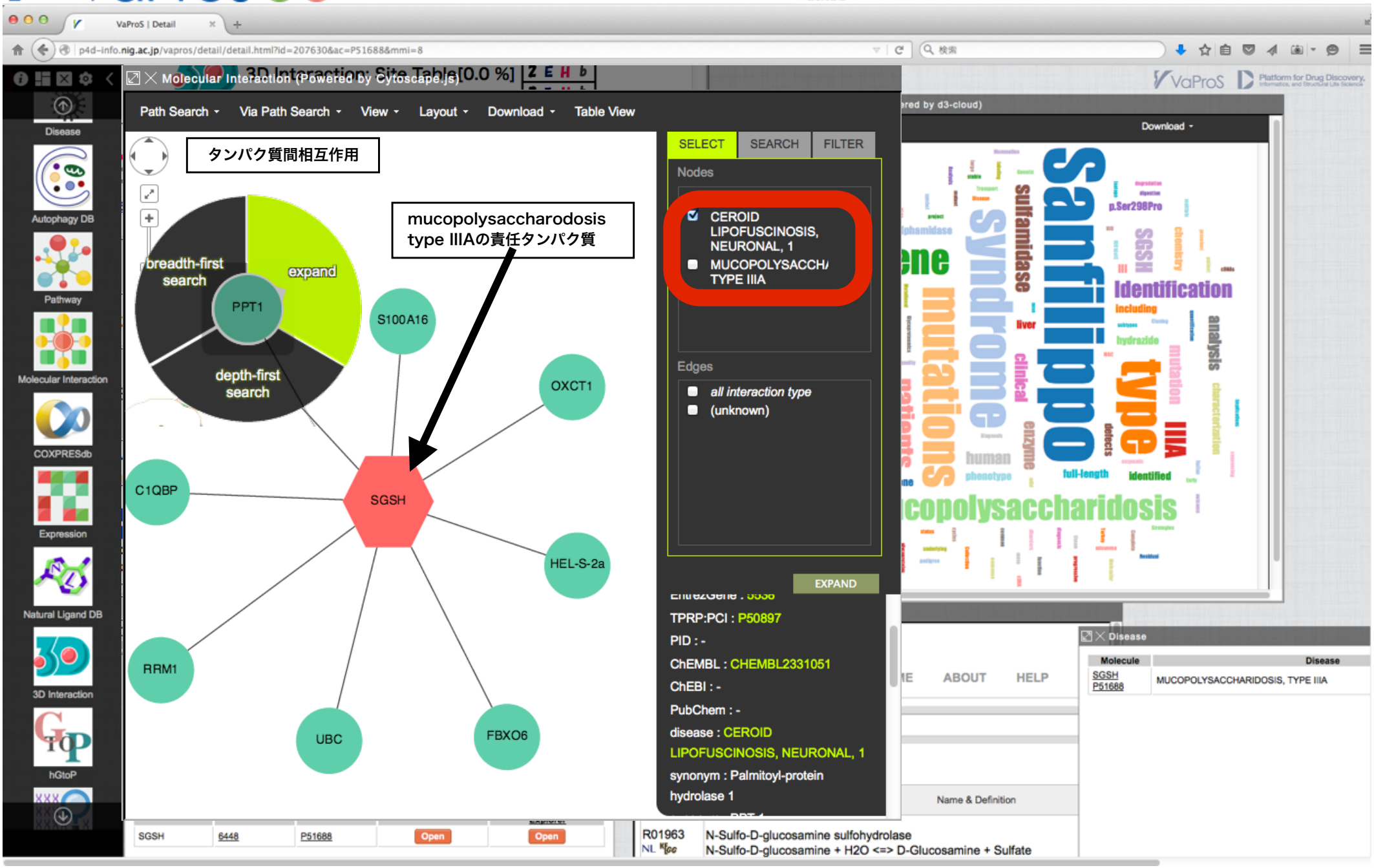

実験的に相互作用が明らかになっているタンパク質群

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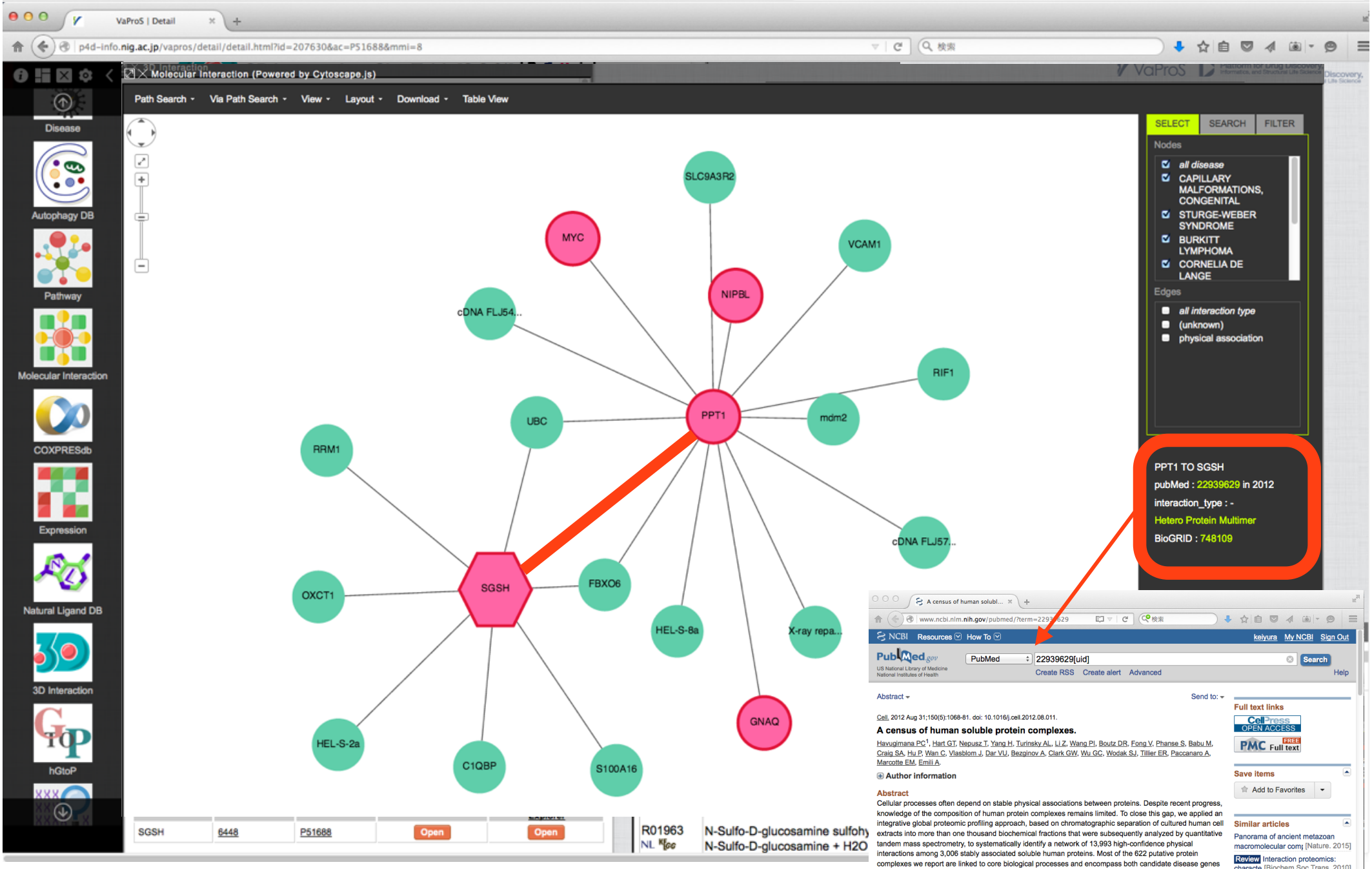

実験的に相互作用が明らかになっているタンパク質群

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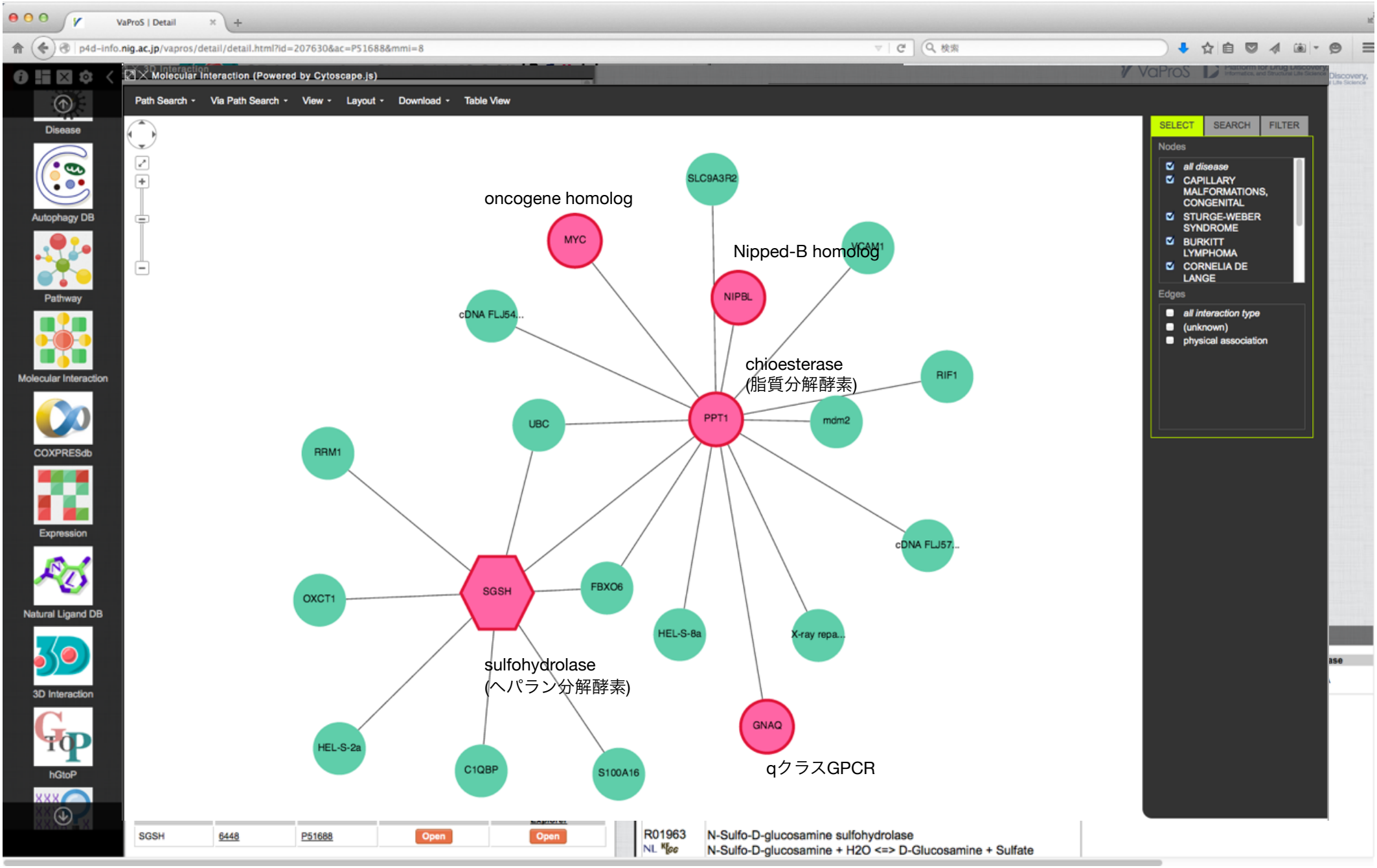
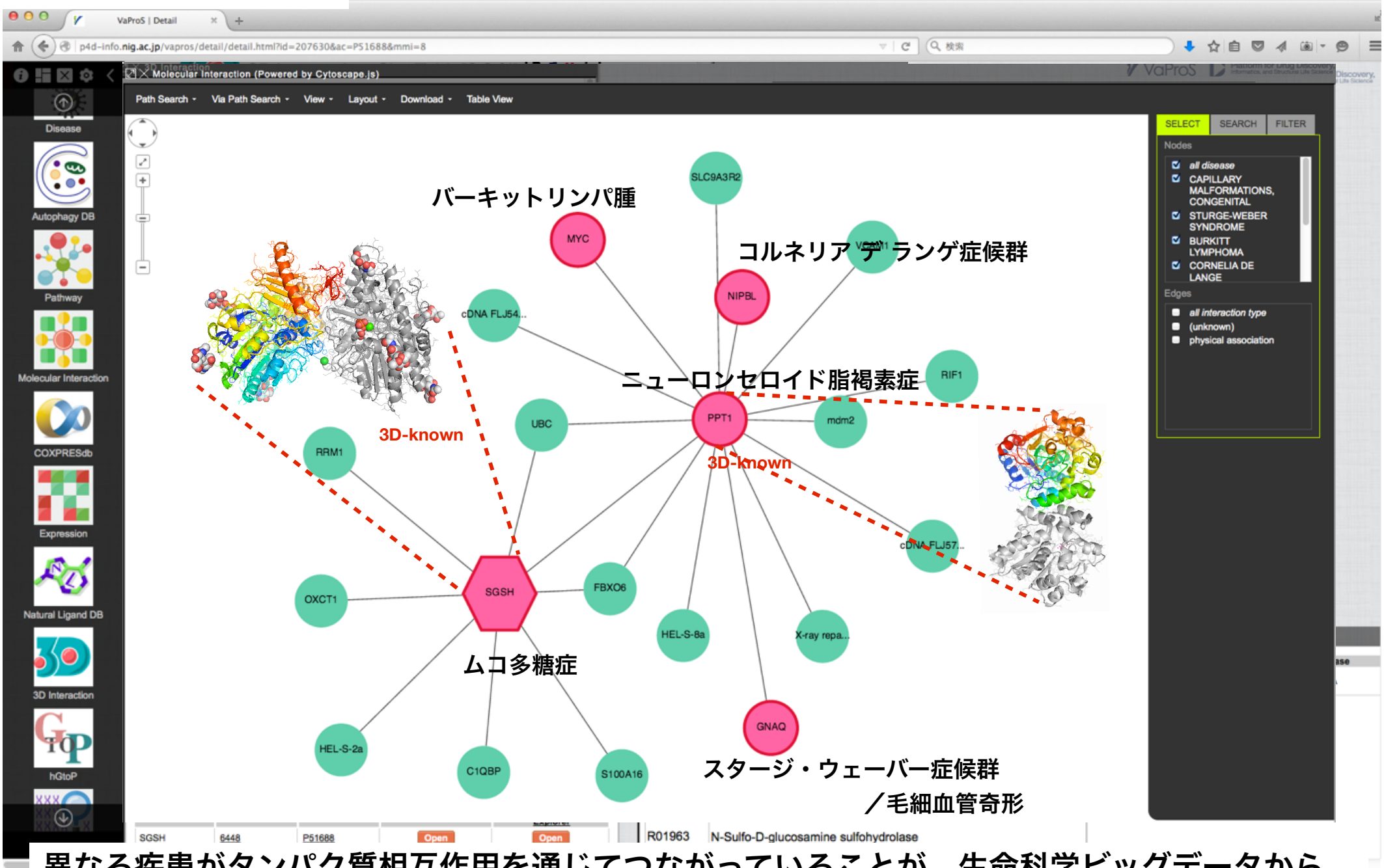
VAriation effect on PROtein Structure and function
VaProS



実験的に相互作用が明らかになっているタンパク質群

ムコ多糖症



異なる疾患がタンパク質相互作用を通じてつながっていることが、生命科学ビッグデータからわかった。