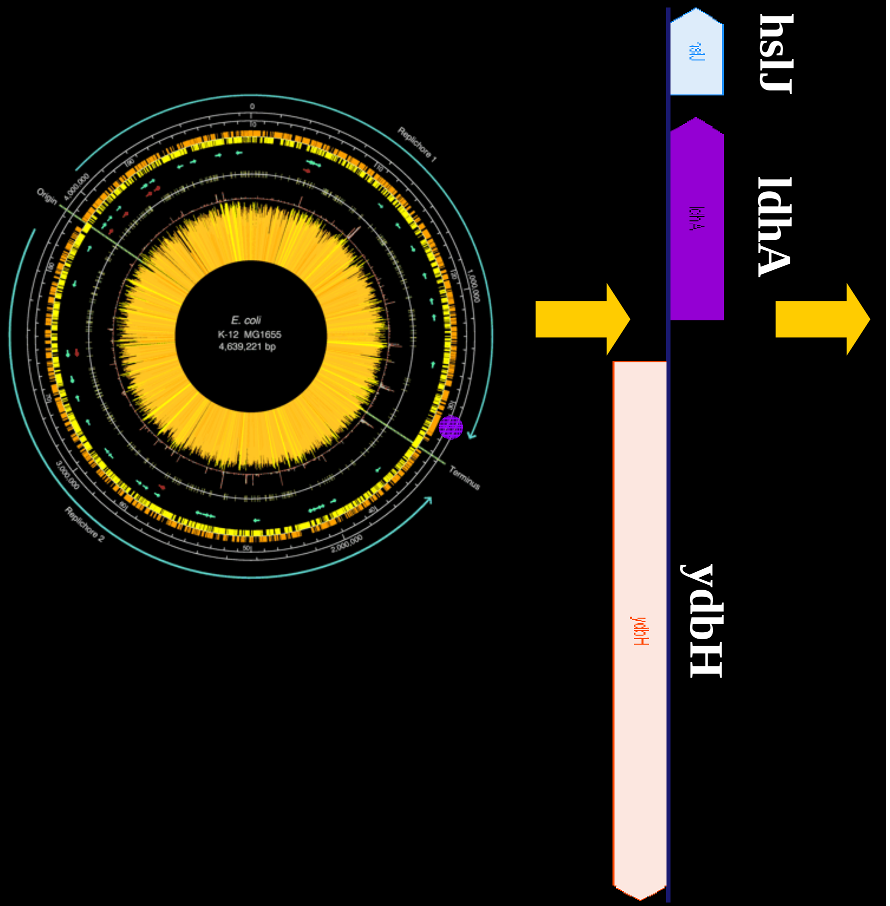
Constraint-Based Workshops

2. Reconstruction Databases

November 29th, 2007

Defining Metabolic Reactions



Lactate Dehydrogenase

1st level: Metabolite Specificity

Primary metabolites: LAC, PYR

Coenzymes: NAD, NADH

2nd level: Metabolite Formulas

Neutral Formulas

$C_3H_6O_3$ $C_3H_4O_3$ $C_{21}H_{26}N_7O_{14}P_2$ $C_{21}H_{27}N_7O_{14}P_2$

Charged Formulas

$C_3H_5O_3^{1-}$ $C_3H_3O_3^{1-}$ $C_{21}H_{26}N_7O_{14}P_2^{1-}$ $C_{21}H_{27}N_7O_{14}P_2^{1-}$

3rd level: Stoichiometry

1 LAC + 1 NAD ? 1 PYR + 1 NADH + 1 H

4th level: Thermodynamic Considerations: Directionality

1 LAC + 1 NAD ⟷ 1 PYR + 1 NADH + 1 H

5th level: Localization

prokaryotes

[c]: cytoplasm
[e]: extracellular
[p]: periplasm

[n]: nucleus
[g]: golgi aparatus
[v]: vacuole
[l]: lysosome

[m]: mitochondria
[x]: peroxisome
[h]: chloroplast
[r]: endoplasmic reticulum

eukaryotes

1 LAC [c] + 1 NAD [c] ⟷ 1 PYR [c] + 1 NADH [c] + 1 H [c]

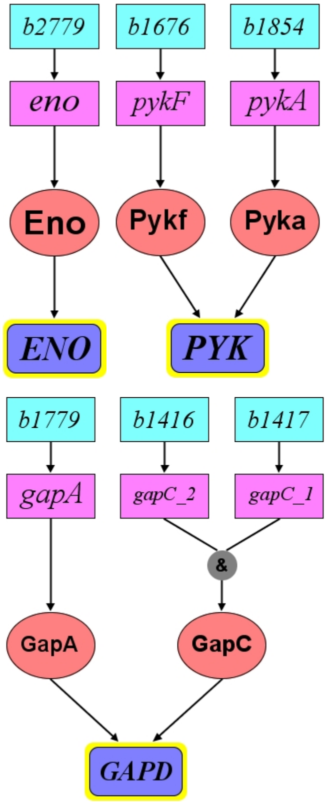
STEPWISE INCORPORATION OF INFORMATION

Network Assembly and Representation

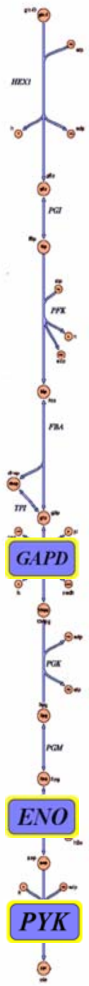
Reconstruction of Glycolytic Pathway

Abbr.	Glycolytic Reactions	Genes
HEX1	[c]glc +atp → g6p + adp	glk
PGI	[c]g6p ↔ f6p	pgi
PFK	[c]atp + f6p → adp + fdp + h	pfkA,pfkB
FBA	[c]fdp ↔ dhap + g3p	fbaA,fbaB
TPI	[c]dhap ↔ g3p	tpiA
GAPD	[c]g3p + nad + pi ↔ 13dpg + h + nadh	gapA,gapC_1,gapC_2
PGK	[c]13dpg + adp ↔ 3pg + atp	pgk
PGM	[c]3pg ↔ 2pg	gpmA,gpmB
ENO	[c]2pg ↔ h2o + pep	eno
PYK	[c]adp + h + pep → atp + pyr	pykA,pykF

	HEX1	PGI	PFK	FBA	TPI	GAPD	PGK	PGM	ENO	PYK
atp	-1	0	-1	0	0	0	1	0	0	1
glc	-1	0	0	0	0	0	0	0	0	0
adp	1	0	1	0	0	0	-1	0	0	-1
g6p	1	-1	0	0	0	0	0	0	0	0
h	1	0	1	0	0	1	0	0	0	-1
f6p	0	1	-1	0	0	0	0	0	0	0
fdp	0	0	1	-1	0	0	0	0	0	0
dhap	0	0	0	1	-1	0	0	0	0	0
g3p	0	0	0	1	1	-1	0	0	0	0
nad	0	0	0	0	0	-1	0	0	0	0
pi	0	0	0	0	0	-1	0	0	0	0
13dpg	0	0	0	0	0	1	-1	0	0	0
nadh	0	0	0	0	0	1	0	0	0	0
3pg	0	0	0	0	0	0	1	-1	0	0
2pg	0	0	0	0	0	0	0	1	-1	0
pep	0	0	0	0	0	0	0	0	1	-1
h2o	0	0	0	0	0	0	0	0	1	0
pyr	0	0	0	0	0	0	0	0	0	1



PYK: IF *pykA* OR *pykF*
ENO: IF *eno*
GAPD: IF *gapA* OR (*gapC_1* AND *gapC_2*)



Outline

- Quick tour of KEGG
- Using KEGG to reconstruct a metabolic network
- Reconstruction of a simple pathway

Quick Tour of KEGG

http://www.genome.ad.jp/kegg/kegg2.html

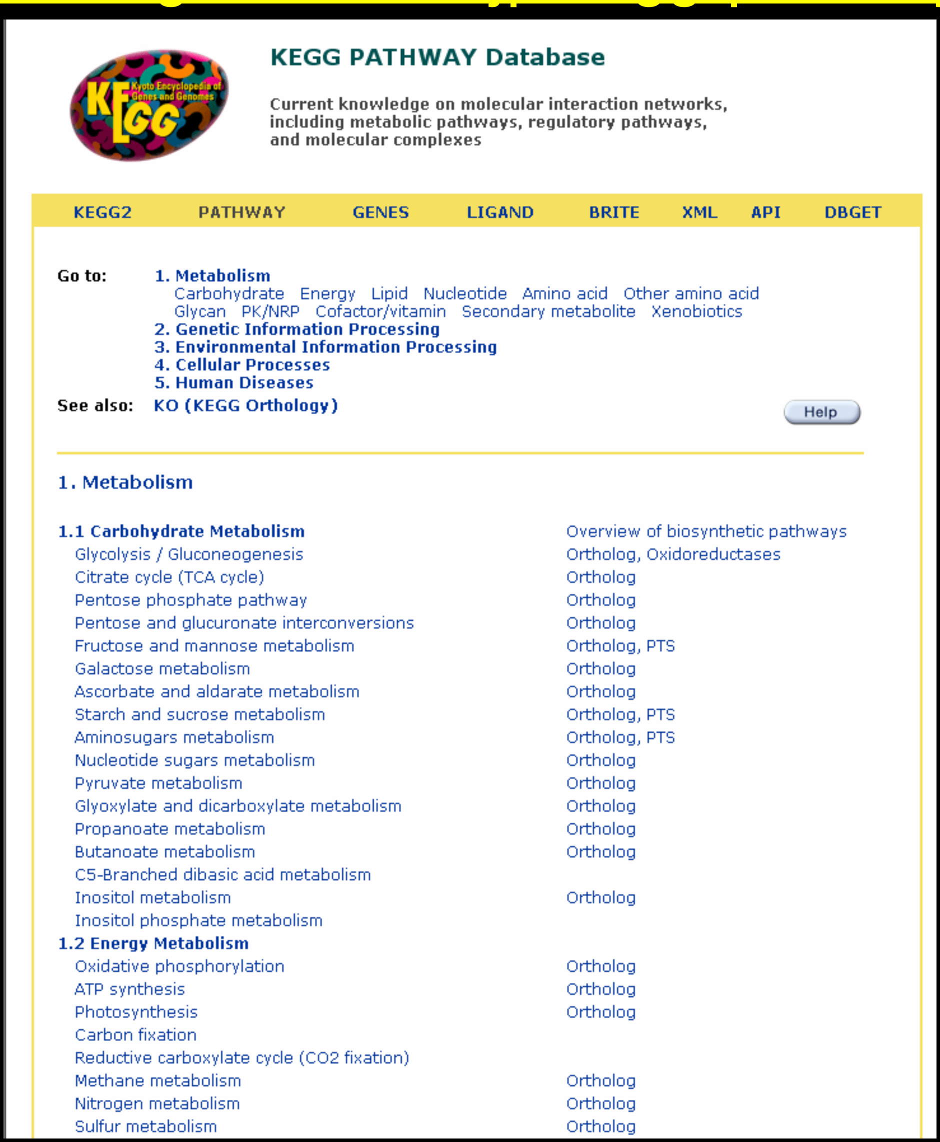
KEGG - Table of Contents

Generalized KEGG

Content	Database	Search & Compute	DBGET Search	
Pathway information	**KEGG PATHWAY**	Search objects in KEGG pathways Color objects in KEGG pathways KEGG pathways in XML	PATHWAY	
Genomic information	**KEGG GENES**	BLAST search against GENES/GENOME FASTA search against GENES/GENOME KEGG EXPRESSION	GENES DGENES / EGENES GENOME	
Chemical information	**KEGG LIGAND**	Search similar compound structures Search similar glycan structures Predict reactions and assign EC numbers Generate possible reaction paths	COMPOUND DRUG GLYCAN REACTION RPAIR ENZYME	LIGAND
Binary relations and hierarchies	**KEGG BRITE**	KEGG Orthology (KO) Automatic annotaion (KO assignment) Therapeutic category of drugs	KO	

KEGG’s Pathway Database

http://www.genome.ad.jp/kegg/pathway.html



KEGG PATHWAY Database

Current knowledge on molecular interaction networks,
including metabolic pathways, regulatory pathways,
and molecular complexes

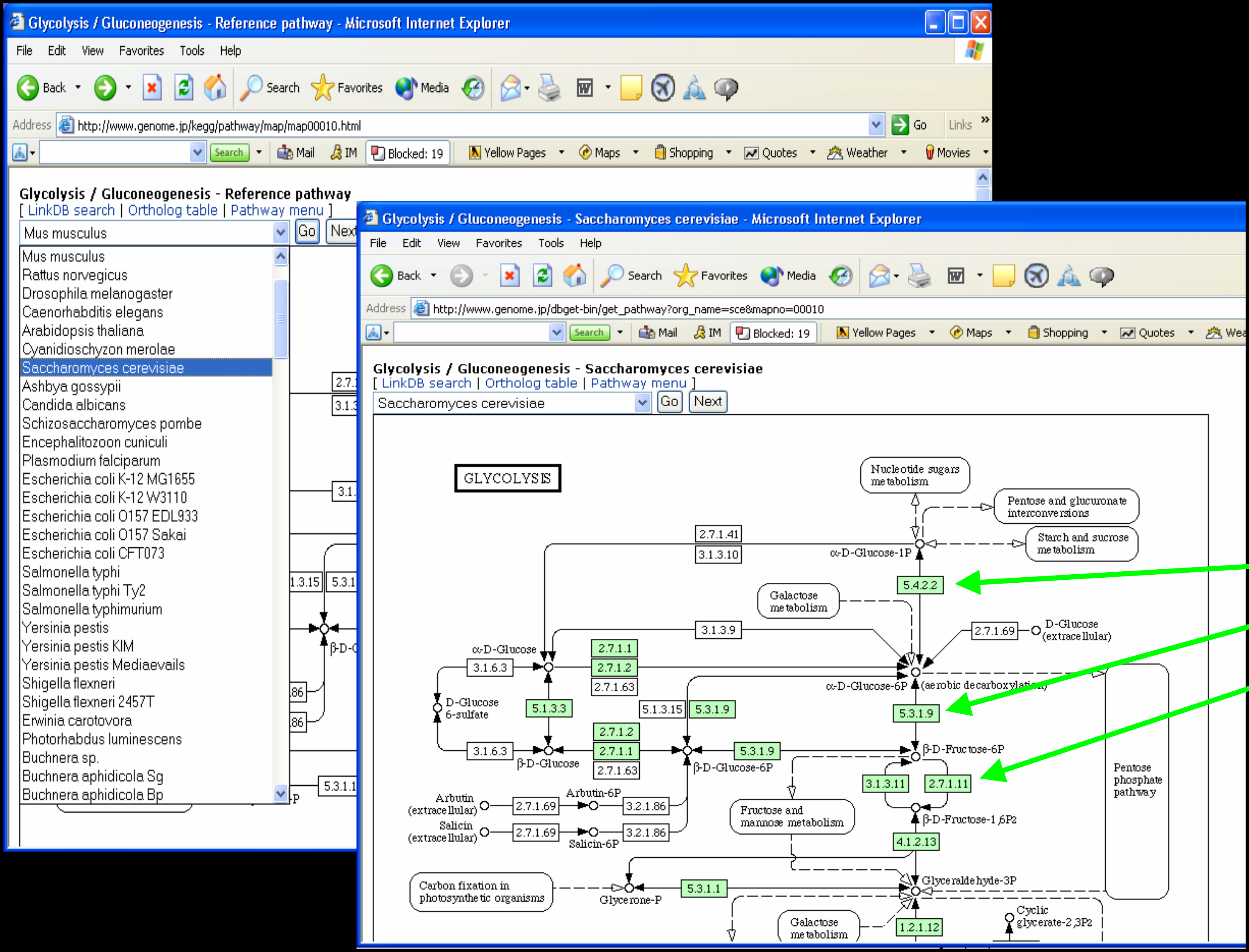
Go to: **1. Metabolism**
Carbohydrate Energy Lipid Nucleotide Amino acid Other amino acid
Glycan PK/NRP Cofactor/vitamin Secondary metabolite Xenobiotics
2. Genetic Information Processing
3. Environmental Information Processing
4. Cellular Processes
5. Human Diseases

See also: **KO (KEGG Orthology)**

1. Metabolism

1.1 Carbohydrate Metabolism	Overview of biosynthetic pathways
Glycolysis / Gluconeogenesis	Ortholog, Oxidoreductases
Citrate cycle (TCA cycle)	Ortholog
Pentose phosphate pathway	Ortholog
Pentose and glucuronate interconversions	Ortholog
Fructose and mannose metabolism	Ortholog, PTS
Galactose metabolism	Ortholog
Ascorbate and aldarate metabolism	Ortholog
Starch and sucrose metabolism	Ortholog, PTS
Aminosugars metabolism	Ortholog, PTS
Nucleotide sugars metabolism	Ortholog
Pyruvate metabolism	Ortholog
Glyoxylate and dicarboxylate metabolism	Ortholog
Propanoate metabolism	Ortholog
Butanoate metabolism	Ortholog
C5-Branched dibasic acid metabolism	
Inositol metabolism	Ortholog
Inositol phosphate metabolism	
1.2 Energy Metabolism	
Oxidative phosphorylation	Ortholog
ATP synthesis	Ortholog
Photosynthesis	Ortholog
Carbon fixation	
Reductive carboxylate cycle (CO2 fixation)	
Methane metabolism	Ortholog
Nitrogen metabolism	Ortholog
Sulfur metabolism	Ortholog

Making an organism-specific map



Glycolysis / Gluconeogenesis - Reference pathway - Microsoft Internet Explorer

Address http://www.genome.jp/kegg/pathway/map/map00010.html

Glycolysis / Gluconeogenesis - Reference pathway

[LinkDB search | Ortholog table | Pathway menu]

Mus musculus

- Mus musculus
- Rattus norvegicus
- Drosophila melanogaster
- Caenorhabditis elegans
- Arabidopsis thaliana
- Cyanidioschyzon merolae
- Saccharomyces cerevisiae
- Ashbya gossypii
- Candida albicans
- Schizosaccharomyces pombe
- Encephalitozoon cuniculi
- Plasmodium falciparum
- Escherichia coli K-12 MG1655
- Escherichia coli K-12 W3110
- Escherichia coli O157 EDL933
- Escherichia coli O157 Sakai
- Escherichia coli CFT073
- Salmonella typhi
- Salmonella typhi Ty2
- Salmonella typhimurium
- Yersinia pestis
- Yersinia pestis KIM
- Yersinia pestis Mediaevails
- Shigella flexneri
- Shigella flexneri 2457T
- Erwinia carotovora
- Photorhabdus luminescens
- Buchnera sp.
- Buchnera aphidicola Sg
- Buchnera aphidicola Bp

Glycolysis / Gluconeogenesis - Saccharomyces cerevisiae - Microsoft Internet Explorer

Address http://www.genome.jp/dbget-bin/get_pathway?org_name=sce&mapno=00010

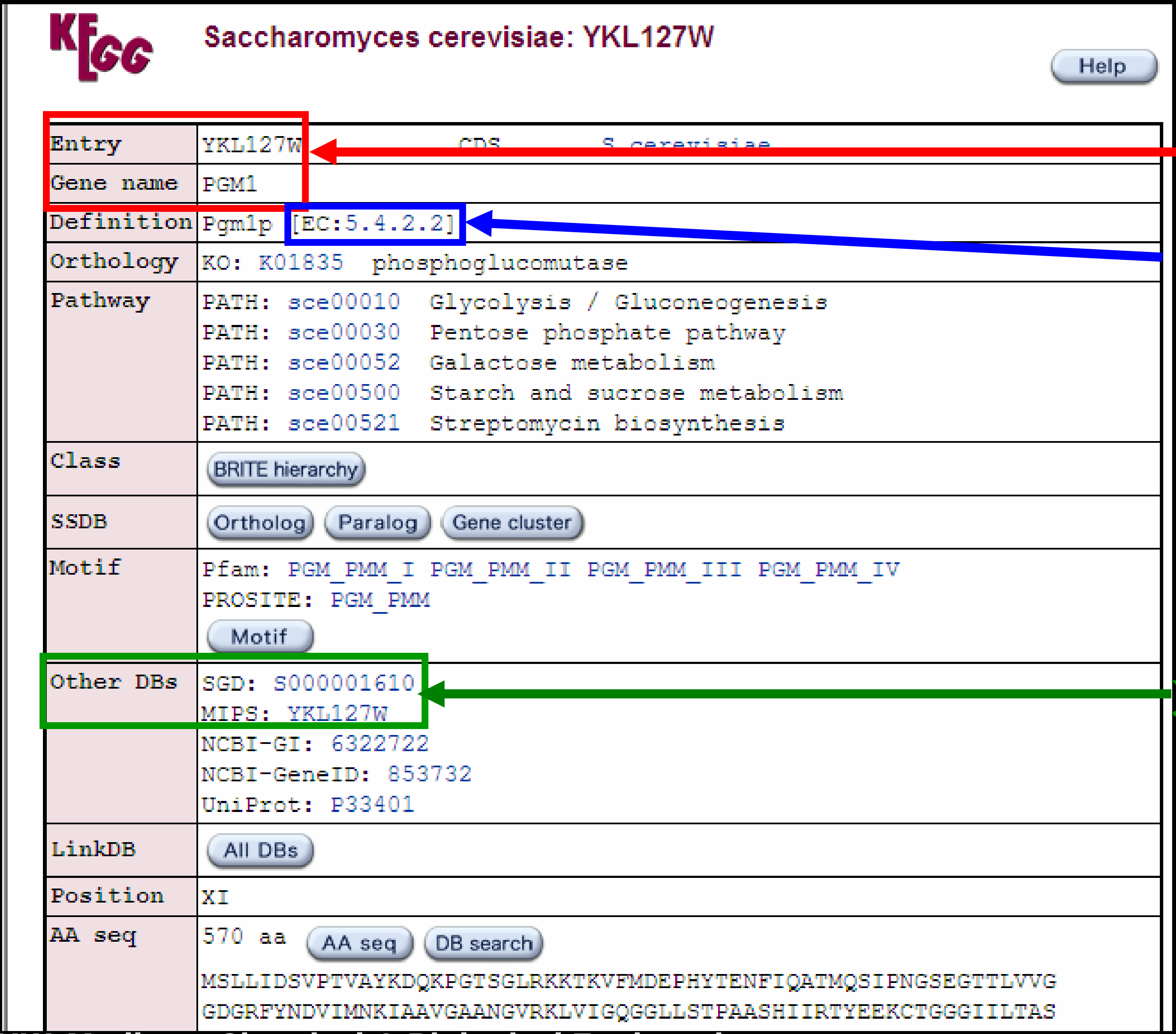
Glycolysis / Gluconeogenesis - Saccharomyces cerevisiae

[LinkDB search | Ortholog table | Pathway menu]

Saccharomyces cerevisiae

Enzymes in yeast are now shaded in green

Yeast-specific information about EC 5.4.2.2



Saccharomyces cerevisiae: YKL127W

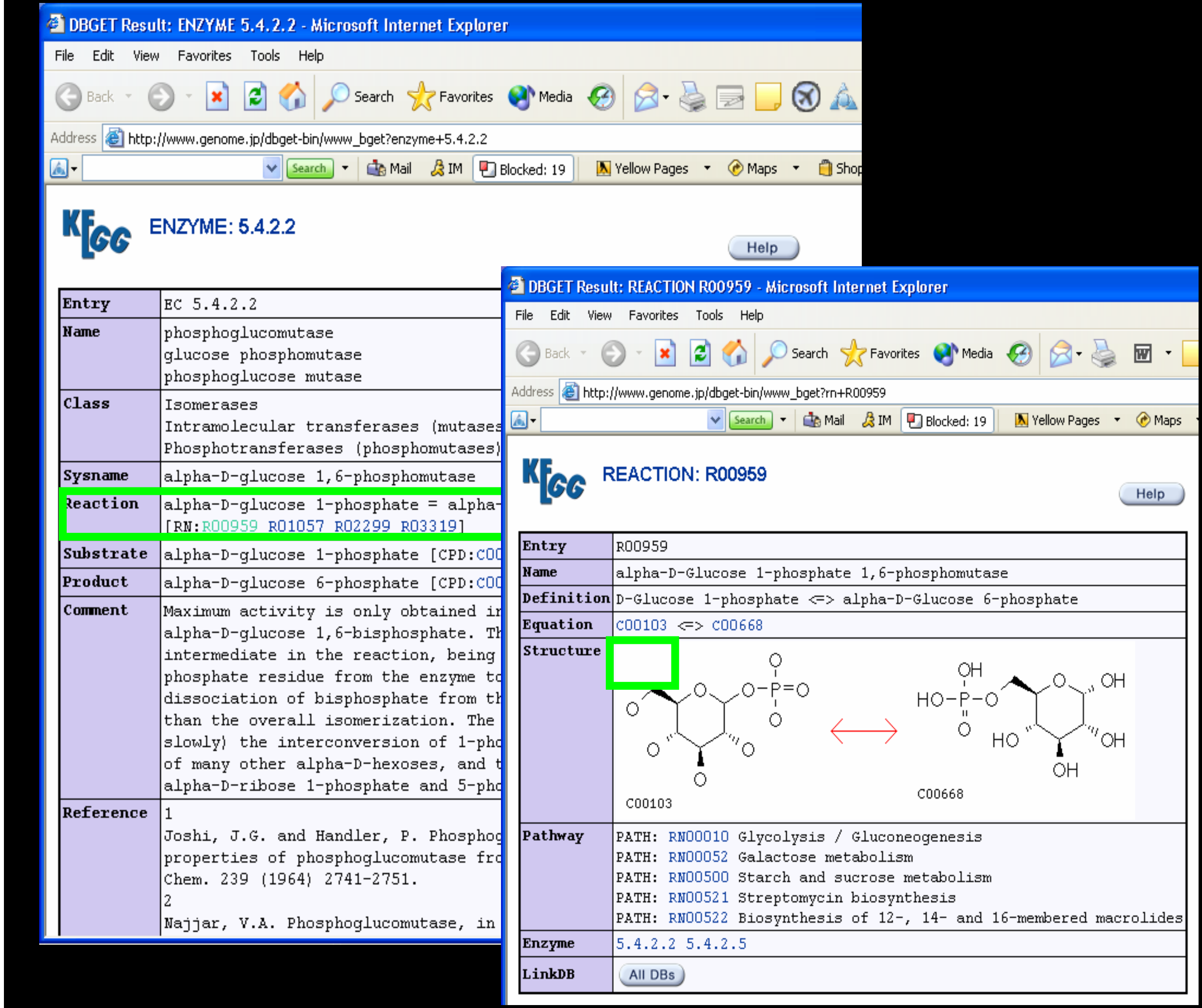
Entry	YKL127W CDS S cerevisiae
Gene name	PGM1
Definition	Pgm1p [EC:5.4.2.2]
Orthology	KO: K01835 phosphoglucomutase
Pathway	PATH: sce00010 Glycolysis / Gluconeogenesis PATH: sce00030 Pentose phosphate pathway PATH: sce00052 Galactose metabolism PATH: sce00500 Starch and sucrose metabolism PATH: sce00521 Streptomycin biosynthesis
Class	BRITE hierarchy
SSDB	Ortholog Paralog Gene cluster
Motif	Pfam: PGM_PMM_I PGM_PMM_II PGM_PMM_III PGM_PMM_IV PROSITE: PGM_PMM Motif
Other DBs	SGD: S000001610 MIPS: YKL127W NCBI-GI: 6322722 NCBI-GeneID: 853732 UniProt: P33401
LinkDB	All DBs
Position	XI
AA seq	570 aa AA seq DB search MSLLIDSVPTVAYKDQKPGTSGLRKKTKVFMDEPHYTENFIQATMQSIPNGSEGTTLVVG GDGRFYNDVIMNKIAAVGAANGVRKLVIGQGGLLSTPAASHIIRTYEEKCTGGGIILTAS

ORF, gene nam

reaction information

yeast databases

Reaction Information

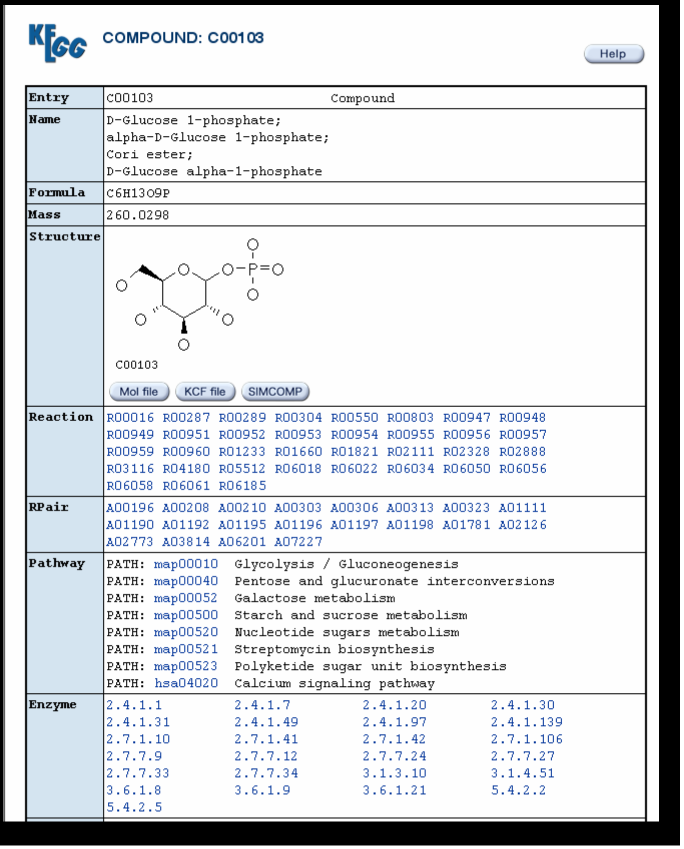


ENZYME: 5.4.2.2

Entry	EC 5.4.2.2
Name	phosphoglucomutase glucose phosphomutase phosphoglucose mutase
Class	Isomerases Intramolecular transferases (mutases Phosphotransferases (phosphomutases)
Sysname	alpha-D-glucose 1,6-phosphomutase
Reaction	alpha-D-glucose 1-phosphate = alpha- [RN:R00959 R01057 R02299 R03319]
Substrate	alpha-D-glucose 1-phosphate [CPD:C00
Product	alpha-D-glucose 6-phosphate [CPD:C00
Comment	Maximum activity is only obtained in alpha-D-glucose 1,6-bisphosphate. Th intermediate in the reaction, being phosphate residue from the enzyme to dissociation of bisphosphate from th than the overall isomerization. The slowly) the interconversion of 1-pho of many other alpha-D-hexoses, and t alpha-D-ribose 1-phosphate and 5-pho
Reference	1 Joshi, J.G. and Handler, P. Phosphog properties of phosphoglucomutase fro Chem. 239 (1964) 2741-2751. 2 Najjar, V.A. Phosphoglucomutase, in

REACTION: R00959

Entry	R00959
Name	alpha-D-Glucose 1-phosphate 1,6-phosphomutase
Definition	D-Glucose 1-phosphate <=> alpha-D-Glucose 6-phosphate
Equation	C00103 <=> C00668
Structure	
Pathway	PATH: RN00010 Glycolysis / Gluconeogenesis PATH: RN00052 Galactose metabolism PATH: RN00500 Starch and sucrose metabolism PATH: RN00521 Streptomycin biosynthesis PATH: RN00522 Biosynthesis of 12-, 14- and 16-membered macrolides
Enzyme	5.4.2.2 5.4.2.5
LinkDB	All DBs

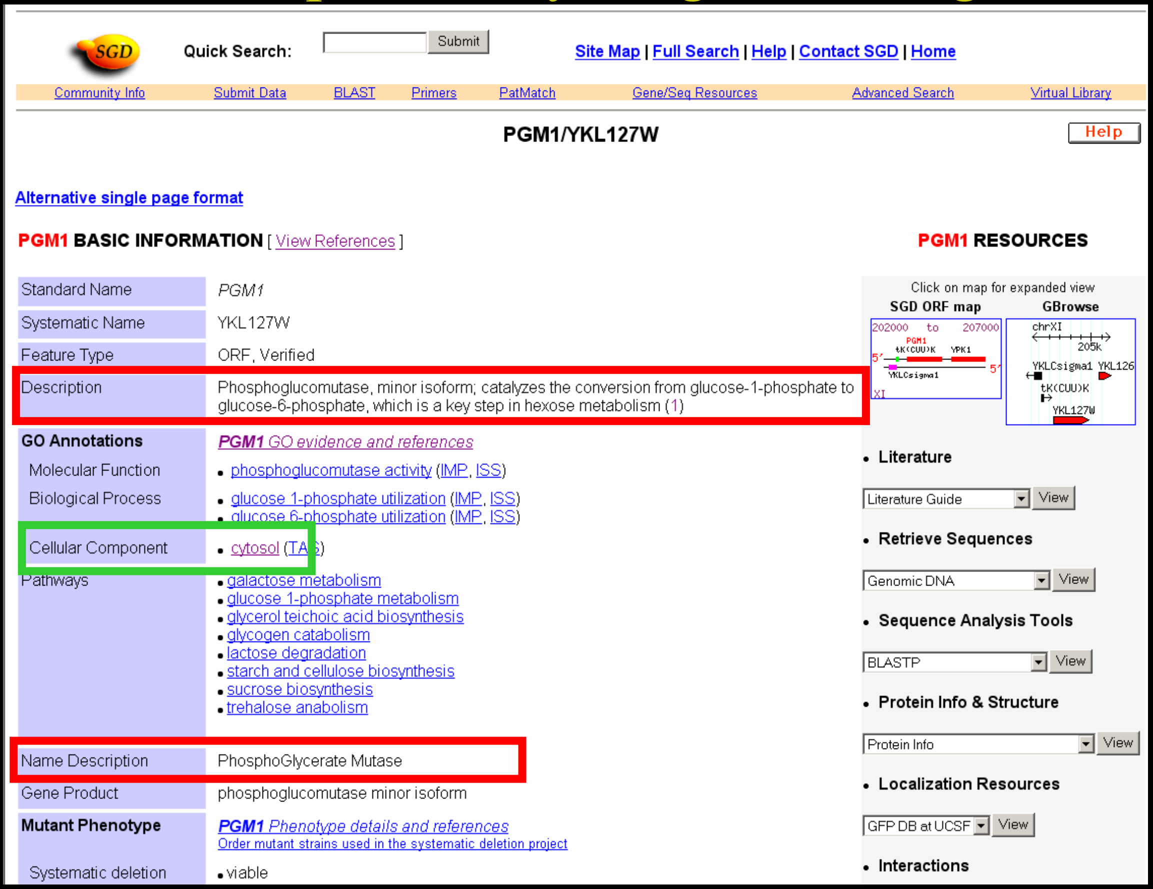


COMPOUND: C00103

Entry	C00103 Compound
Name	D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate
Formula	C6H13O9P
Mass	260.0298
Structure	C00103
Reaction	R00016 R00287 R00289 R00304 R00550 R00803 R00947 R00948 R00949 R00951 R00952 R00953 R00954 R00955 R00956 R00957 R00959 R00960 R01233 R01660 R01821 R02111 R02328 R02888 R03116 R04180 R05512 R06018 R06022 R06034 R06050 R06056 R06058 R06061 R06185
RPair	A00196 A00208 A00210 A00303 A00306 A00313 A00323 A01111 A01190 A01192 A01195 A01196 A01197 A01198 A01781 A02126 A02773 A03814 A06201 A07227
Pathway	PATH: map00010 Glycolysis / Gluconeogenesis PATH: map00040 Pentose and glucuronate interconversions PATH: map00052 Galactose metabolism PATH: map00500 Starch and sucrose metabolism PATH: map00520 Nucleotide sugars metabolism PATH: map00521 Streptomycin biosynthesis PATH: map00523 Polyketide sugar unit biosynthesis PATH: hsa04020 Calcium signaling pathway
Enzyme	2.4.1.1 2.4.1.7 2.4.1.20 2.4.1.30 2.4.1.31 2.4.1.49 2.4.1.97 2.4.1.139 2.7.1.10 2.7.1.41 2.7.1.42 2.7.1.106 2.7.7.9 2.7.7.12 2.7.7.24 2.7.7.27 2.7.7.33 2.7.7.34 3.1.3.10 3.1.4.51 3.6.1.8 3.6.1.9 3.6.1.21 5.4.2.2 5.4.2.5

Yeast Databases

SGD: http://www.yeastgenome.org/



PGM1/YKL127W

PGM1 BASIC INFORMATION [View References]

Standard Name	*PGM1*
Systematic Name	YKL127W
Feature Type	ORF, Verified
Description	Phosphoglucomutase, minor isoform; catalyzes the conversion from glucose-1-phosphate to glucose-6-phosphate, which is a key step in hexose metabolism (1)
GO Annotations	*PGM1 GO evidence and references*
Molecular Function	- phosphoglucomutase activity (IMP, ISS)
Biological Process	- glucose 1-phosphate utilization (IMP, ISS) - glucose 6-phosphate utilization (IMP, ISS)
Cellular Component	- cytosol (TAS)
Pathways	- galactose metabolism - glucose 1-phosphate metabolism - glycerol teichoic acid biosynthesis - glycogen catabolism - lactose degradation - starch and cellulose biosynthesis - sucrose biosynthesis - trehalose anabolism
Name Description	PhosphoGlycerate Mutase
Gene Product	phosphoglucomutase minor isoform
Mutant Phenotype	*PGM1 Phenotype details and references* Order mutant strains used in the systematic deletion project
Systematic deletion	- viable

PGM1 RESOURCES

- **Literature**
- **Retrieve Sequences**
- **Sequence Analysis Tools**
- **Protein Info & Structure**
- **Localization Resources**
- **Interactions**

Localization:
cytosol

Gene-protein-reaction association:
“minor isoform” suggests that there is an isozyme

Yeast Databases

CYGD: http://mips.gsf.de/genre/proj/yeast/

Search Gene/ORF:

Search Description/Remarks:

Catalogues/Tables:

Chromosome View:
I II III IV V VI VII
VIII IX X XI XII XIII
XIV XV XVI Mito

Search / View
Fungi Connection
Tables
Reviews
Pathways
Transcription
About CYGD
Help

PGM1 YKL127w

PGM1 **phosphoglucomutase, minor isoform**

Standard Name: YKL127w
Classification: known protein | *3708 Entries*
Feature Type: CDS

Features

PROTEIN VIEW *PEDANT help*
BLASTP INTERPRO PROSITE PFAM COGs

Taxonomy of Closest Homolog:
- Eucarya
  ..Fungi
  ....Ascomycota
  ......Hemiascomycetes
  ....**Saccharomyces paradoxus** | *4984 Entries*
  Closest..Homolog: 13962 Saccharomyces_paradoxus_NRRL_Y17217 (88.4%)

Similarity:
Paralogs | Homologs in Hemiascomycetes (88.4%) | Ascomycota no Hemiascomycetes (57.6%) | Fungi no Ascomycota (53.7%)) | Eucarya no Fungi (46.5%) | (Plants (42.1%) | Mammalia (43.8%)) || Bacteria (46.8%) || Archaea (14.4%) |||| SWISS-PROT

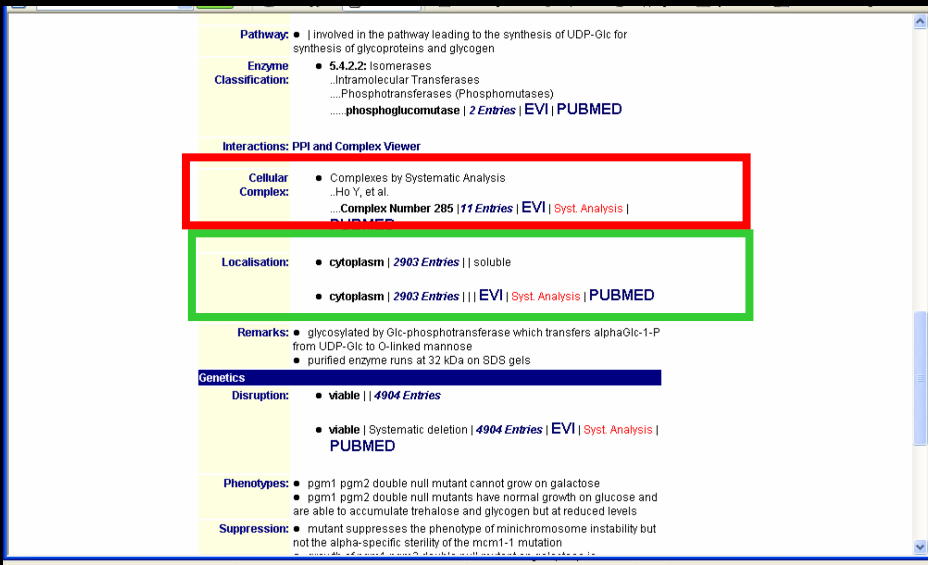
- 'Seed Extraction Sequence Analysis Method' to find paralogs

Search Genolevures I (RST) homologs

FunCat:
- METABOLISM
  ..C-compound and carbohydrate metabolism
  ....**C-compound and carbohydrate utilization** | *261 Entries*
- ENERGY
  ..**metabolism of energy reserves (e.g. glycogen, trehalose)** | *37 Entries*

Function:
- participates in both the breakdown and synthesis of glucose; can also act on mannose
- interconverts glc-1-P and glc-6-P
- needed for utilisation of glycogen and for growth on galactose
- needed for synthesis of trehalose

Interpro:
- IPR005841 Phosphoglucomutase/phosphomannomutase | *4 Entries*
- IPR005843 Phosphoglucomutase/phosphomannomutase C terminal | *3 Entries*
- IPR005844 Phosphoglucomutase/phosphomannomutase alpha/beta/alpha domain I | *4 Entries*
- IPR005845 Phosphoglucomutase/phosphomannomutase alpha/beta/alpha domain II | *2 Entries*
- IPR005846 Phosphoglucomutase/phosphomannomutase alpha/beta/alpha domain III | *2 Entries*



Pathway:
- | involved in the pathway leading to the synthesis of UDP-Glc for synthesis of glycoproteins and glycogen

Enzyme Classification:
- **5.4.2.2:** Isomerases
  ..Intramolecular Transferases
  ....Phosphotransferases (Phosphomutases)
  ......**phosphoglucomutase** | *2 Entries* | EVI | PUBMED

Interactions: PPI and Complex Viewer

Cellular Complex:
- Complexes by Systematic Analysis
  ..Ho Y, et al.
  ....**Complex Number 285** | *11 Entries* | EVI | Syst. Analysis |

Localisation:
- **cytoplasm** | *2903 Entries* | | soluble
- **cytoplasm** | *2903 Entries* | | | EVI | Syst. Analysis | PUBMED

Remarks:
- glycosylated by Glc-phosphotransferase which transfers alphaGlc-1-P from UDP-Glc to O-linked mannose
- purified enzyme runs at 32 kDa on SDS gels

Genetics

Disruption:
- **viable** | | *4904 Entries*
- **viable** | Systematic deletion | *4904 Entries* | EVI | Syst. Analysis | PUBMED

Phenotypes:
- pgm1 pgm2 double null mutant cannot grow on galactose
- pgm1 pgm2 double null mutants have normal growth on glucose and are able to accumulate trehalose and glycogen but at reduced levels

Suppression:
- mutant suppresses the phenotype of minichromosome instability but not the alpha-specific sterility of the mcm1-1 mutation

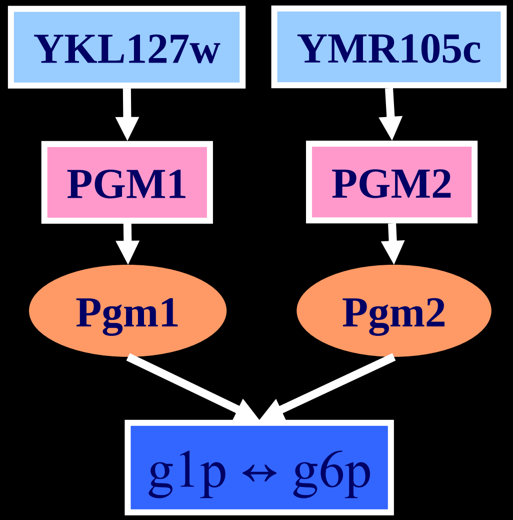
Localization:
cytosol

Gene-protein-reaction
association:
isozyme isYMR105c (PGM2)

The first entry in our reconstruction:

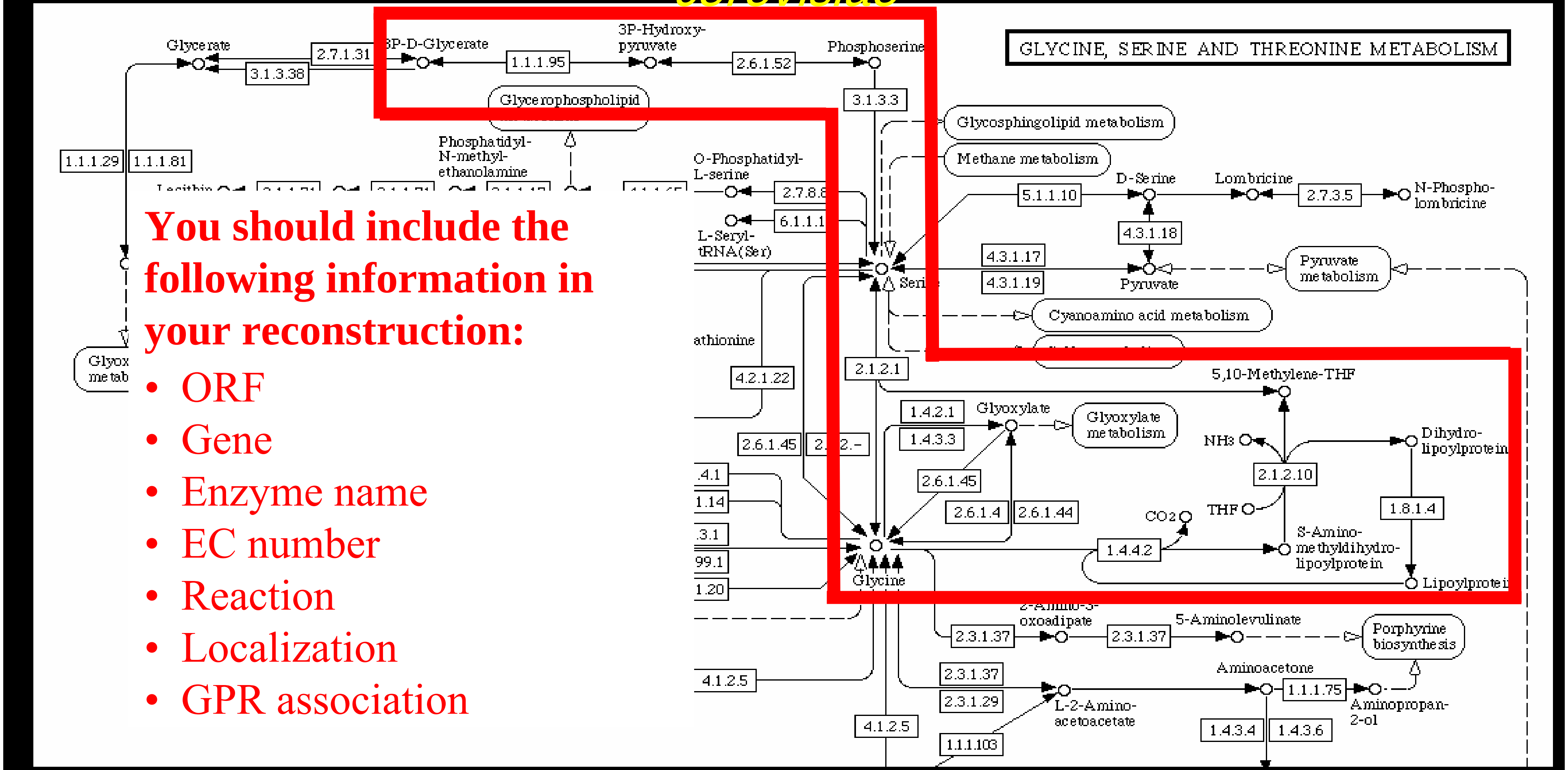
ORF	YKL127w
GENE	PGM1
NAME	Phosphoglucomutase, minor isoform
EC NUMBER	5.4.2.2
REACTION	g1p ↔ g6p
LOCALIZATION	cytosol

GPR ASSOCIATION



Now it’s *your* turn!

Reconstruct this segment of the glycine, serine, and threonine metabolism map for *Saccharomyces cerevisiae*



You should include the following information in your reconstruction:

- ORF
- Gene
- Enzyme name
- EC number
- Reaction
- Localization
- GPR association

Results

ORF	(YER081W or YIL074C)	YOR184W	YGR208W
Gene	(Ser3) or (Ser33)	Ser1	Ser2
Name	phosphoglycerate dehydrogenase	phosphoserine transaminase	phosphoserine phosphatase
EC #r	EC-1.1.1.95	EC-2.6.1.52	EC-3.1.3.3
Reaction	3-phosphoglycerate + nad <==> 3phosphohydroxypyruvate + h + nadh	3phosphonooxypyruvate + L-glutamate <==> 2-oxoglutarate + O-phopspho-L-serine	O-phopspho-L-serine + h2o <==> L-serine + pi
Localization	cytoplasm	cytoplasm	cytoplasm

ORF	YGR208W	YBR263W	YLR058C
Gene	Ser2-n	Shm1-m	Shm2
Name	phosphoserine phosphatase	glycine hydroxymethyltransferase	glycine hydroxymethyltransferase
EC #r	EC-3.1.3.3	EC-2.1.2.1	EC-2.1.2.1
Reaction	O-phopspho-L-serine + h2o <==> L-serine + pi	L-serine + tetrahydrofolate <==> 5,10-methylenetetrahydrofolate + glycine + h2o	L-serine + tetrahydrofolate <==> 5,10-methylenetetrahydrofolate + glycine + h2o
Localization	nucleus	mitochondrion	cytoplasm

ORF	(YDR019C and YMR189W and YAL044C and YFL018C)	(YDR019C and YMR189W and YAL044C and YFL018C)	(YDR019C and YMR189W and YAL044C and YFL018C)
Gene	(Gcv1-m and Gcv2-m and Gcv3-m and Lpd1-m)	(Gcv1-m and Gcv2-m and Gcv3-m and Lpd1-m)	(Gcv1-m and Gcv2-m and Gcv3-m and Lpd1-m)
Name	glycine-cleavage complex	glycine-cleavage complex	glycine-cleavage complex
EC #r	EC-2.1.2.10	EC-1.4.4.2	EC-1.8.1.4
Reaction	protein-S-aminomethyldihydrolipoyllysne + tetrahydrofolate --> protein-dihydrolipoyllysine + 5,10-methylenetetrahydrofolate + nh3	glycine + H-protein-lipoyllysine <==> H-protein-S-aminomethyldihydrolipoyllysine + co2	protein-N6-(dihydrolipoyl)lysine + nad <==> protein-N6-(lipoyl)lysine + nadh + h
Localization	mitochondrion	mitochondrion	mitochondrion

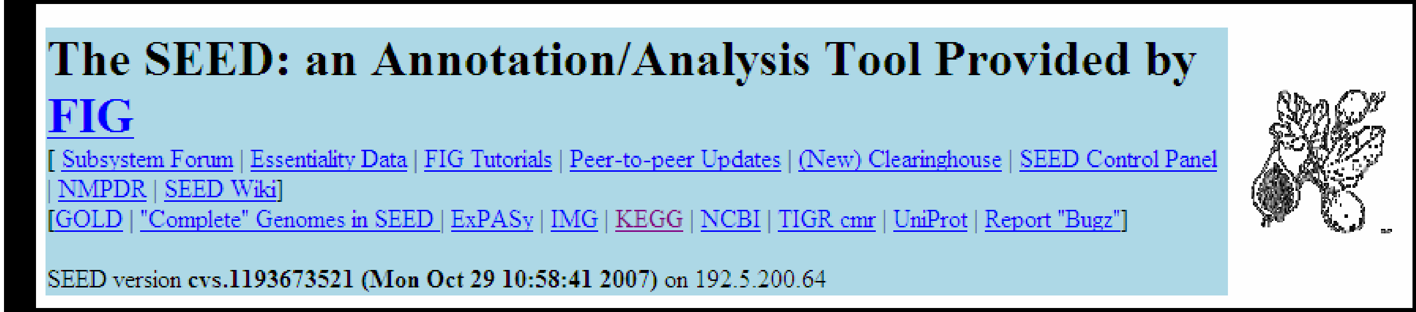
What else is needed in our reconstruction?

- Need to reconcile the different metabolite names are used in the KEGG maps and reactions.
- Need to determine reaction reversibility. Sometimes this can be inferred from the genome annotation, but usually we need to go to the literature.
- Need to identify alternate substrates. This can typically be found in BRENDA, the enzyme database.
- Need to collect evidence. The genome annotation databases are useful for collecting this information.
- Need to assign confidence scores. This is based on the methods used to collect the evidence.
- Need to determine the formula and charge of each compound.
- Need to elementally and charge balance the reactions.

Other Useful Databases

- BRENDA: http://www.brenda.uni-koeln.de/
- ExPASy: http://us.expasy.org/enzyme/
- MetaCyc: http://metacyc.org/
- The SEED: http://theseed.uchicago.edu/FIG/index.cgi
- PSORT: http://www.psort.org/
- PROLINKS: http://128.97.39.94/cgi-bin/functionator/pronav
- Transport Classification Database: http://www.tcdb.org/

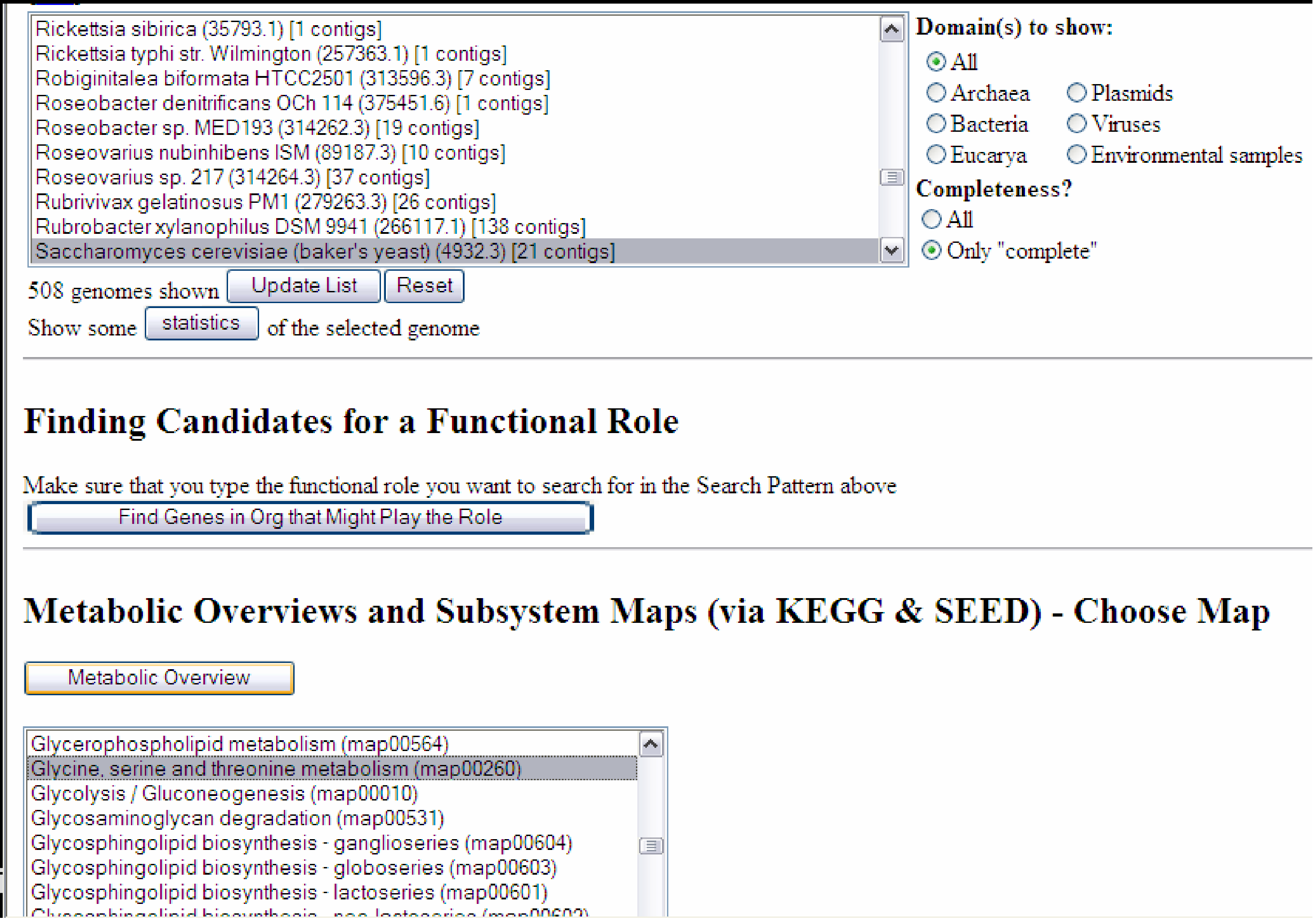
http://theseed.uchicago.edu/FIG/index.cgi



The SEED: an Annotation/Analysis Tool Provided by FIG

[Subsystem Forum | Essentiality Data | FIG Tutorials | Peer-to-peer Updates | (New) Clearinghouse | SEED Control Panel | NMPDR | SEED Wiki]
[GOLD | "Complete" Genomes in SEED | ExPASy | IMG | KEGG | NCBI | TIGR cmr | UniProt | Report "Bugz"]

SEED version **cvs.1193673521 (Mon Oct 29 10:58:41 2007)** on 192.5.200.64



Rickettsia sibirica (35793.1) [1 contigs]
Rickettsia typhi str. Wilmington (257363.1) [1 contigs]
Robiginitalea biformata HTCC2501 (313596.3) [7 contigs]
Roseobacter denitrificans OCh 114 (375451.6) [1 contigs]
Roseobacter sp. MED193 (314262.3) [19 contigs]
Roseovarius nubinhibens ISM (89187.3) [10 contigs]
Roseovarius sp. 217 (314264.3) [37 contigs]
Rubrivivax gelatinosus PM1 (279263.3) [26 contigs]
Rubrobacter xylanophilus DSM 9941 (266117.1) [138 contigs]
Saccharomyces cerevisiae (baker's yeast) (4932.3) [21 contigs]

Domain(s) to show:
● All
○ Archaea ○ Plasmids
○ Bacteria ○ Viruses
○ Eucarya ○ Environmental samples

Completeness?
○ All
● Only "complete"

508 genomes shown

Show some of the selected genome

Finding Candidates for a Functional Role

Make sure that you type the functional role you want to search for in the Search Pattern above

Metabolic Overviews and Subsystem Maps (via KEGG & SEED) - Choose Map

Glycerophospholipid metabolism (map00564)
Glycine, serine and threonine metabolism (map00260)
Glycolysis / Gluconeogenesis (map00010)
Glycosaminoglycan degradation (map00531)
Glycosphingolipid biosynthesis - ganglioseries (map00604)
Glycosphingolipid biosynthesis - globoseries (map00603)
Glycosphingolipid biosynthesis - lactoseries (map00601)

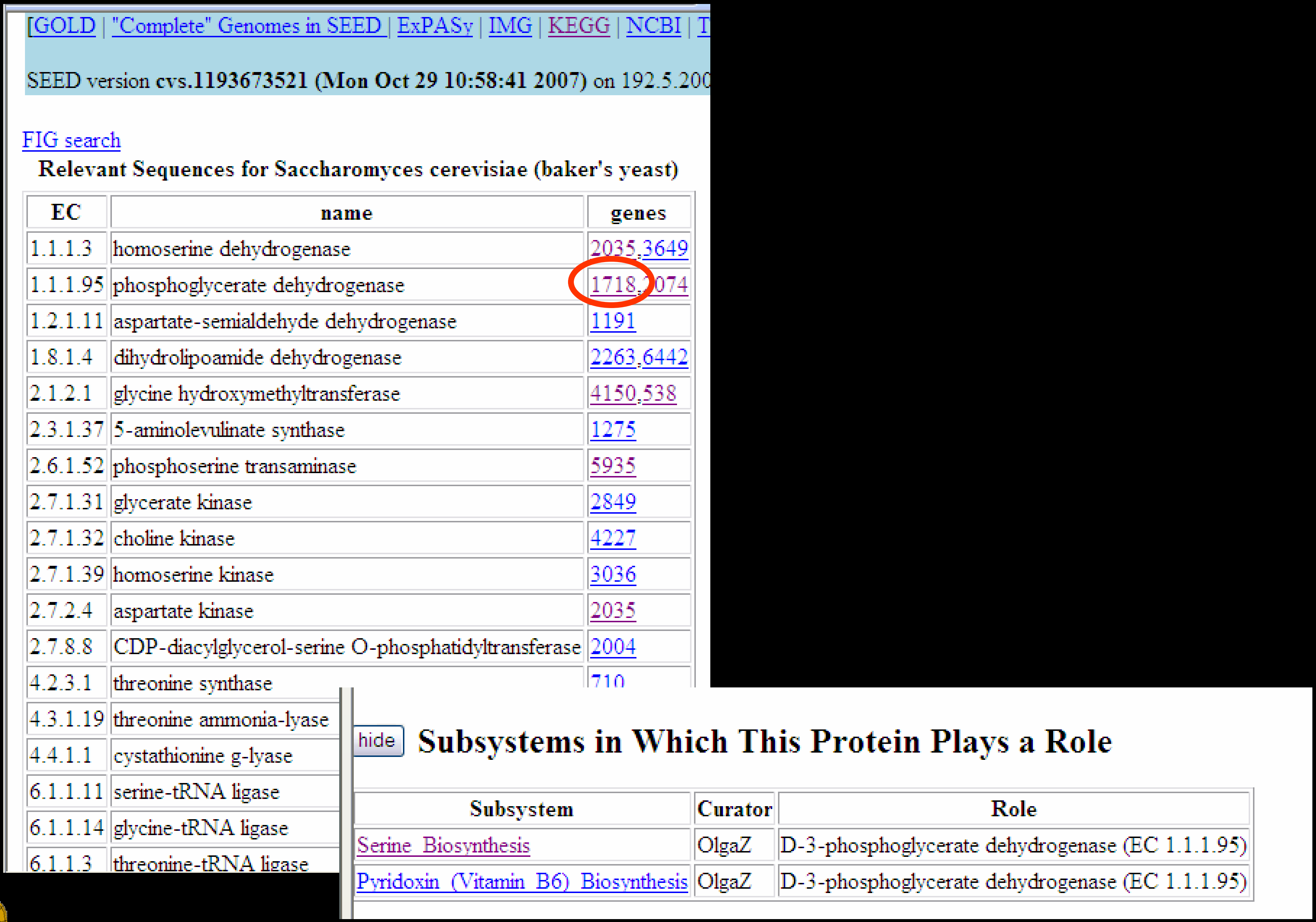


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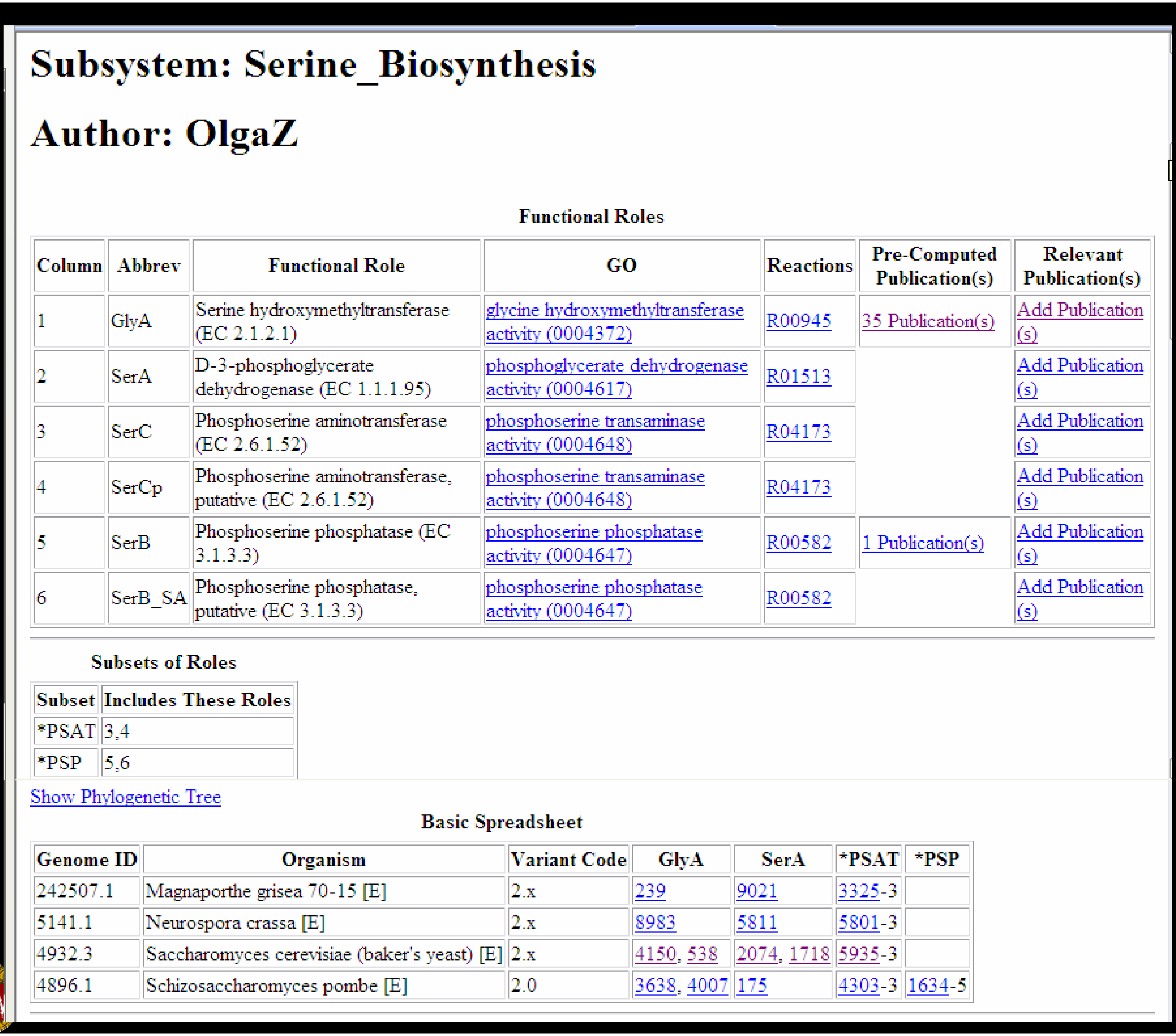
FIG search

Relevant Sequences for Saccharomyces cerevisiae (baker's yeast)

EC	name	genes
1.1.1.3	homoserine dehydrogenase	2035,3649
1.1.1.95	phosphoglycerate dehydrogenase	1718,2074
1.2.1.11	aspartate-semialdehyde dehydrogenase	1191
1.8.1.4	dihydrolipoamide dehydrogenase	2263,6442
2.1.2.1	glycine hydroxymethyltransferase	4150,538
2.3.1.37	5-aminolevulinate synthase	1275
2.6.1.52	phosphoserine transaminase	5935
2.7.1.31	glycerate kinase	2849
2.7.1.32	choline kinase	4227
2.7.1.39	homoserine kinase	3036
2.7.2.4	aspartate kinase	2035
2.7.8.8	CDP-diacylglycerol-serine O-phosphatidyltransferase	2004
4.2.3.1	threonine synthase	710
4.3.1.19	threonine ammonia-lyase	
4.4.1.1	cystathionine g-lyase	
6.1.1.11	serine-tRNA ligase	
6.1.1.14	glycine-tRNA ligase	
6.1.1.3	threonine-tRNA ligase	

Subsystems in Which This Protein Plays a Role

Subsystem	Curator	Role
Serine Biosynthesis	OlgaZ	D-3-phosphoglycerate dehydrogenase (EC 1.1.1.95)
Pyridoxin (Vitamin B6) Biosynthesis	OlgaZ	D-3-phosphoglycerate dehydrogenase (EC 1.1.1.95)



Subsystem: Serine_Biosynthesis

Author: OlgaZ

Functional Roles

Column	Abbrev	Functional Role	GO	Reactions	Pre-Computed Publication(s)	Relevant Publication(s)
1	GlyA	Serine hydroxymethyltransferase (EC 2.1.2.1)	glycine hydroxymethyltransferase activity (0004372)	R00945	35 Publication(s)	Add Publication (s)
2	SerA	D-3-phosphoglycerate dehydrogenase (EC 1.1.1.95)	phosphoglycerate dehydrogenase activity (0004617)	R01513		Add Publication (s)
3	SerC	Phosphoserine aminotransferase (EC 2.6.1.52)	phosphoserine transaminase activity (0004648)	R04173		Add Publication (s)
4	SerCp	Phosphoserine aminotransferase, putative (EC 2.6.1.52)	phosphoserine transaminase activity (0004648)	R04173		Add Publication (s)
5	SerB	Phosphoserine phosphatase (EC 3.1.3.3)	phosphoserine phosphatase activity (0004647)	R00582	1 Publication(s)	Add Publication (s)
6	SerB_SA	Phosphoserine phosphatase, putative (EC 3.1.3.3)	phosphoserine phosphatase activity (0004647)	R00582		Add Publication (s)

Subsets of Roles

Subset	Includes These Roles
*PSAT	3,4
*PSP	5,6

Show Phylogenetic Tree

Basic Spreadsheet

Genome ID	Organism	Variant Code	GlyA	SerA	*PSAT	*PSP
242507.1	Magnaporthe grisea 70-15 [E]	2.x	239	9021	3325-3	
5141.1	Neurospora crassa [E]	2.x	8983	5811	5801-3	
4932.3	Saccharomyces cerevisiae (baker's yeast) [E]	2.x	4150, 538	2074, 1718	5935-3	
4896.1	Schizosaccharomyces pombe [E]	2.0	3638, 4007	175	4303-3	1634-5

Summary

- KEGG maps are a great starting point for metabolic reconstructions.
- Organism-specific databases are also useful since they collect many data types in one location.
- Metabolic reconstruction is a time-consuming process that requires manual curation.