

# KEGG/GenomeNetの利用法

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統合データベース講習会：AJACS蝦夷3 2013/11/6

# 内容

- ・ ブラウザを使ったKEGG/GenomeNetの利用法
  - ・ KEGGとGenomeNetの概要
  - ・ ゲノム情報（配列データ）
  - ・ システム情報（パスウェイと階層分類）
  - ・ ケミカル情報（化合物と反応データ）

# Web

<http://www.genome.jp/ja/>

“genomenet” “ゲノムネット”でWeb検索

# GenomeNet

- ・ゲノム情報を基盤とした生命科学研究を促進するためのインターネットサービス
- ・KEGGを主幹とするデータベース群と、それらデータを解析するために計算ツール群からなっている

The screenshot shows the GenomeNet homepage with several key features highlighted:

- Search Bar:** A search bar at the top right allows users to search across the integrated databases.
- Navigation Links:** A sidebar on the left provides links to various sections: ゲノムネット (GenomeNet), 総合データベース (Integrated Database), 医薬品データベース (Drug Database), KEGG, varDB, 研究支援データベース (Research Support Database), 計算ツール (Computational Tools), and FTP.
- Highlighted Sections:**
  - ゲノムネットデータベースリソース (GenomeNet Database Resources):** This section contains links to the integrated database, DBGET search, LinkDB search, KEGG MEDICUS (disease and drug integration), KEGG:命のシステム情報統合データベース (KEGG Life System Information Integration Database), KEGG PATHWAY, KEGG BRITE, KEGG Organisms, KEGG GENES, KEGG LIGAND, Reaction Ontology, varDB (antigen variation database), CYORF (ciliate proteome), BSORF (bacterial proteome), and EXPRESSION (expression profile).
  - ゲノムネット計算ツール (GenomeNet Computational Tools):** This section includes links for BLAST / FASTA (homology search), MOTIF (motif search), CLUSTALW / MAFFT / PRRN (multiple sequence alignment), and various genome information analysis tools like OC Viewer, REST services, and KAAS.
- Right Sidebar:** Includes links to KEGG Pathway Browser, BRITE Functional Layer (Japanese), KEGG Species List, MetaGenome, DraftGenome, and a diagram illustrating database links.
- Bottom Right:** A graph showing the growth of databases over time.

# KEGG

## Kyoto Encyclopedia of Genes and Genomes

- ・ゲノムや分子レベルの情報から細胞、個体、エコシステムといった生命システムレベルの機能を理解するためのデータベースリソース
- ・遺伝子や化合物などの分子部品のデータベースと、それらをつなぐネットワークのデータベースからなっている

The screenshot shows the KEGG homepage with a sidebar containing links to various databases and tools. The main content area features a brief introduction to KEGG and a list of entry points categorized by type.

**KEGG Home**  
Release notes  
Current statistics  
Plea from KEGG

**KEGG Database**  
KEGG の概要  
Searching KEGG  
KEGG mapping  
Color codes

**KEGG Objects**  
Pathway maps  
Brite hierarchies

**KEGG Software**  
KegTools  
KEGG API  
KGML

**KEGG FTP**  
利用申し込み

ゲノムネット  
DBGET/LinkDB  
Feedback  
Kanehisa Labs

**KEGG: Kyoto Encyclopedia of Genes and Genomes**

KEGG は分子レベルの情報から細胞、個体、エコシステムといった高次生命システムの機能や有用性を理解するためのリソースです。とくにゲノムをはじめとしたハイスクロットデータの生物学的意味解釈に広く利用されています。また KEGG MEDICUS で薬品添付文書など社会的ニーズの高いデータとの統合も行われています。医薬品相互作用検索や KEGG お薬手帳をお試しください。

**KEGG の主要エントリーポイント**

**KEGG2** KEGG 全体の目次のページ [Update notes](#)

**データタイプごとのエントリーポイント**

<b>KEGG PATHWAY</b>	パスウェイマップ [パスウェイ一覧]
<b>KEGG BRITE</b>	機能階層・オントロジー (一部日本語) [Brite 一覧]
<b>KEGG MODULE</b>	KEGG モジュール [モジュール一覧]
<b>KEGG DISEASE</b>	病気 (日本語) [がん   感染症]
<b>KEGG DRUG</b>	医薬品 (日本語) [薬効分類 ATC 分類]
<b>KEGG ORTHOLOGY</b>	オーソログアノテーション
<b>KEGG GENOME</b>	ゲノム [KEGG 生物種一覧]
<b>KEGG GENES</b>	遺伝子・タンパク質
<b>KEGG COMPOUND</b>	化合物 [化合物分類]
<b>KEGG REACTION</b>	化学反応 [反応モジュール]

**一般向けのエントリーポイント**

**KEGG MEDICUS** ゲノムと疾患・医薬品の統合リソース (日本語) [お薬手帳]

**生物種ごとのエントリーポイント**

**KEGG Organisms** 生物種コード(複数可)  Go hsa hsa eco

**解析ツール**

# KEGG



# Kyoto Encyclo

KEGG: Kyoto Encyclopedia of Genes and Genomes

KEGG Home  
Release notes  
Current statistics  
Plea from KEGG

KEGG Database  
KEGG の概要  
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Feedback

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KEGG2  
データタイプごとのエントリーポイント  
KEGG2

KEGG の主要エントリーポイント  
KEGG2

KEGG PATHWAY  
KEGG BRITE  
KEGG MODULE  
KEGG MEDICUS  
KEGG ORTHOLOGY  
KEGG GENES  
KEGG GENOME  
KEGG Organisms  
KEGG LIGAND  
KEGG COMPOUND  
KEGG GLYCAN  
KEGG REACTION  
Reaction Modules  
KEGG MEDICUS  
KEGG Organisms  
KEGG REACTION

KEGG – Table of Contents

KEGG – Table of Contents

KEGG2 PATHWAY BRITE MODULE DISEASE DRUG KO GENOME GENES LIGAND DBGET

Search KEGG for  Go Clear

Category	Entry Point	Release Info	Search & Compute	DBGET Search
Systems information	<a href="#">KEGG PATHWAY</a> <a href="#">KEGG BRITE</a> <a href="#">KEGG MODULE</a> <a href="#">KEGG Mapper</a> <a href="#">KEGG Atlas</a>	New maps Update history New hierarchies Update history	Search Pathway Search Brite Search Module KEGG pathway maps BRITE functional hierarchies KEGG modules	PATHWAY BRITE MODULE
	<a href="#">KEGG DISEASE</a> <a href="#">KEGG DRUG</a> <a href="#">KEGG ENVIRON</a> <a href="#">KEGG MEDICUS</a>	New drug maps Update history	Human diseases Infectious diseases ATC drug classification	DISEASE DRUG ENVIRON
	<a href="#">KEGG ORTHOLOGY</a>		KEGG Orthology (KO)	ORTHOLOGY
Genomic information	<a href="#">KEGG GENES</a> <a href="#">KEGG GENOME</a> <a href="#">KEGG Organisms</a>	New organisms Update history	SSDB search OC viewer† BLAST / FASTA search† KAAS automatic annotation† Map organisms to taxonomy Generate taxonomy tree KEGG organisms	GENES DGENES EGENEST† MGENEST† GENOME EGENOMET† MGENOMET†
Chemical information	<a href="#">KEGG LIGAND</a> <a href="#">KEGG COMPOUND</a> <a href="#">KEGG GLYCAN</a> <a href="#">KEGG REACTION</a> Reaction Modules		SIMCOMP / SUBCOMP search† KCAM search† E-zyme reaction prediction† PathPred pathway prediction† PathComp path computation† PathSearch reaction search†	COMPOUND GLYCAN REACTION RPAIR RCLASS ENZYME

KEGG is developed by Kanehisa Laboratories. See [Kanehisa et al. \(2012\)](#) for the new features of KEGG.  
† Developed and maintained by Kyoto University Bioinformatics Center as part of its GenomeNet service.

KEGG for specific organisms

KEGG Organisms - the list of currently available organisms

Select  Organism   (examples) hsa mmu sce eco bsu syn

# ゲノム情報

配列データ

# KEGG GENES

KEGG GENES Database

Molecular building blocks of life in the genomic space

KEGG2 PATHWAY BRITE MODULE KO GENOME GENES SSDB Organisms

Enter org:gene (Example) syn:ssr3451

Entry Gene cluster Ortholog Paralog Motif Clear

**Gene Catalogs**

KEGG GENES is a collection of gene catalogs for all complete genomes (see [release history](#)) generated from publicly available resources, mostly NCBI RefSeq. They are subject to SSDB computation and KO assignment (gene annotation) by KOALA tool. KEGG DGENES for draft genomes of some eukaryotes and KEGG EGENES for EST datasets of mostly plants are supplementary gene catalogs, which are given automatic KO assignment by KAAS with GENES used as a reference data set. There is now a fourth type of gene catalogs, MGENES for metagenomes (see also [KEGG GENOME](#)) with automatic annotation. The viral gene catalog, VGENES, is not yet fully integrated in the KEGG system.

Gene catalog	Category	Remark
GENES	complete genomes	High-quality genomes with KOALA and manual annotations
DGENES		Draft genomes with automatic (KAAS) annotation
EGENES	EST datasets	EST contigs with automatic (KAAS) annotation
MGENES	Metagenomes	Metagenomes with automatic (KAAS) annotation
VGENES	Viruses	No annotation; available only in DBGET

Search GENES for  Go Clear  
 bfind mode  bget mode

Search Organism hsa for  Go Clear  
 bfind mode  bget mode

**Gene Annotation**

遺伝子・タンパク質配列を集めたデータベース

サブカテゴリ

GENES：コンプリートゲノム

DGENES：ドラフトゲノム

EGENES：ESTコンティグ

MGENES：メタゲノム

VGENES：ウイルスゲノム

# KEGG GENES

KEGG Organisms: Complete Genomes

Eukaryotes

Eukaryotes: 202 Bacteria: 2510 Archaea: 161

[ Genomes | Draft | ESTs | Meta | Pan ]

EGENES  
DGENES  
MGENES

Category	Species	Source	
Vertebrates	Mammals	hsa Homo sapiens (human)	RefSeq
		ptr Pan troglodytes (chimpanzee)	RefSeq
		pps Pan paniscus (bonobo)	RefSeq
		ggo Gorilla gorilla gorilla (western lowland gorilla)	RefSeq
		pon Pongo abelii (Sumatran orangutan)	RefSeq
		mcc Macaca mulatta (rhesus monkey)	RefSeq
		mmu Mus musculus (mouse)	RefSeq
		rno Rattus norvegicus (rat)	RefSeq
		cge Cricetulus griseus (Chinese hamster)	RefSeq
		hgl Heterocephalus glaber (naked mole rat)	RefSeq
		cfa Canis familiaris (dog)	RefSeq
		aml Ailuropoda melanoleuca (giant panda)	RefSeq
		fca Felis catus (domestic cat)	RefSeq
		bta Bos taurus (cow)	RefSeq
		ssc Sus scrofa (pig)	RefSeq
ecb Equus caballus (horse)	RefSeq		
mdo Monodelphis domestica (opossum)	RefSeq		
shr Sarcophilus harrisii (Tasmanian devil)	RefSeq		

- KEGGに登録されている生物種のリスト
- 各生物には生物種コードがつけられている

# KEGG GENES

KEGG GENOME: Homo sapiens (human)

**KEGG** **Homo sapiens (human)**

Genome info    Pathway map    Brite hierarchy    Module    Genome map    Blast

Search genes:  Go Clear

**Genome information**

<b>T number</b>	T01001
<b>Org code</b>	hsa
<b>Aliases</b>	HUMAN, 9606
<b>Full name</b>	Homo sapiens (human)
<b>Definition</b>	Homo sapiens (human)
<b>Annotation</b>	manual
<b>Taxonomy</b>	TAX: 9606

Lineage Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini; Catarrhini; Hominidae; Homo

Data source RefSeq (Project:168)

Original DB NCBI, OMIM, HGNC, HPRD, Ensembl

Statistics Number of protein genes: 20124  
Number of RNA genes: 8818

Reference PMID: 11237011

Authors Lander ES, et al.

アノテーション作業の進度

manual : 手作業

KOALA : 自動 (SSEARCHベース)

KAAS : 自動 (BLASTベース)

Annotation manual ← →

# KEGG GENES

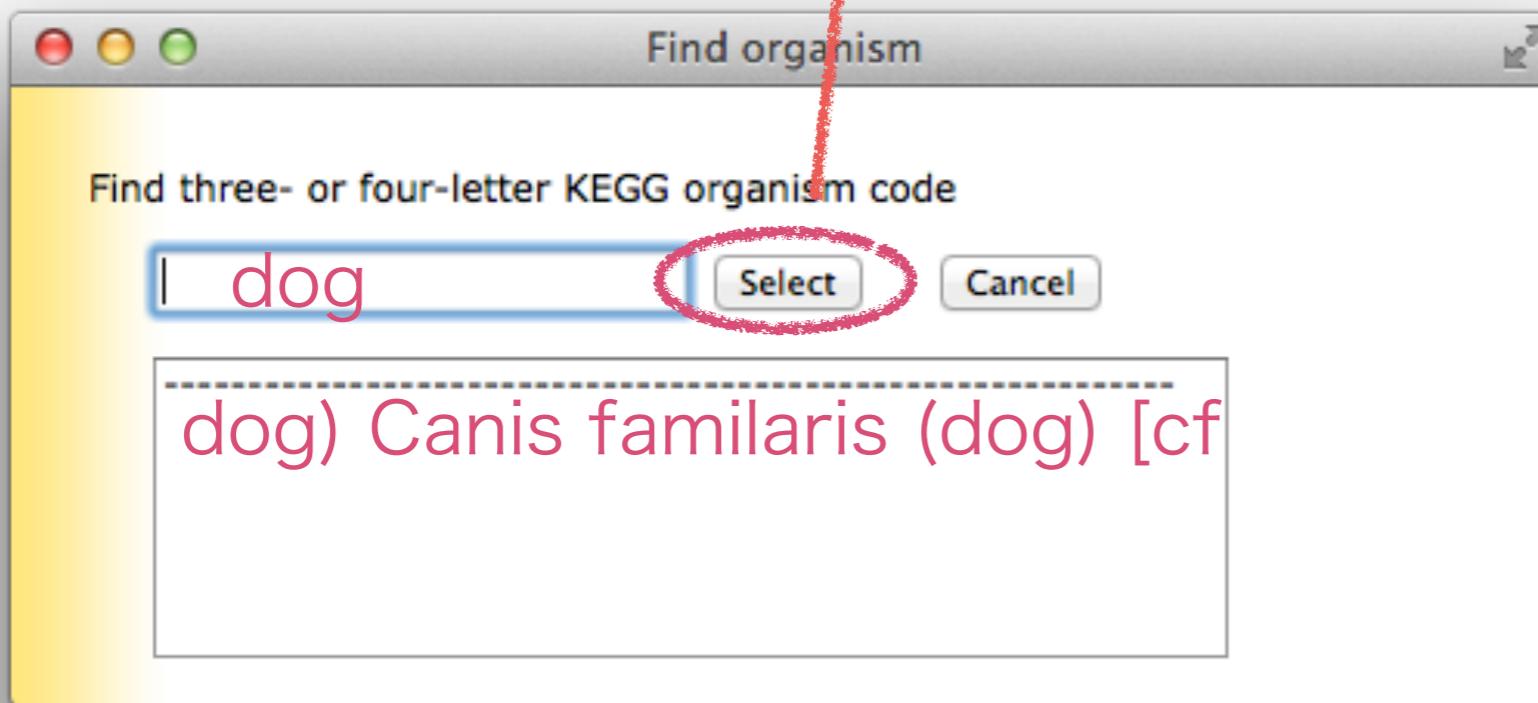
GENESエントリのキーワード検索

Search GENES for  Go Clear

bfind mode  bget mode

Search Organism [cfa] for RNA polymerase Go Clear

bfind mode  bget mode



# KEGG GENES

- GENESエントリ
- 配列の他、モチーフ、機能アノテーションや他のデータベースへのリンクが記載されている

Definition :

オリジナルサイトでの記述

Orthology :

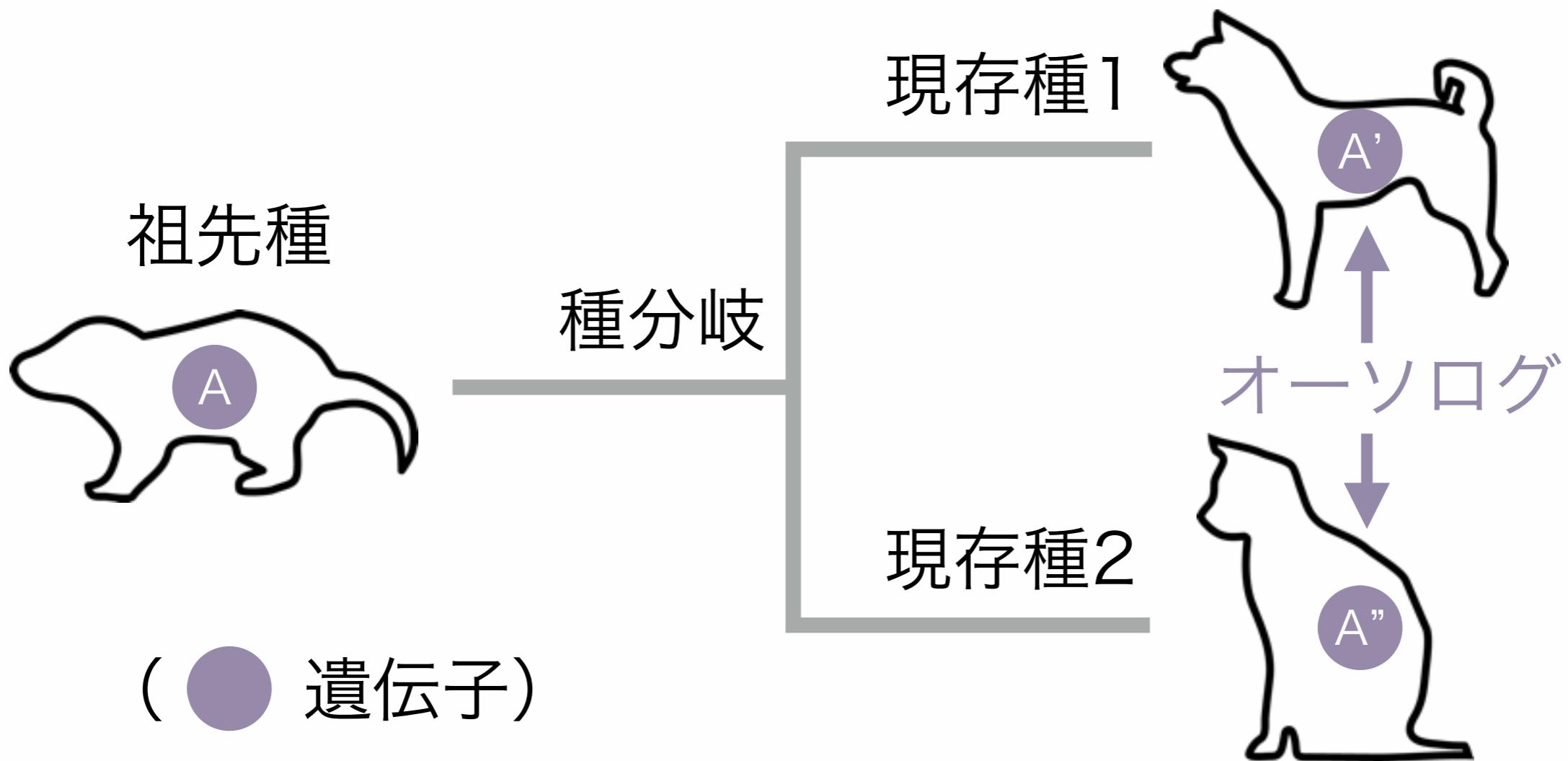
KEGGでつけられたアノテーション

KEGG T01007: 476158

**Kegg** Canis familiaris (dog): 476158 Help

Entry	476158	CDS	T01007
Gene name	CTDP1		
Definition	CTD (carboxy-terminal domain, RNA polymerase II, polypeptide A) phosphatase, subunit 1		
Orthology	K15732 RNA polymerase II subunit A C-terminal domain phosphatase [EC:3.1.3.16]		
Organism	cfa Canis familiaris (dog)		
Class	BRITE hierarchy		
SSDB	Ortholog Paralog GFIT		
Motif	Pfam: FCP1_C NIF PTCB-BRCT Biotin_lipoyl BRCT Biotin_lipoyl_2 Motif		
Other DBs	NCBI-GI: 73945347 NCBI-GeneID: 476158 Ensembl: ENSCAFG000000000010 UniProt: E2R1Y2		
Position	1		
AA seq	933 aa AA seq DB search	MEAPPAGRVPAEGAPPANVAVCPGPGLRLLEWRVAAGAAVRIGSVLAVCEAAAASAQP AGSAPARAGSGGCVRAERRLRSERAGVVRELCAQPGQVVVPGAVLVRLEGCSHPVVMKGL CAECGQDLTQLQSKNGQQVPLSTATVSMVHSVPelmanvssseqaeqlgredqqrlnhrnrkl VLMVDLDQTLIHTTEQHQCQMSNKGIFHFQLGRGEPMHLTRVRPHCREFLEKIARLYELH VFTFGSRLYAHTIAGFLPEKKLFSHRILSRDECIDPFSKTGNLRNLFP CGDSMVCIID REDVWKFAPNLITVKKYVYFQGIGDINAPSGSRESQARRKVNQSSRGADGPEQAPSIREI EEGRQVSGVEQSNGL GKPMRELNGGASPRGDWPLPGQEERGARPTTRGPLADKGPPAC AQHQHGRTLPEKRPQAQGTASGDLDFDLSSES DSAQSSDGESGEGKSLERPQGARDAGKAA QRGGPSGPGGERPTGVSPCAESAPDAQEEGERDGLCGLAGGSADRKEAETESQNSEQSGI TAGESLDQSVEEEEDEDGGDEDDHLVYLEEILARVHSDDYYAKYDRYLRGDSQEAPDIRK IVPELKSRVLADVAII FSGLHPTNFPIEKTRHYHATALGAKILTQLVLDPDNPDRATHL IAARAGTEKVRQAQECGQLHVVNPDWLSCLERWDRVEQLFPLRDDYGRAQREDGPAAF PDRQGALPTALFHPTPVHPRTQPGPEVRIYDANTGKLIRKGAVGPGPPGSLAVHTEHSSF RVVQPPRQMLAQLPDSRPGEQPGPSGRKRQPSMSETMPLYTLCKEDLESMDKEVDDILG EGSDDSDNEKRRPEEERKERPPPBPQATPEATPSSERTRAGSRGPRGHKRKLPEEDAGS ASSGESESGEDEEGSSSEADEMAAALAEALNDLM	
NT seq	2802 nt NT seq atggaggcgccgccccgcggggccgcgttcccggcggggcgccccggccggccgtggcc gaggtgcgtgcggccggccggccgtgcgcctgcgcgactggagggttgcggccggcc gcggccgtgcgcgtgcgtgtggcggtgtgtggccggccgtgcgtgcgcgcggcc gcgggggtcccccctgcggccggccgtccggggctgcgtgcgcgcggcc aggtcggagcgtgcgggtgtgtgcggggagctgtgcgcgcagccggcc cccggggcggttctggtacgggtggaaaggatgtagccaccgggttgtcat tgtgtgtactggggccaggacctaaccggcttcaggatgtaaaaggcc tgtgtgtactggggccaggacctaaccggcttcaggatgtaaaaggcc		

# オーソログ遺伝子



種分岐によって生じた生物間で対応する遺伝子で、配列相同性を持ち、同一の生物学的機能を持っていると考えられる遺伝子で、オーソログ遺伝子を見つけることが、機能アノテーションを行う上で重要



# KEGG ORTHOLOGY (KO)

- KOエントリ
- K番号
- オーソロググループの名前、機能、KEGG PATHWAY/BRITEへのリンク、グループに分類されている遺伝子、グループ作成の基となった文献情報などが記載
- KOエントリのDefinitionが、GENESエントリのOrthologyに対応

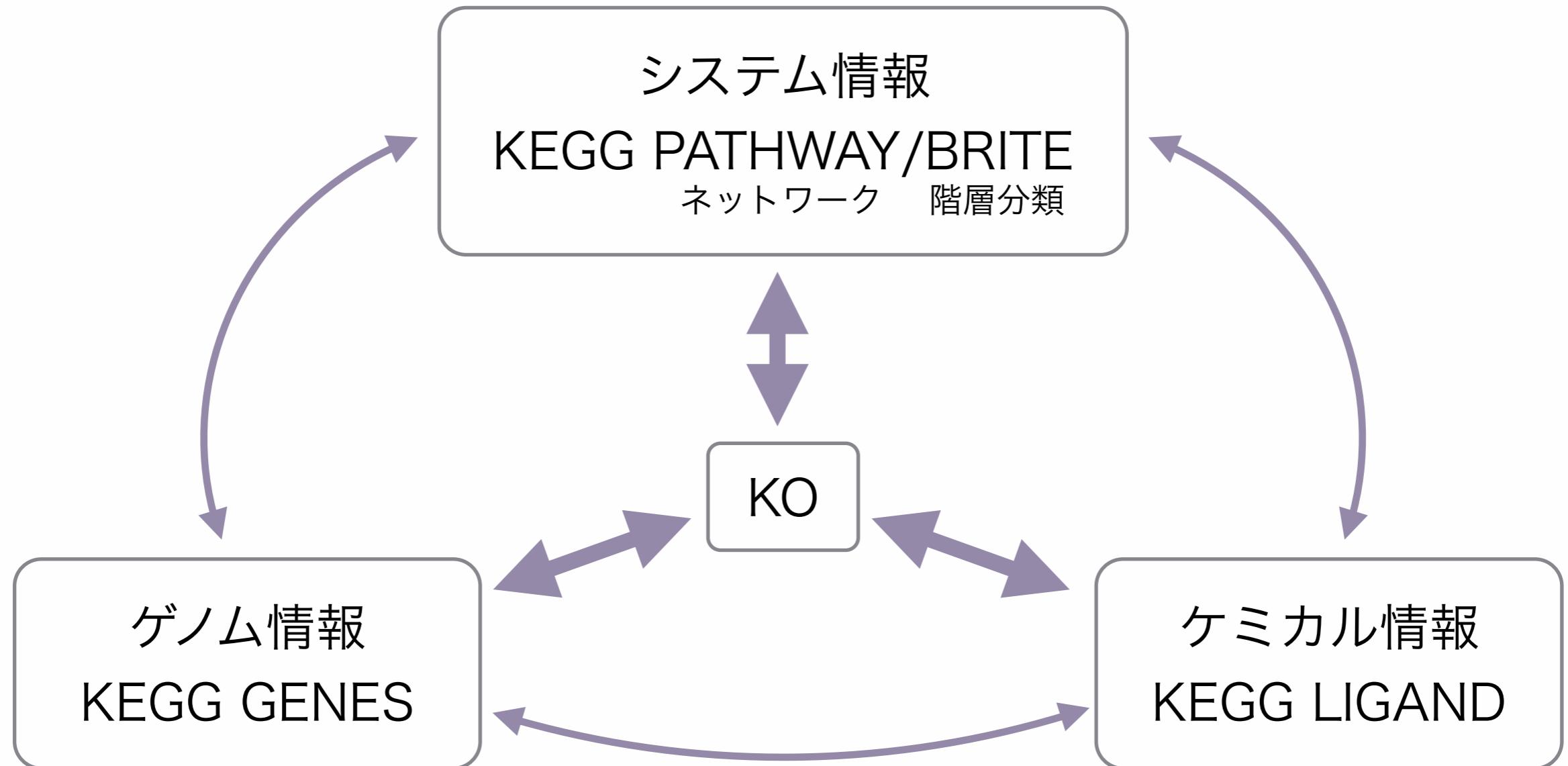
KEGG ORTHOLOGY: K15732

ORTHOLOGY: K15732

Help

Entry	K15732	KO
Name	CTDP1, FCP1	
Definition	RNA polymerase II subunit A C-terminal domain phosphatase [EC:3.1.3.16]	
Disease	H01220 Congenital cataracts, facial dysmorphism, and neuropathy (CCFDN)	
Brite	Enzymes [BR:ko01000] 3. Hydrolases 3.1 Acting on ester bonds 3.1.3 Phosphoric-monoester hydrolases 3.1.3.16 phosphoprotein phosphatase K15732 CTDP1, FCP1; RNA polymerase II subunit A C-terminal d Transcription machinery [BR:ko03021] Eukaryotic type RNA polymerase II system Other transcription-related factors Others K15732 CTDP1, FCP1; RNA polymerase II subunit A C-terminal d <a href="#">BRITE hierarchy</a>	
Other DBs	COG: COG5190 GO: 0008420	
Genes	HSA: 9150(CTDP1) PTR: 468592(CTDP1) PPS: 100968379(CTDP1) GGO: 101143233(CTDP1) PON: 100436593(CTDP1) MCC: 698467(CTDP1) MMU: 67655(Ctdp1) RNO: 291414(Ctdp1) CGE: 100764255(Ctdp1) HGL: 101696942(Ctdp1) » show all <a href="#">Taxonomy</a> <a href="#">KOALA</a> <a href="#">UniProt</a>	
Reference	PMID:15304220	
Authors	Kamenski T, Heilmeier S, Meinhart A, Cramer P	
Title	Structure and mechanism of RNA polymerase II CTD phosphatases.	
Journal	Mol Cell 15:399-407 (2004)	

KOグループに割り当てられていない、KEGG外部の配列データ、ユーザがシーケンスした配列データからはKEGGのシステムが利用できない？



3つのタイプのデータベースの多くは、KOを介してリンクされているため、KEGGを利用する上で非常に重要

# KAAS

- ・ 入力
  - ・ 大規模シークエンスによって得られた生物種のアミノ酸や塩基配列
- ・ 出力
- ・ 配列名とKOの対応表
- ・ PATHWAYマップ
- ・ BRITE階層分類

KAAS – KEGG Automatic Annotation Server



**KAAS - KEGG Automatic Annotation Server**  
for ortholog assignment and pathway mapping

**Request** **Help**

**About KAAS**

KAAS (KEGG Automatic Annotation Server) provides functional annotation of genes by BLAST comparisons against the manually curated KEGG GENES database. The result contains KO (KEGG Orthology) assignments and automatically generated KEGG pathways.

- [KAAS Help](#)

**Complete or Draft Genome**

KAAS works best when a complete set of genes in a genome is known. Prepare query amino acid sequences and use the BBH (bi-directional best hit) method to assign orthologs.

- [KAAS job request \(BBH method\)](#)

**Partial Genome**

KAAS can also be used for a limited number of genes. Prepare query amino acid sequences and use the SBH (single-directional best hit) method to assign orthologs.

- [KAAS job request \(SBH method\)](#)  
- [KAAS interactive](#)

**ESTs**

When ESTs are comprehensive enough, a set of consensus contigs can be generated by the EGassembler server and used as a gene set for KAAS with the BBH method. Otherwise, use ESTs as they

**Example of Results**

**KO assignment**

**KO Assignment Results**

Home [KO list] [BRITE hierarchies] [Pathway map]

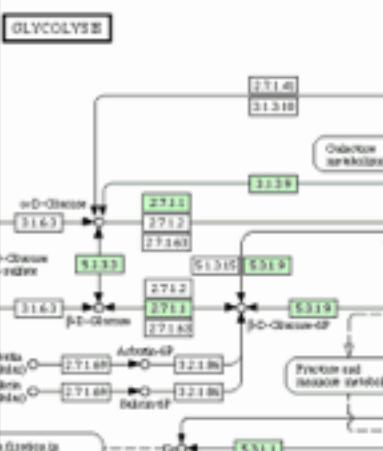
Query gene : KO assignment

testS70411

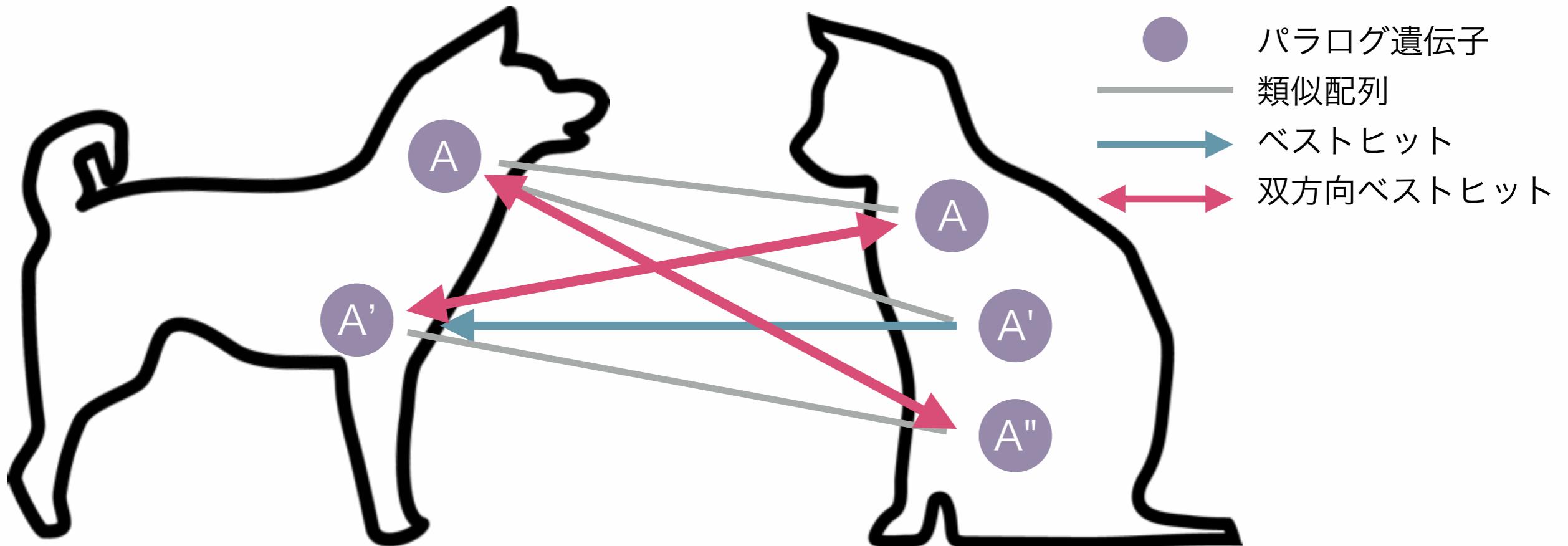
```
query_0001
query_0002 K0003
query_0003 K00872
query_0004 K01733
query_0005
query_0006
query_0007 K03310
query_0008 K0016
query_0009 K03031
query_0010 K07034
query_0011
query_0012
query_0013
query_0014 K04043
query_0015 K03000
query_0016
```

**KEGG pathway mapping**

GLYCOLYSIS



# KAAS



ただ似ているより、ベストヒットである遺伝子同士が、よりオーソログの関係にある可能性が高く、双向方向ベストヒットである遺伝子がさらにオーソログの関係にある可能性が高い

# KAAS

- ・入力データがコンプリートゲノムの遺伝子であるなど、ある程度の網羅性がある場合双方向ベストヒットを用いたモード
- ・部分的な配列であったり、メタゲノムなど複数の生物の配列が混ざっている場合にはベストヒットを用いたモード

KAAS – KEGG Automatic Annotation Server

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**Example of Results**

**KO assignment**

**KO Assignment Results**

Home [KO list] [BRUTE hierarchies] [Pathway map]

Query gene : KO assignment

testS70411

- query\_0001
- query\_0002 KO0072
- query\_0003 KO1733
- query\_0004 KO0310
- query\_0005 KO0116
- query\_0006 KO0093
- query\_0007 KO07034
- query\_0008 KO0111
- query\_0009 KO0112
- query\_0010 KO0113
- query\_0011 KO0114
- query\_0012 KO0115
- query\_0013 KO0116
- query\_0014 KO0117
- query\_0015 KO0118

**KEGG pathway mapping**

GLYCOLYSIS

<img alt="Diagram of the Glycolysis pathway showing various enzymes and metabolites. Nodes are labeled with KEGG IDs such as 31318, 27140, 27111, 27112, 27113, 27114, 27115, 27116, 27117, 27118, 27119, 27120, 27121, 27122, 27123, 27124, 27125, 27126, 27127, 27128, 27129, 27130, 27131, 27132, 27133, 27134, 27135, 27136, 27137, 27138, 27139, 27140, 27141, 27142, 27143, 27144, 27145, 27146, 27147, 27148, 27149, 27150, 27151, 27152, 27153, 27154, 27155, 27156, 27157, 27158, 27159, 27160, 27161, 27162, 27163, 27164, 27165, 27166, 27167, 27168, 27169, 27170, 27171, 27172, 27173, 27174, 27175, 27176, 27177, 27178, 27179, 27180, 27181, 27182, 27183, 27184, 27185, 27186, 27187, 27188, 27189, 27190, 27191, 27192, 27193, 27194, 27195, 27196, 27197, 27198, 27199, 27110, 27111, 27112, 27113, 27114, 27115, 27116, 27117, 27118, 27119, 27120, 27121, 27122, 27123, 27124, 27125, 27126, 27127, 27128, 27129, 27130, 27131, 27132, 27133, 27134, 27135, 27136, 27137, 27138, 27139, 27140, 27141, 27142, 27143, 27144, 27145, 27146, 27147, 27148, 27149, 27150, 27151, 27152, 27153, 27154, 27155, 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## ・ 入力データがコンプリート

KAAS – KEGG Automatic Annotation Server

manually annotated organisms

color : selected / not selected

Eukaryotes

Animals

Vertebrates

Mammals

hsa	Homo sapiens (human)
ptr	Pan troglodytes (chimpanzee)
pon	Pongo abelii (Sumatran orangutan)
mcc	Macaca mulatta (rhesus monkey)
mmu	Mus musculus (mouse)
rno	Rattus norvegicus (rat)
cfa	Canis familiaris (dog)
aml	Ailuropoda melanoleuca (giant panda)
bta	Bos taurus (cow)
ssc	Sus scrofa (pig)
ecb	Equus caballus (horse)
mdo	Monodelphis domestica (opossum)
oaa	Ornithorhynchus anatinus (platypus)

KEGG Automatic Annotation Server  
www.genome.jp/kaas-bin/kaas\_main

Compute Clear

Query sequences (in multi-FASTA)

Text data ( Nucleotide) 遺伝子領域の配列

```
>Query01  
MAALTRDPQFQKLQQWYREHRSELNLRR  
LFDANKDRFNHFSLTLNNTNHGHILVDYSKN  
>Query02
```

File upload ( Nucleotide)  
ファイルを選択 ファイル未選択

Query name  
query 自由に名前を入力

E-mail address  
メールを入力

GENES data set (javascript button or text box)  
Representative set  
   データベース側の生物種の選択

Manual selection  
 (popup window)

Selected organisms (up to 40 organisms)  
hsa, dme, cel, ath, sce, cho, eco, nme, hpy, rpr, bsu, lla, cac, mge, mtu, ctr, bbu, syn, bth, dra, aae, mja, ape

(Example) eco, bsu, syn

Assignment method  
 BBH (bi-directional best hit)

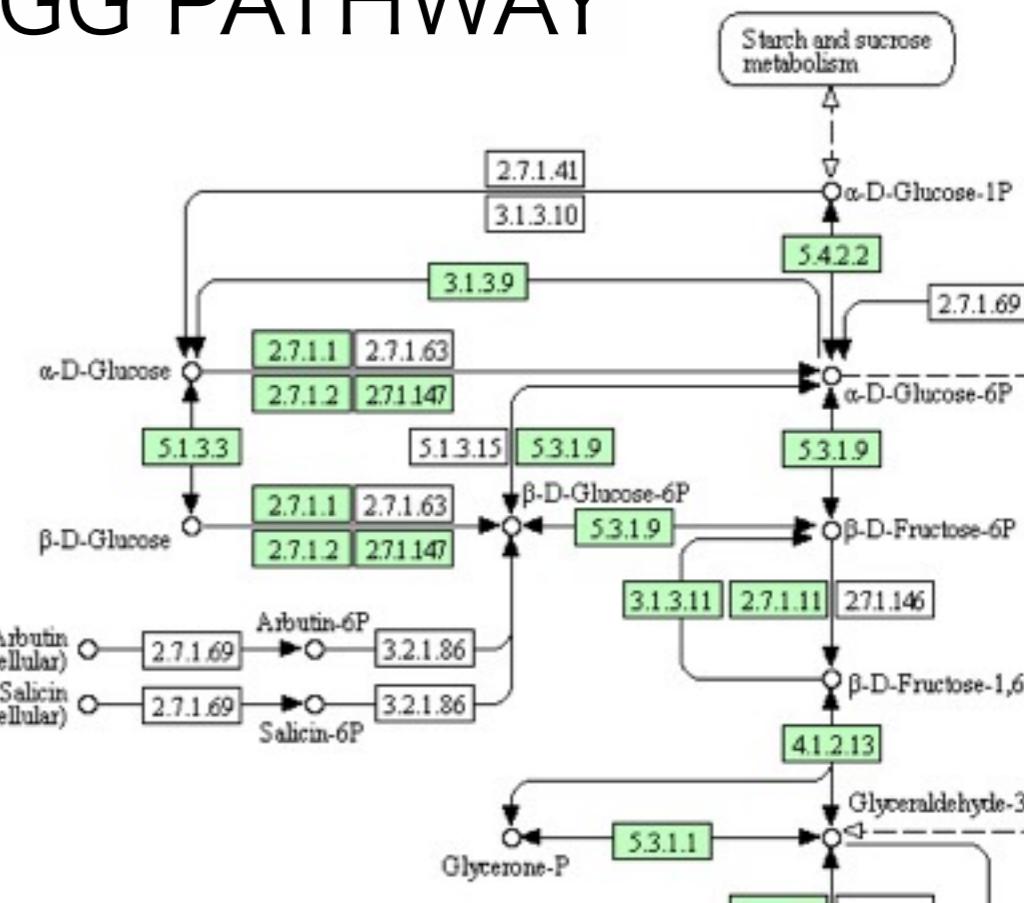
# KAAS

KAASによる  
アノテーション

配列名	KO
Query01	K00234
Query02	K01423
Query03	K15231
Query04	K04352
Query05	K06331
Query06	K00075
Query07	K03561
Query08	K00780
Query09	K03060
Query10	K11988

KOを介して  
システム情報へ  
→

## KEGG PATHWAY



## KEGG BRITE

▼ ▼ ▼  One-click mode

### ▼ Aspartic Peptidases

#### ▼ Family A1: pepsin family

- K06002 PGA; pepsin A [EC:3.4.23.1]
- K01377 PGC; gastricsin [EC:3.4.23.3]
- K04521 BACE1; beta-site APP-cleaving enzyme 1 (memapsin 2) [EC:3.4.23.4]
- K07747 BACE2; beta-site APP-cleaving enzyme 2 (memapsin 1) [EC:3.4.23.5]
- K01378 CYM; chymosin [EC:3.4.23.4]
- K01380 REN; renin [EC:3.4.23.15]
- K01379 CTSD; cathepsin D [EC:3.4.23.5]
- K01382 CTSE; cathepsin E [EC:3.4.23.34]
- K01383 E3.4.23.35; barrierpepsin [EC:3.4.23.35]
- K06004 E3.4.23.18; aspergillopepsin I [EC:3.4.23.18]
- K01381 E3.4.23.25; saccharopepsin [EC:3.4.23.25]
- K08245 E3.4.23.40; phytpepsin [EC:3.4.23.40]
- K06007 E3.4.23.38; plasmepsin I [EC:3.4.23.38]
- K06008 E3.4.23.39; plasmepsin II [EC:3.4.23.39]
- K06009 E3.4.23.41; yapsin 1 [EC:3.4.23.41]
- K06005 S1P; serine/arginine-rich endonuclease [EC:3.4.23.24]

# システム情報

分子の相互作用ネットワーク

# KEGG PATHWAY

- ・代謝系（1）
  - ・12カテゴリ
  - ・中間代謝、二次代謝、薬の代謝、全体像
- ・制御系（2－5）
  - ・20カテゴリ
  - ・遺伝子制御、環境シグナル、細胞プロセス、生態システム他
- ・疾患（6）
  - ・がん、免疫、神経編成、循環器・代謝疾患、感染症
- ・薬の開発（7）
  - ・開発の歴史、標的ベース、構造ベース

KEGG PATHWAY Database

KEGG PATHWAY Database

Wiring diagrams of molecular interactions, reactions, and relations

KEGG2 PATHWAY BRITE MODULE DISEASE DRUG KO GENOME GENES LIGAND DBG

Select prefix  Enter keywords   Help

**Pathway Maps**

KEGG PATHWAY is a collection of manually drawn pathway maps (see [new maps](#) and [update history](#)) representing our knowledge on the molecular interaction and reaction networks for:

1. Metabolism
2. Genetic Information Processing
3. Environmental Information Processing
4. Cellular Processes
5. Organismal Systems
6. Human Diseases

and also on the structure relationships (KEGG drug structure maps) in:

1. Metabolism
2. Genetic Information Processing
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5. Organismal Systems
6. Human Diseases
7. Drug Development

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KEGG PATHWAY mapping is the process to map molecular datasets, especially large-scale datasets in genomics, transcriptomics, proteomics, and metabolomics, to the KEGG pathway maps for biological interpretation of higher-level systemic functions.

- Search Pathway - basic pathway mapping tool
- Search&Color Pathway - advanced pathway mapping tool
- Color Pathway - selected pathway map coloring tool

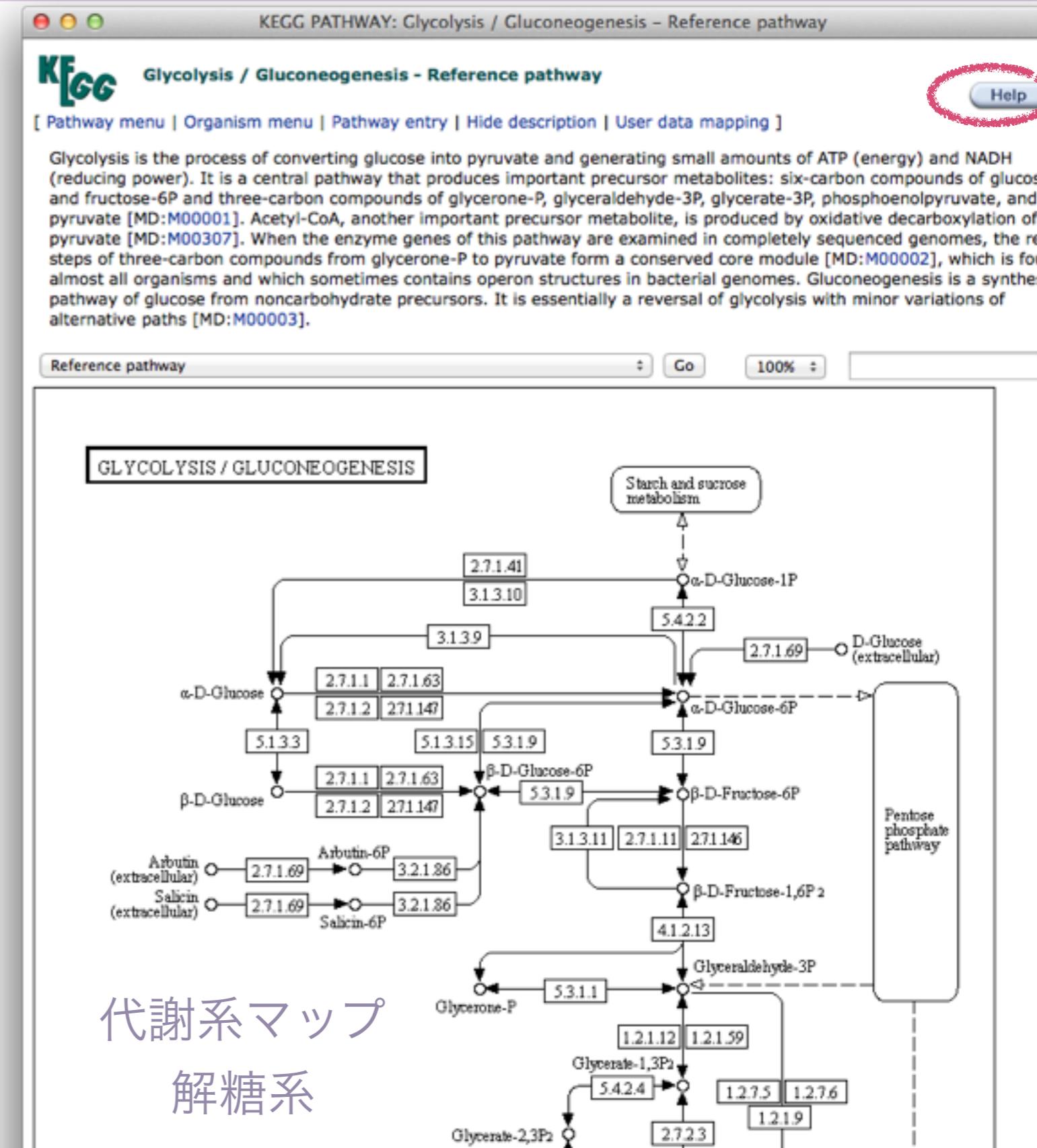
**1. Metabolism**

**1.0 Global and overview maps**

Metabolic pathways	[KEGG Atlas]	KEGG modules
Biosynthesis of secondary metabolites	[KEGG Atlas]	KEGG reaction modules
Microbial metabolism in diverse environments	[KEGG Atlas]	
Carbon metabolism	[KEGG Atlas]	
2-Oxocarboxylic acid metabolism	[KEGG Atlas]	
Fatty acid metabolism	[KEGG Atlas]	

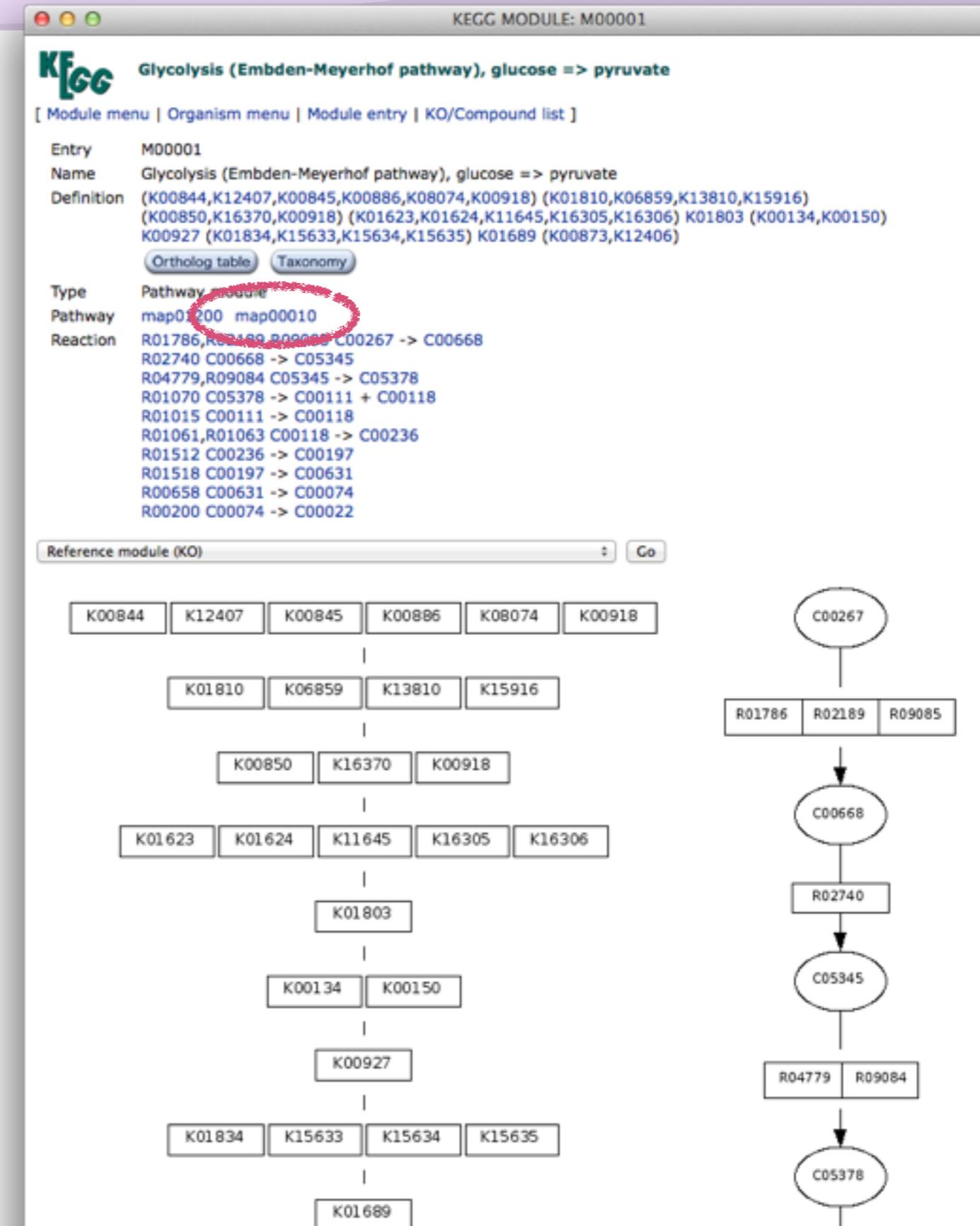
# KEGG PATHWAY

- 酵素・遺伝子と化合物のネットワーク
- Pathway menu
  - BRITE形式の階層分類
- Organism menu
  - 生物種リスト
- Pathway entry
  - PATHWAYデータベースのエントリ形式
- Show (Hide) description
  - マップの説明
- User data mapping
  - マップの中のオブジェクトへの色づけ



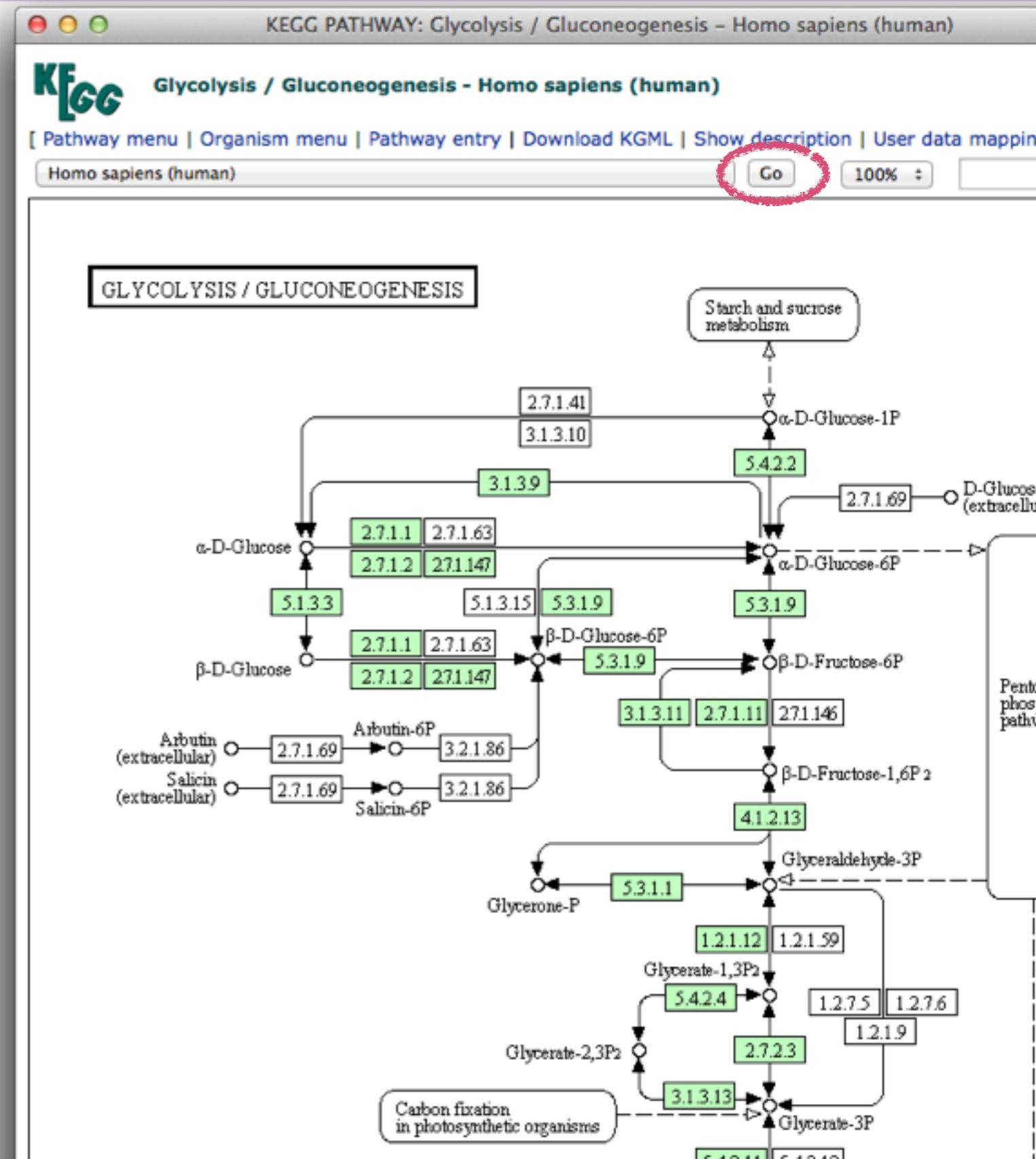
# KEGG MODULE

- ・ パスウェイモジュール
- ・ M番号
- ・ PATHWAYマップより小さい単位
- ・ 生物種間での保存度合い、複合体の形成、オペロンなどを考慮した機能単位
- ・ オーソロググループ (KO) の組み合わせで表現

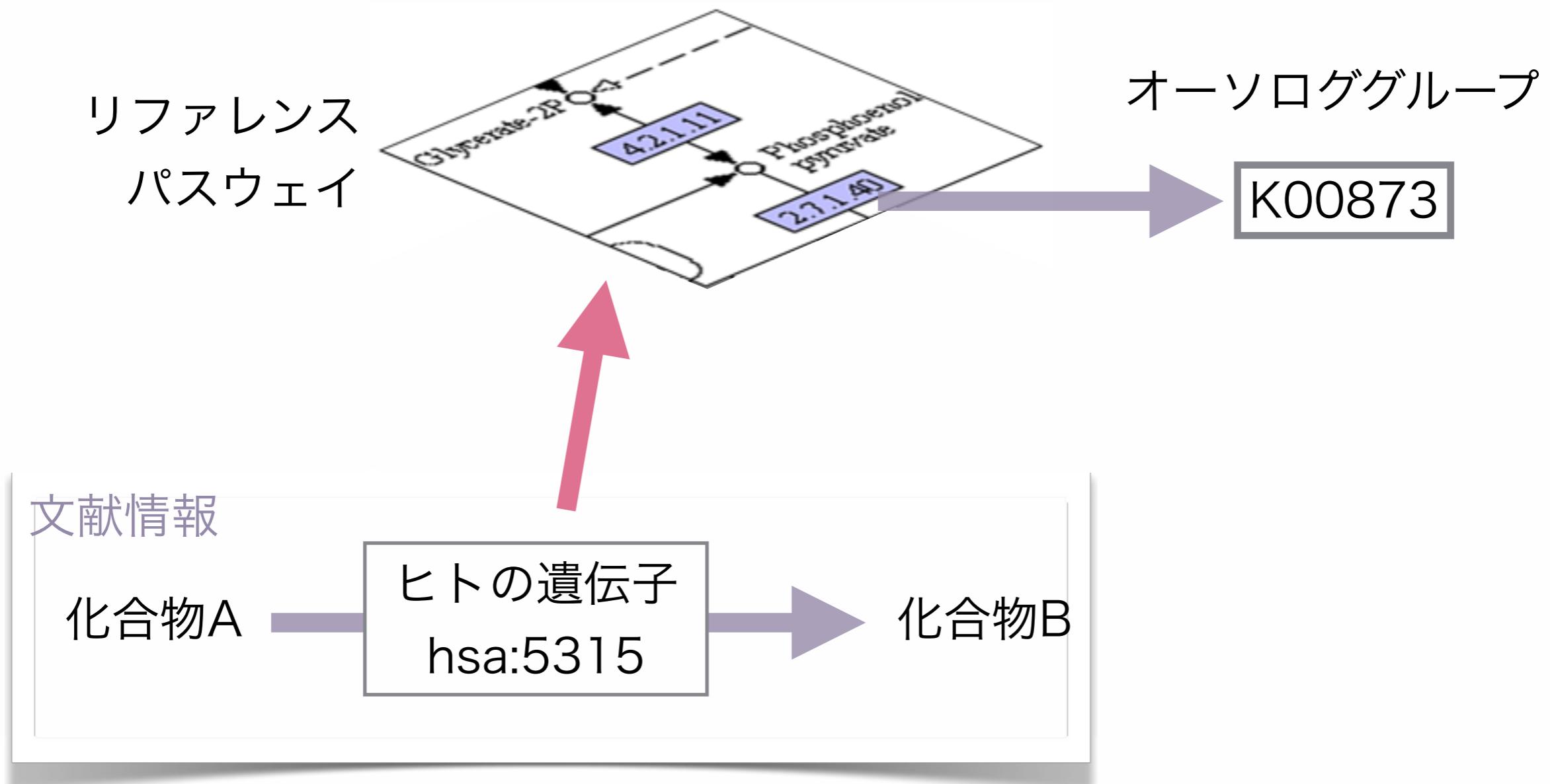


# KEGG PATHWAY

- Reference Pathway (KO)
  - KOだけにリンクしているマップ
- Reference Pathway (EC)
  - ECだけにリンクしているマップ
- Reference Pathway (Reaction)
  - 反応だけにリンクしているマップ
- 生物種名
  - 生物種の遺伝子にリンクしているマップ

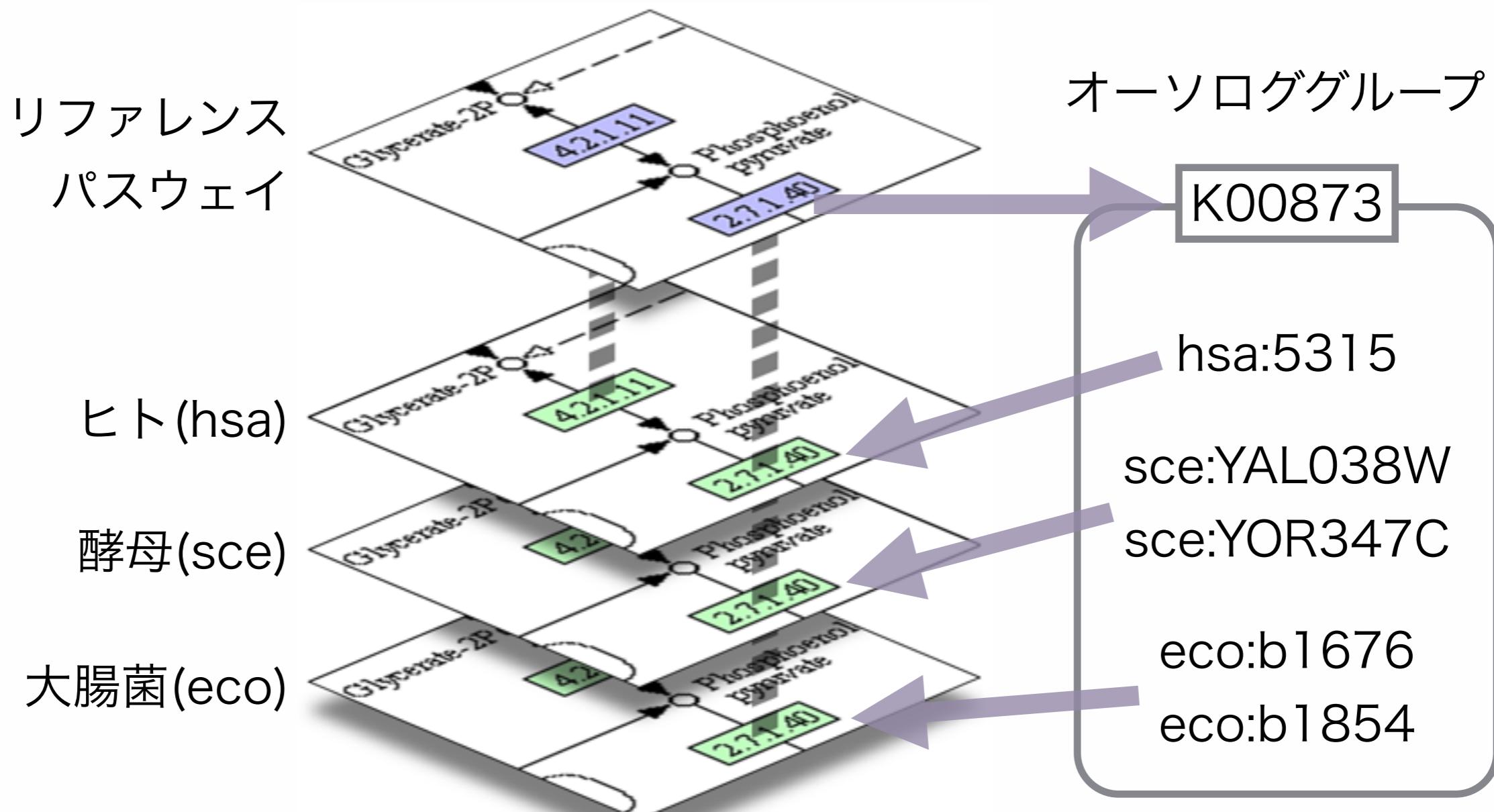


# KEGG PATHWAY



文献情報からリファレンスパスウェイが作成される

# KEGG PATHWAY



KOと化合物のネットワークであるリファレンスパスウェイを基に、生物種毎のパスウェイが作られる

# KEGG PATHWAY

- ・代謝系（1）
  - ・12カテゴリ
  - ・中間代謝、二次代謝、薬の代謝、全体像
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KEGG PATHWAY Database

KEGG PATHWAY Database

Wiring diagrams of molecular interactions, reactions, and relations

KEGG2 PATHWAY BRITE MODULE DISEASE DRUG KO GENOME GENES LIGAND DBG

Select prefix Enter keywords

map Organism Go Help

**Pathway Maps**

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1. **Metabolism** (Global/overview, Carbohydrate, Energy, Lipid, Nucleotide, Amino acid, Other amino, Glycan, Cofactor/vitamin, Terpenoid/PK, Other secondary metabolite, Xenobiotics, Chemical structure)
2. **Genetic Information Processing**
3. **Environmental Information Processing**
4. **Cellular Processes**
5. **Organismal Systems**
6. **Human Diseases**

and also on the structure relationships (KEGG drug structure maps) in:

7. **Drug Development**

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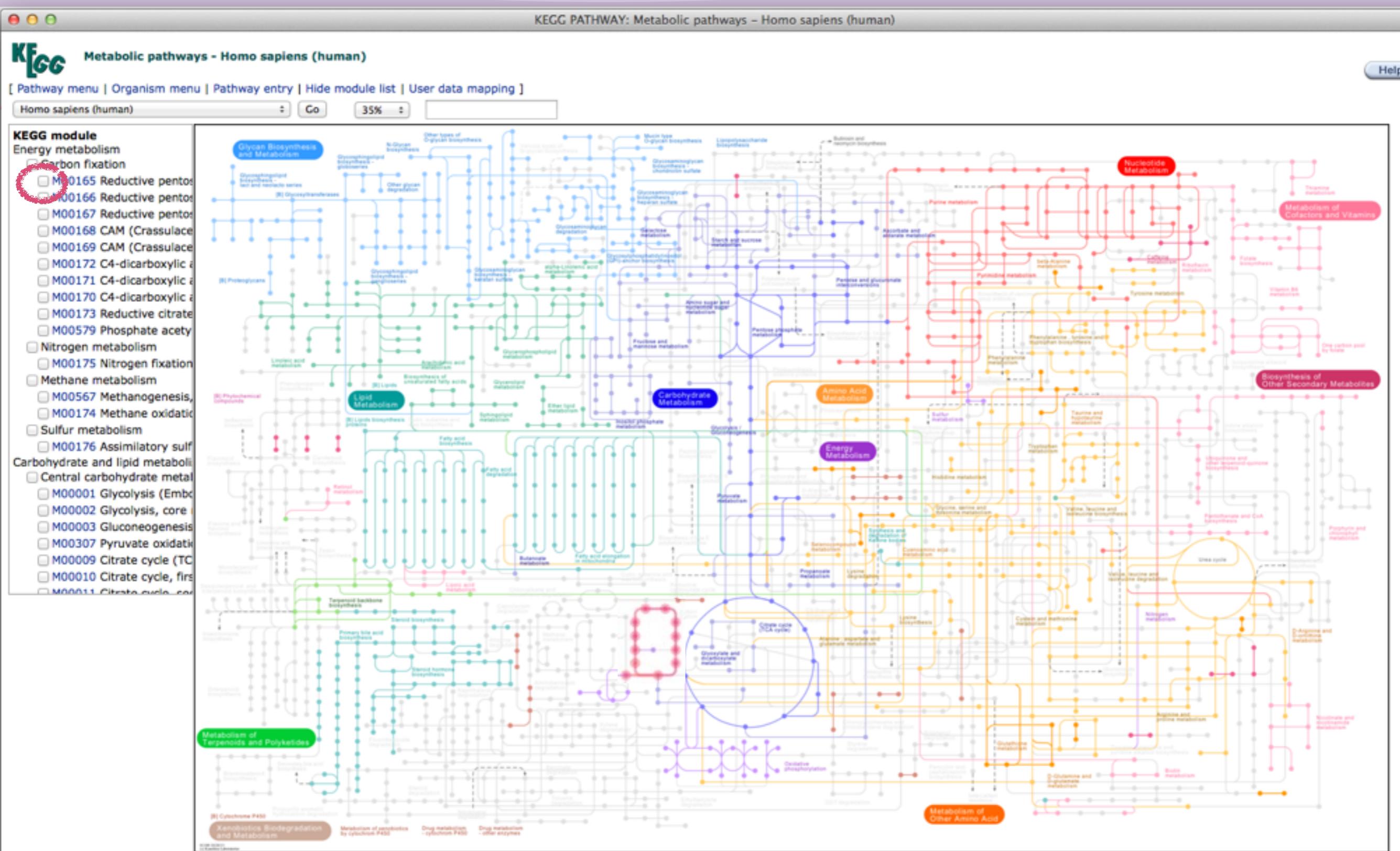
- [Search Pathway](#) - basic pathway mapping tool
- [Search&Color Pathway](#) - advanced pathway mapping tool
- [Color Pathway](#) - selected pathway map coloring tool

**1. Metabolism**

**1.0 Global and overview maps**

Metabolic pathways	[KEGG Atlas]	KEGG modules
Biosynthesis of secondary metabolites	[KEGG Atlas]	KEGG reaction modules
Microbial metabolism in diverse environments	[KEGG Atlas]	
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2-Oxocarboxylic acid metabolism	[KEGG Atlas]	
Fatty acid metabolism	[KEGG Atlas]	

# KEGG PATHWAY



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KEGG PATHWAY Database

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Wiring diagrams of molecular interactions, reactions, and relations

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6. Human Diseases

and also on the structure relationships (KEGG drug structure maps) in:

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**Pathway Mapping**

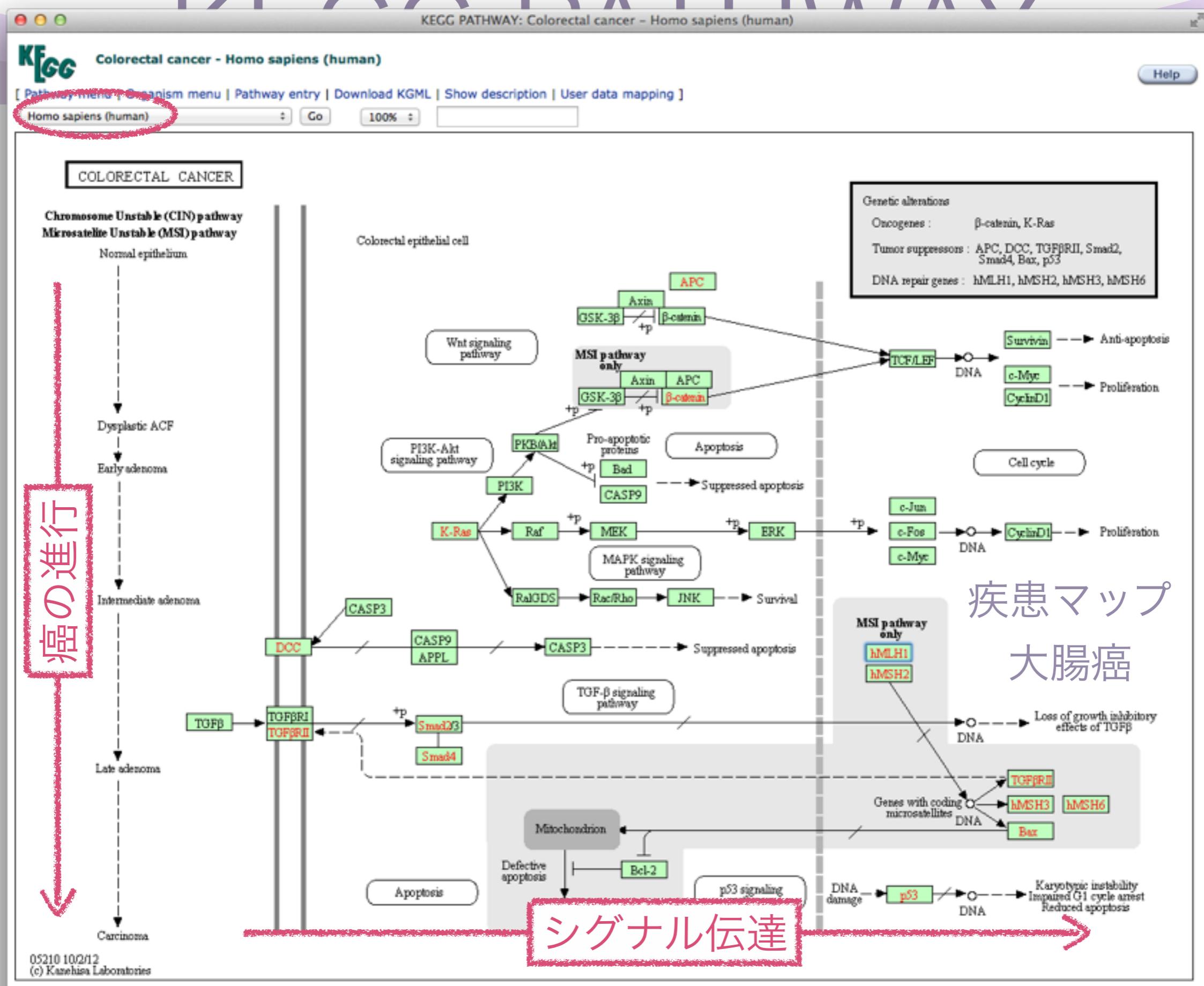
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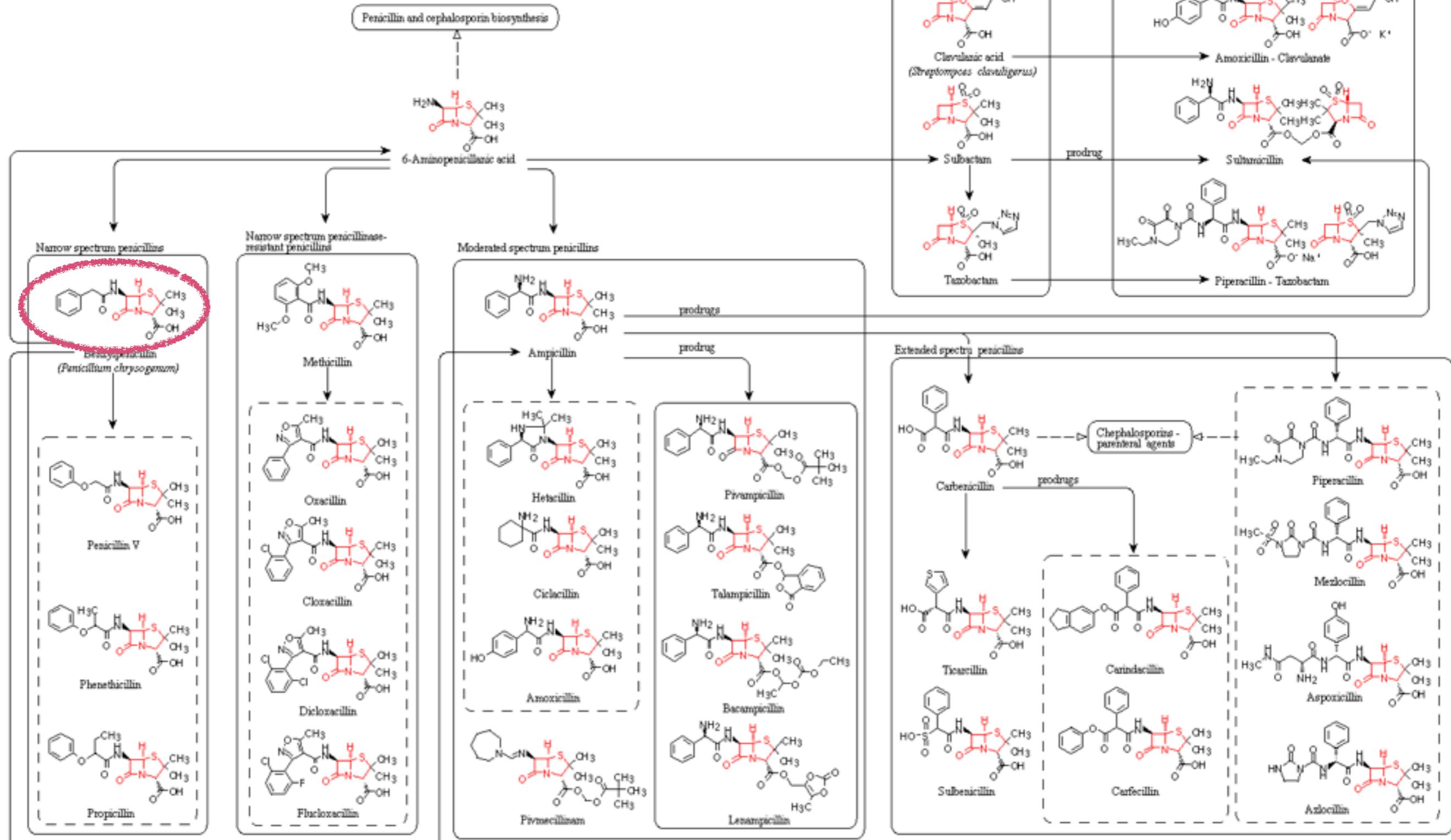


# KEGG PATHWAY

KEGG PATHWAY Database

PENICILLINS

## ペニシリン系抗生物質



# KEGG Mapper

## Pathway Mapping

- マップの中の丸や四角のオブジェクトを指定してパスウェイにマッピングできる
- 複数のオブジェクトにそれぞれ自由な色を塗ることが可能

KEGG PATHWAY Database

KEGG PATHWAY Database

Wiring diagrams of molecular interactions, reactions, and relations

KEGG2 PATHWAY BRITE MODULE DISEASE DRUG KO GENOME GENES LIGAND DBG

Select prefix: map Enter keywords Go Help

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- [Search Pathway](#) - basic pathway mapping tool
- [Search&Color Pathway](#) - Advanced pathway mapping tool
- [Color Pathway](#) - selected pathway map coloring tool

### 1. Metabolism

#### 1.0 Global and overview maps

Metabolic pathways	[KEGG Atlas]	KEGG modules
Biosynthesis of secondary metabolites	[KEGG Atlas]	KEGG reaction modules
Microbial metabolism in diverse environments	[KEGG Atlas]	
Carbon metabolism	[KEGG Atlas]	
2-Oxocarboxylic acid metabolism	[KEGG Atlas]	
Fatty acid metabolism	[KEGG Atlas]	

# KEGG Mapper

- Pathway Mapping
  - マップの中の丸や四角のオブジェクトを指定してパスウェイにマッピングできる
  - 複数のオブジェクトにそれぞれ自由な色を塗ることが可能

KEGG Mapper – Search&Color Pathway

**KEGG Mapper – Search&Color Pathway**

KEGG Mapper    Search Pathway    Search&Color Pathway    Color Pathway    Reconstruct  
KEGG Atlas    Search Brite    Search&Color Brite    Color Pathway 3D    Reconstruct  
KEGG            Search Module    Search&Color Module    Join Brite    Reconstruct

Search against: ko    Enter: map, ko, ec, rn, hsadd, or org

Primary ID: KEGG identifiers (NCBI and UniProt IDs may be used for organism-specific pathways)

Enter objects one per line followed by bgcolor, fgcolor:

K01803 red,blue  
C00118 pink

Examples:  
(Reference pathway (KO))  
K01803 red,blue  
C00118 pink

←

(Homo sapiens pathway)  
7167 red,blue  
C00118 pink

Alternatively, enter the file name containing the data:  
ファイルを選択 ファイル未選択

If necessary, change default bgcolor: pink

Include aliases  
 Use uncolored diagrams  
 Display objects not found in the search  
 Search pathways containing all the objects (AND search)

Exec    Clear

# KEGG Mapper

- ・入力形式は“ID 背景色,文字色”
- ・色はWebカラーが使用可能
- ・IDはNCBI-GenelD、NCBI-gi、UniProtも使用可能

KEGG Mapper – Search&Color Pathway

KEGG Mapper – Search&Color Pathway

KEGG Mapper KEGG Atlas KEGG Search Pathway Search Brite Search Module Search&Color Pathway Search&Color Brite Search&Color Module Color Pathway Color Pathway 3D Join Brite Reconstruct Reconstruct Reconstruct

Search against:  Enter: map, ko, ec, rn, hsadd, or

Primary ID:  KEGG identifiers NCBI-GenelD NCBI-gi UniProt

Enter object ID by bgcolor, fgcolor:

474487 #f0e68c,red

Examples:  
(Reference pathway (KO))  
K01803 red,blue  
C00118 pink  
(Homo sapiens pathway)  
7167 red,blue  
C00118 pink

Alternatively, enter the file name containing the data:

If necessary, change default bgcolor:

Include aliases  
 Use uncolored diagrams  
 Display objects not found in the search  
 Search pathways containing all the objects (AND search)

KEGG GENOME Database  
[www.genome.jp/kegg/genome.html](http://www.genome.jp/kegg/genome.html)

Draft genomes	GENOMES	T1 numbers	DGENES	KAAS
EST datasets	EGENOME	T2 numbers	EGENES	KAAS
Metagenomes	MGENOME	T3 numbers	MGENES	KAAS
Pangenomes		Generic species names	GENES	KOALA
Viruses	VGENOME	RefSeq identifiers	VGENES	None

**Search** **GENOME** for  **Go** **Clear**

bfind mode  bget mode

### KEGG Mapping for Genome Comparison and Combination

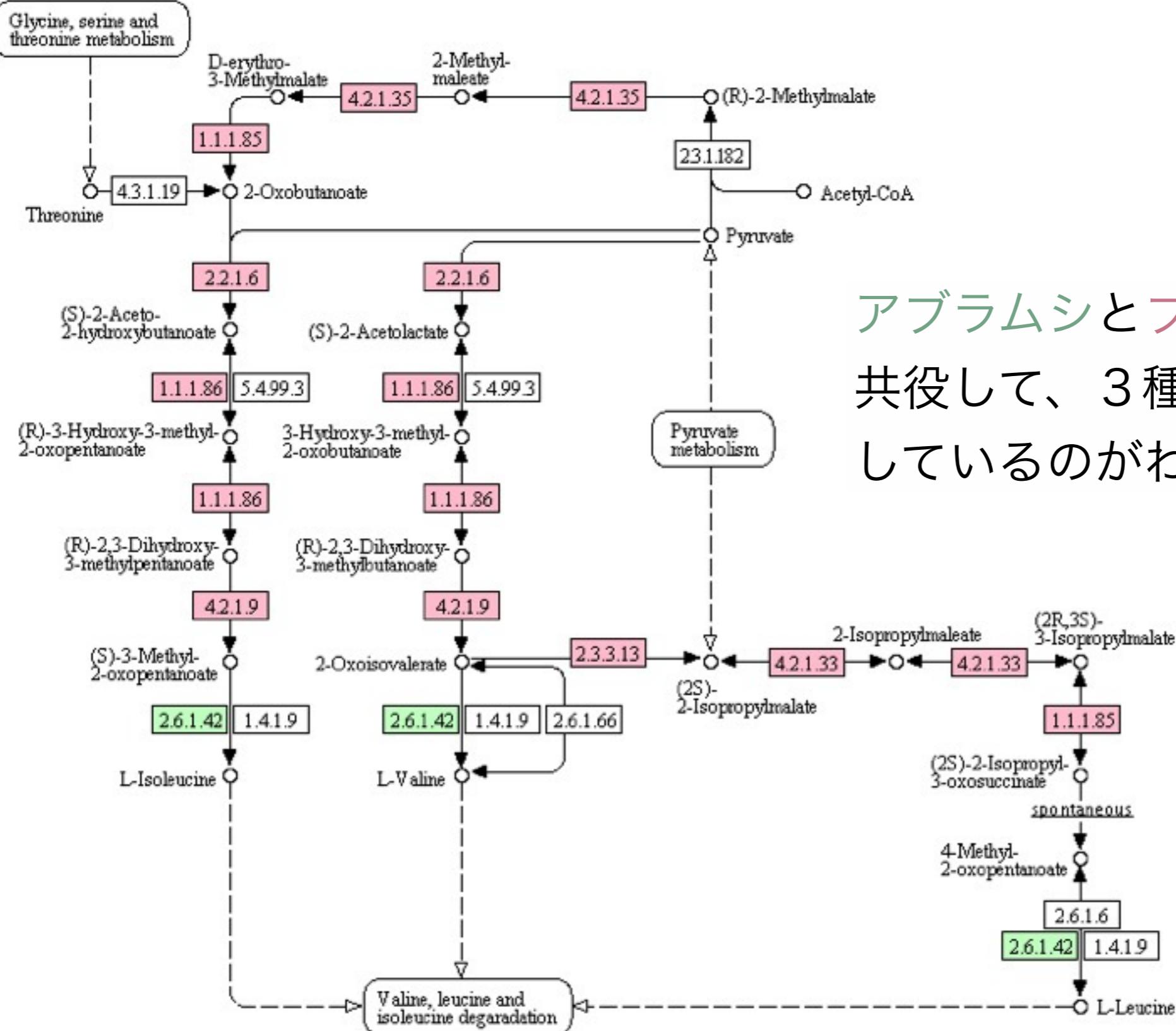
An organism group may be defined to compare or combine KEGG organisms, enabling the analysis of combined pathway maps for the group.

Define organism group (enter organism codes or T numbers):  **Go**

(Genome comparison)

- hsa eco Homo sapiens (human) vs. Escherichia coli K-12 strain such as Terpenoid backbone biosynthesis where green for human, red for E.coli, and split for both
- (Host-microbiome relationship)
- hsa+T30003 Homo sapiens (human) + gut microbiome such as Global metabolism map where green for human, red for gut microbiome, and blue for both
- (Host-symbiont relationship)
- dlia+mlo *Lactuca sativa* (lettuce) + *Morcharizobium loti* *Agrobacterium tumefaciens* + *Agrobacterium rhizogenes* + *Rhizobium leguminosarum* + *Rhizobium etli* + *Rhizobium fredii* + *Rhizobium meliloti* + *Rhizobium phaseoli* + *Rhizobium phaseoli* + *Rhizobium sp. 1* + *Rhizobium sp. 2* + *Rhizobium sp. 3* + *Rhizobium sp. 4* + *Rhizobium sp. 5* + *Rhizobium sp. 6* + *Rhizobium sp. 7* + *Rhizobium sp. 8* + *Rhizobium sp. 9* + *Rhizobium sp. 10* + *Rhizobium sp. 11* + *Rhizobium sp. 12* + *Rhizobium sp. 13* + *Rhizobium sp. 14* + *Rhizobium sp. 15* + *Rhizobium sp. 16* + *Rhizobium sp. 17* + *Rhizobium sp. 18* + *Rhizobium sp. 19* + *Rhizobium sp. 20* + *Rhizobium sp. 21* + *Rhizobium sp. 22* + *Rhizobium sp. 23* + *Rhizobium sp. 24* + *Rhizobium sp. 25* + *Rhizobium sp. 26* + *Rhizobium sp. 27* + *Rhizobium sp. 28* + *Rhizobium sp. 29* + *Rhizobium sp. 30* + *Rhizobium sp. 31* + *Rhizobium sp. 32* + *Rhizobium sp. 33* + *Rhizobium sp. 34* + *Rhizobium sp. 35* + *Rhizobium sp. 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VALINE, LEUCINE AND ISOLEUCINE BIOSYNTHESIS



アブラムシとブフネラの遺伝子が  
共役して、3種のアミノ酸を合成  
しているのがわかる

# KEGG BRITE

- ・機能や知識の階層分類
- ・パスウェイにある遺伝子はパスウェイの階層で分類されていると言える
- ・パスウェイには入らないような遺伝子の分類が必要
- ・化合物や薬の分類も必要
- ・様々な視点で文献情報の知識を基に分類

KEGG BRITE Database

www.genome.jp/kegg/brite.html リーダー

 KEGG BRITE Database  
Functional hierarchies and binary relationships of biological entities

KEGG2 PATHWAY BRITE MODULE DISEASE DRUG KO GENOME GENES LIGAND DBGET

**Functional Hierarchies**

KEGG BRITE is a collection of hierarchical classifications (see [new hierarchies and update history](#)) representing our knowledge on various aspects of biological systems. In contrast to KEGG PATHWAY, which is limited to molecular interactions and reactions, KEGG BRITE incorporates many different types of relationships.

The hierarchies, especially those with additional tab-delimited fields, can better be examined with a desktop application called KegHier, which works on Mac, Windows, and Linux platforms.

- [Download KegHier](#)

Search BRITE hierarchies for  Go Clear  
 KEGG identifiers only

**Brite Mapping**

KEGG BRITE mapping is the process to map molecular datasets, especially large-scale datasets in genomics, transcriptomics, proteomics, and metabolomics, to the BRITE functional hierarchies for biological interpretation of higher-level systemic functions.

- [Search Brite - basic brite mapping tool](#)
- [Search&Color Brite - advanced brite mapping tool](#)
- [Join Brite - selected brite hierarchy manipulation tool](#)

**Pathways and Ontologies**  
KEGG pathway maps  
BRITE functional hierarchies

**Genes and Proteins**  
Network hierarchy  
KEGG Orthology (KO) (K numbers)  
KEGG modules (M/K numbers)  
KEGG reaction modules

**Diseases and Drugs**  
» Japanese  
Diseases (H numbers)  
Human diseases [+ gene]  
Infectious diseases [+ genome]  
Human diseases in ICD-10 classification

**Protein families (K numbers)**  
Enzymes  
Protein kinases

**Disease genes and markers**  
Cancer stages  
Cancer-associated carbohydrates (table)

**Prescription drugs (D numbers)**  
ATC classification [+ target]  
USP drug classification  
Therapeutic categories of drugs in Japan

# KEGG

- Pathway and Ontologies
  - PATHWAYデータベースやBRITEデータベースの一覧
- Genes and Proteins
  - 遺伝子やタンパク質の機能やネットワークの分類
- Drugs and Diseases
  - 薬や疾患の分類
- Compounds and Reactions
  - 化合物の機能による分類、酵素反応の種類による分類
- Organisms and Cells
  - 生物の系統分類、器官や細胞の分類

www.genome.jp/kegg/brite\_ja.html リーダー

**Pathways and Ontologies**

- KEGG パスウェイマップ
- BRITE 機能階層
- BRITE 機能階層 (日本語ファイル)

**Genes and Proteins**

Network hierarchy

- KEGG Orthology (KO) (K numbers)
- KEGG modules (M/K numbers)
- KEGG reaction modules

Protein families (K numbers)

- Enzymes
- Protein kinases
- Peptidases
- Glycosyltransferases
- LPS biosynthesis proteins
- Lipid biosynthesis proteins
- Polyketide biosynthesis proteins
- Prenyltransferases
- Amino acid related enzymes
- Cytochrome P450
- Photosynthesis proteins

- Transcription factors
- Transcription machinery
- Spliceosome
- Ribosome
- Ribosome biogenesis
- Transfer RNA biogenesis
- Translation factors
- Chaperones and folding catalysts
- SNAREs
- Ubiquitin system
- Proteasome
- DNA replication proteins
- Chromosome
- DNA repair and recombination proteins

- Transporters
- Secretion system
- Bacterial toxins
- Two-component system
- Bacterial motility proteins
- Cytoskeleton proteins
- Exosome *New!*

- G protein-coupled receptors
- Enzyme-linked receptors
- Cytokine receptors
- Nuclear receptors
- Ion channels
- GTP-binding proteins
- Cytokines
- CAMs and their ligands
- CD molecules

- Proteoglycans
- HS/Hep binding proteins
- Lectins

RNA family (K numbers)

- Non-coding RNAs

**Diseases and Drugs**

Diseases (H numbers)

- ヒト疾患 [+ 遺伝子]
- 感染症疾患 [+ グノム]
- ICD-10 による疾患分類
- 感染症法による感染症分類

Disease genes and markers

- Cancer stages
- Cancer-associated carbohydrates (table)

Prescription drugs (D numbers)

- 医療用医薬品の薬効分類 [+ 商品]
- 医療用医薬品のATC分類 [+ ターゲット]
- 医療用医薬品のUSP分類
- ステロイド外用薬のランク [+ 商品] *New!*
- ターゲットに基づく医薬品分類
- 抗感染薬
- 抗悪性腫瘍薬
- 米国のゲノムバイオマーカー (table)
- 日本のゲノムバイオマーカー (table)
- 日本薬局方収載医薬品

OTC and other drugs (D/E/C numbers)

- 一般用医薬品の分類 [+ 商品]
- 一般用医薬品のリスク区分 [+ 商品]
- 日本のスイッチOTC薬 (table)
- 医薬品添加物
- 漢方方剤と生薬
- 生薬
- 精油
- メディカルハーブ
- Phytochemicals used as drugs
- 動物用医薬品分類

**Compounds and Reactions**

Compounds (C numbers)

- 生体物質
- Lipids
- Phytochemical compounds
- Bioactive peptides
- 内分泌擾乱物質
- 農薬
- 発がん物質
- 自然毒

Reactions (R/RC numbers)

- Enzymatic reactions
- IUBMB reaction hierarchy
- Reaction class
- Glycosyltransferase reactions

**Organisms and Cells**

Organisms

- KEGG 生物種 [+ キーワード]
- 動物分類
- 植物分類
- Photosynthetic organisms
- 植物病原体

Cells, tissues, and organs

- ヒトの器官系
- ヒトの細胞

# KEGG BRITE

- BRITEデータベースでも  
PATHWAYデータベースと同様  
に、キーワード検索やBRITEへ  
のマッピングが可能

KEGG BRITE Database

www.genome.jp/kegg/brite.html リーダー



**KEGG BRITE Database**  
Functional hierarchies and binary relationships of biological entities

KEGG2 PATHWAY BRITE MODULE DISEASE DRUG KO GENOME GENES LIGAND DBGET

**Functional Hierarchies**

KEGG BRITE is a collection of hierarchical classifications (see [new hierarchies](#) and [update history](#)) representing our knowledge on various aspects of biological systems. In contrast to KEGG PATHWAY, which is limited to molecular interactions and reactions, KEGG BRITE incorporates many different types of relationships.

The hierarchies, especially those with additional tab-delimited fields, can better be examined with a desktop application called KegHier, which works on Mac, Windows, and Linux platforms.

- Download KegHier

Search BRITE hierarchies for  Go Clear  
 KEGG identifiers only

**Brite Mapping**

KEGG BRITE mapping is the process to map molecular datasets, especially large-scale datasets in genomics, transcriptomics, proteomics, and metabolomics, to the BRITE functional hierarchies for biological interpretation of higher-level systemic functions.

- Search Brite - basic brite mapping tool
- Search&Color Brite - advanced brite mapping tool
- Join Brite - selected brite hierarchy manipulation tool

---

**Pathways and Ontologies**  
KEGG pathway maps  
BRITE functional hierarchies

**Genes and Proteins**  
Network hierarchy  
KEGG Orthology (KO) (K numbers)  
KEGG modules (M/K numbers)  
KEGG reaction modules

**Protein families (K numbers)**  
Enzymes

**Diseases and Drugs**  
» Japanese  
Diseases (H numbers)  
Human diseases [+ gene]  
Infectious diseases [+ genome]  
Human diseases in ICD-10 classification

**Disease genes and markers**  
Cancer stages  
Cancer-associated carbohydrates (table)

**Prescription drugs (D numbers)**  
ATC classification [+ target]  
USP drug classification

# ケミカル情報

化合物・反応データ

# KEGG LIGAND

- ・ ケミカル情報データベース
- ・ 6つのデータベースからなる
- ・ KEGG COMPOUND
  - ・ 中間代謝、二次代謝産物などの化合物データベース
- ・ KEGG GLYCAN
  - ・ 糖鎖構造データベース
- ・ KEGG REACTION/RPAIR/RCLASS/ENZYME
  - ・ 生化学反応データベース

KEGG – Table of Contents  
KEGG LIGAND Database

Database	Identifier	Content	Specialized entry point
LIGAND	COMPOUND	C number	Chemical compound structures
	GLYCAN	G number	Glycan structures
	REACTION	R number	Biochemical reactions
	RPAIR	RP number	Reactant pair alignments
	RCLASS	RC number	Reaction class
	ENZYME	EC number	Enzyme nomenclature

Search LIGAND for  Go Clear  
 bfind mode  bget mode

**LIGAND Relational Database**  
The primary database of KEGG LIGAND is a relational database with the KegDraw interface, which is used to generate the secondary (flat file) database for DBGET. A read-only copy of the LIGAND relational database is made publicly accessible.

Search COMPOUND  
Compound ID  example) C00010 Go Clear  
Name   
Formula   
Exact Mass   
Reaction   
Pathway   
Enzyme   
DBlinks

Search GLYCAN  
Name   
Formula   
Exact Mass   
Reaction   
Pathway   
Enzyme   
DBlinks

Search REACTION  
Reaction ID  example) R00259 Go Clear

Search RPAIR  
Rpair ID  example) RP00010 Go Clear

Chemical Structure Search  
Search similar compound structures

# KEGG COMPOUND

- COMPOUNDエントリ
- C番号
- 化合物名、組成式、分子量、構造の記載
- 関連する生化学反応、パスウェイ、酵素番号、BRITE階層分類、他のデータベースへのリンク
- 構造は2次元情報のみ
- 立体異性が判明している場合はその情報を含む

KEGG COMPOUND: C00163

**Compound: C00163**

Entry	C00163	Compound
Name	Propanoate; Propionate; Propanoic acid; Propionic acid	
Formula	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	
Exact mass	74.0368	
Mol weight	74.0785	
Structure		
	C00163	
	<a href="#">Mol file</a> <a href="#">KCF file</a> <a href="#">DB search</a> <a href="#">Jmol</a> <a href="#">KegDraw</a>	
Remark	Same as: D02310	
Reaction	R00920 R00925 R00928 R01353 R01354 R01355 R01449 R05366	
Pathway	map00640 Propanoate metabolism map00642 Ethylbenzene degradation map00760 Nicotinate and nicotinamide metabolism map01100 Metabolic pathways map01120 Microbial metabolism in diverse environments map01220 Degradation of aromatic compounds map04973 Carbohydrate digestion and absorption map04974 Protein digestion and absorption	
Enzyme	2.7.2.1 2.7.2.15 2.8.3.1 3.7.1.- 4.1.3.32 6.2.1.1 6.2.1.13 6.2.1.17	
Brite	Compounds with biological roles [BR:br08001] Organic acids Carboxylic acids Monocarboxylic acid C00163 Propionate; Propanoate Lipids [BR:br08002] FA Fatty acyls FA01 Fatty Acids and Conjugates FA0101 Straight chain fatty acids C00163 Propanoic acid <a href="#">BRITE hierarchy</a>	
Other DBs	CAS: 79-09-4 PubChem: 3463 ChEBI: 30768 LIPIDMAPS: LMFA01010003 LipidBank: DFA0003 KNAPSAcK: C00044287 PDB-CCD: PPI 3DMET: B01176 NIKKAJI: J1.963A	
LinkDB	All DBs	
KCF data	Show	

# KCFフォーマット

ENTRY	C00163	KEGG Atom Types				Compound
ATOM	5					
	1	C6a	C	24.7142	-18.7600	
	2	C1b	C	25.9258	-19.4624	
	3	O6a	O	23.5027	-19.4624	
	4	O6a	O	24.7142	-17.3612	
	5	C1a	C	27.1373	-18.7600	
BOND	4					
	1	1	2	1		
	2	1	3	1		
	3	1	4	2		
	4	2	5	1		

KCF

///  
5 4 0 0 0 0 0 0 0 0999 V2000

24.7142 -18.7600 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

25.9258 -19.4624 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

23.5027 -19.4624 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

24.7142 -17.3612 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

27.1373 -18.7600 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0

1 3 1 0 0 0

1 4 2 0 0 0

2 5 1 0 0 0

M END

mol

# KEGG REACTION

- REACTIONエントリ
- R番号
- 反応名、反応式などが記載
- 反応を触媒する遺伝子がKOとして記載
- 内外の他のデータベースへのリンク

KEGG REACTION: R01353

**REACTION: R01353**

**Entry**: R01353      **Reaction**

**Name**: ATP:propanoate phosphotransferase

**Definition**: ATP + Propanoate <=> ADP + Propanoyl phosphate

**Equation**: C00002 + C00163 <=> C00008 + C02876

**RPair**: RP00003 C00002\_C00008\_main  
 RP01451 C00163\_C02876\_main  
 RP00540 C00002\_C02876\_trans

**Enzyme**: 2.7.2.1      2.7.2.15

**Pathway**: rn00640 Propanoate metabolism

**Orthology**: K00925 acetate kinase [EC:2.7.2.1]  
 K00932 propionate kinase [EC:2.7.2.15]

**LinkDB**: All DBs

DBGET integrated database retrieval system

# KEGG RPAIR

- RPAIRエントリ
- RP番号
- 基質・生成物間の原子のアラインメントを色で表現

KEGG RPAIR: RP01451

RPAIR: RP01451

<b>Entry</b>	RP01451	<b>RPair</b>
<b>Name</b>	C00163_C02876	
<b>Compound</b>	C00163 Propanoate C02876 Propanoyl phosphate	
<b>Type</b>	main	
<b>RDM</b>	1 1 O6a-O7a:-P1b:C6a-C7a	
<b>RClass</b>	RC00043	
<b>Related pair</b>	RP00113 RP00180 RP00497 RP00932 RP00967 RP00970 RP01282 RP01453 RP01477 RP01498 RP01501 RP01560 RP01691 RP01694 RP02380 RP03622 RP04397 RP04833 RP11219 RP15339	
<b>Reaction</b>	R01353	
<b>Enzyme</b>	2.7.2.1 2.7.2.15	
<b>KCF data</b>	Show	

The diagram illustrates the chemical reaction and the alignment of atoms between the reactant (Propanoate) and the product (Propanoyl phosphate). The reactant (R atom) is shown with atoms C1a, C1b, and O6a. The product (D atom) is shown with atoms O1c, P1b, and O7a. The intermediate molecule (M atom) is shown with atoms C7a, C1b, C1a, and O6a. The alignment of atoms is indicated by colored lines connecting corresponding atoms between the reactant and the product.

- RPAIR工
- RP番号
- 基質・生
- アライン
- 現

KEGG RPAIR: RP01451

KCF data Hide

ALIGN	
5	
1	1:C6a
2	2:C1b
3	3:O6a
4	4:O6a
5	5:C1a
-	*
	6:C7a #M1
	7:C1b
	2:O7a #R1
	8:O6a
	9:C1a
	1:P1b #D1

ENTRY1

COMPOUND C00163

ATOM 5

1	C6a	C	-0.2862	0.0000
2	C1b	C	0.4276	-0.4138
3	O6a	O	-1.0000	-0.4138
4	O6a	O	-0.2862	0.8241
5	C1a	C	1.1414	0.0000

BOND 4

1	1	2	1
2	1	3	1
3	1	4	2
4	2	5	1

ENTRY2

COMPOUND C02876

ATOM 9

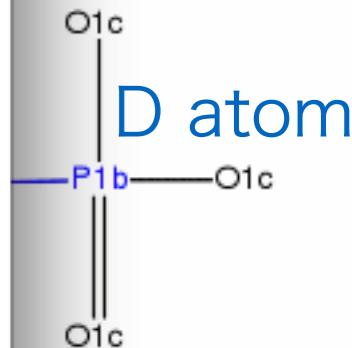
1	P1b	P	20.2552	-14.4472
2	O7a	O	18.8576	-14.4535
3	O1c	O	21.6530	-14.4472
4	O1c	O	20.2488	-13.0428
5	O1c	O	20.2552	-15.8448
6	C7a	C	17.6466	-15.1557
7	C1b	C	16.4292	-14.4535
8	O6a	O	17.6466	-16.5533
9	C1a	C	15.2182	-15.1557

BOND 8

1	1	2	1
2	1	3	1
3	1	4	1
4	1	5	2
5	2	6	1
6	6	7	1
7	6	8	2
8	7	9	1

アラインメント

化合物 1



化合物 2

970 RP01282  
691 RP01694  
339

# KEGG RCLASS

- RCLASSエントリ
- RC番号
- Definition行にRDMパターン
- 全く同じRDMパターンを持つ  
RPAIRエントリが記載
- 関連するREACTION、  
ENZYME、PATHWAY、  
ORTHOLOGYのリスト

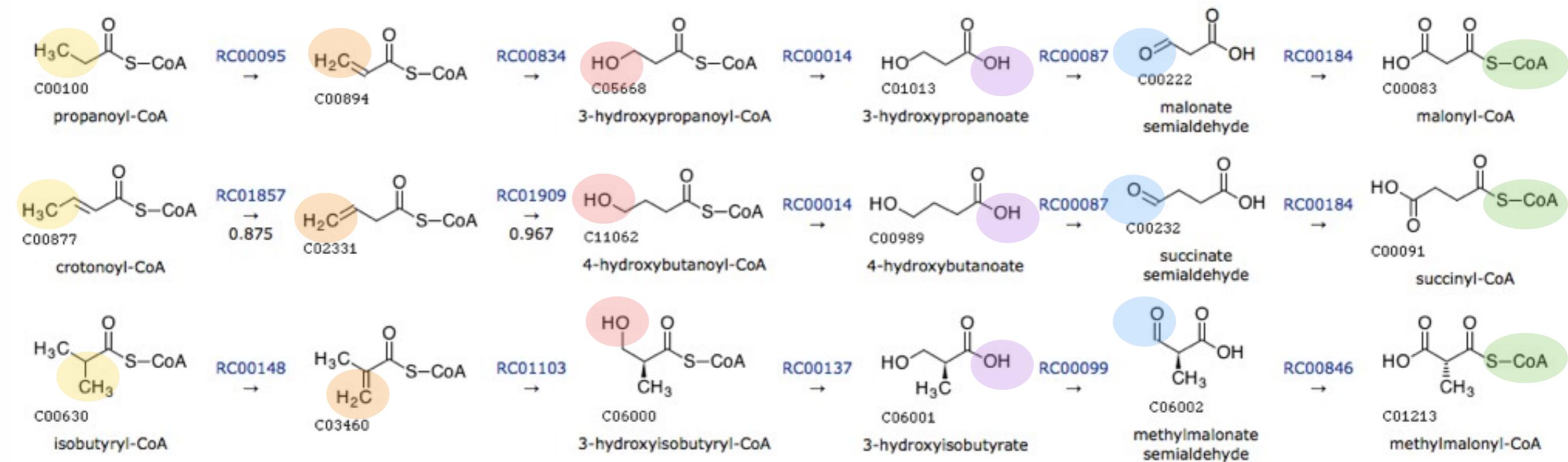
KEGG RCLASS: RC00043

KEGG RCLASS: RC00043

Entry	RC00043	RClass
Definition	O6a-O7a:*-P1b:C6a-C7a	
RPair	<a href="#">RP00113</a> <a href="#">RP00180</a> <a href="#">RP00497</a> <a href="#">RP00932</a> <a href="#">RP00967</a> <a href="#">RP00970</a> <a href="#">RP01282</a> <a href="#">RP01453</a> <a href="#">RP01477</a> <a href="#">RP01498</a> <a href="#">RP01501</a> <a href="#">RP01560</a> <a href="#">RP01691</a> <a href="#">RP01694</a> <a href="#">RP03622</a> <a href="#">RP04397</a> <a href="#">RP04833</a> <a href="#">RP11219</a> <a href="#">RP15339</a>	<a href="#">DB search</a>
Related class		<a href="#">DB search</a>
Reaction	<a href="#">R00239</a> <a href="#">R00315</a> <a href="#">R00316</a> <a href="#">R00317</a> <a href="#">R00320</a> <a href="#">R00322</a> <a href="#">R00480</a> <a href="#">R00539</a> <a href="#">R00542</a> <a href="#">R01074</a> <a href="#">R01353</a> <a href="#">R01354</a> <a href="#">R01395</a> <a href="#">R01421</a> <a href="#">R01423</a> <a href="#">R01504</a> <a href="#">R01512</a> <a href="#">R01515</a> <a href="#">R01517</a> <a href="#">R01660</a> <a href="#">R01688</a> <a href="#">R01690</a> <a href="#">R02188</a> <a href="#">R02649</a> <a href="#">R03098</a> <a href="#">R03841</a> <a href="#">R04002</a> <a href="#">R07770</a> <a href="#">R08404</a> <a href="#">R08405</a> <a href="#">R08406</a> <a href="#">R08407</a> <a href="#">R09776</a>	
Enzyme	<a href="#">1.2.1.31</a> <a href="#">2.7.1.61</a> <a href="#">2.7.1.106</a> <a href="#">2.7.2.1</a> <a href="#">2.7.2.2</a> <a href="#">2.7.2.3</a> <a href="#">2.7.2.4</a> <a href="#">2.7.2.7</a> <a href="#">2.7.2.8</a> <a href="#">2.7.2.10</a> <a href="#">2.7.2.11</a> <a href="#">2.7.2.12</a> <a href="#">2.7.2.14</a> <a href="#">2.7.2.15</a> <a href="#">2.7.2.-</a> <a href="#">2.7.4.17</a> <a href="#">2.7.7.58</a> <a href="#">2.7.7.63</a> <a href="#">3.6.1.7</a> <a href="#">3.6.1.20</a> <a href="#">6.2.1.1</a> <a href="#">6.2.1.11</a> <a href="#">6.2.1.17</a> <a href="#">6.3.4.9</a> <a href="#">6.3.4.10</a> <a href="#">6.3.4.11</a> <a href="#">6.3.4.15</a>	
Pathway	<a href="#">rn00010</a> Glycolysis / Gluconeogenesis <a href="#">rn00260</a> Glycine, serine and threonine metabolism <a href="#">rn00270</a> Cysteine and methionine metabolism <a href="#">rn00300</a> Lysine biosynthesis	

# Reaction Module

RM0019



構造変化パターンの分類から、類似した連続反応によって代謝が進む、Reaction Moduleデータベースを作成

# SIMCOMP

- 配列の類似性検索が  
BLAST/FASTAで可能な  
と同様に、化合物の構造類  
似性検索が可能

SIMCOMP Search



**SIMCOMP Search**

SUBCOMP    SIMCOMP    SIMCOMP2    API    KEGG2

Enter query compound: (in one of the four forms)

Compound ID: C00022 (Example) C00022 [View structure](#)

MOL File Name: [ファイルを選択](#) [ファイル未選択](#)

MOL File Text:

SMILES:

Select target database:

COMPOUND     DRUG     KNAPSAcK     REACTION

Search options:

Global search     Local search     Customized search

▶ Option details

[SIMCOMP help](#)  
[SIMCOMP REST API](#)

[Download KegDraw](#)  
KegDraw is a Java application for drawing compound structure.

**Compute**

# SIMCOMP

- SIMCOMP
  - データベースへの化合物の類似性検索
- SIMCOMP2
  - 問い合わせ化合物間の類似性検索
- SUBCOMP
  - 化合物の部分構造検索

SIMCOMP Search

**SIMCOMP Search**

**SUBCOMP** **SIMCOMP** **SIMCOMP2** API KEGG2

Enter query compound: (in one of the four forms)

Compound ID (Example) C00022 View structure

MOL File Name ファイルを選択 ファイル未選択

MOL File Text

SMILES

Select target database:

COMPOUND  DRUG  KNAPSAcK  REACTION

Search options:

Global search  Local search  Customized search  
Option details

[SIMCOMP help](#) [SIMCOMP REST API](#)

[Download KegDraw](#)  
KegDraw is a Java application for drawing compound structure.

# Feedback

GenomeNet Feedback Form

GenomeNet



**GenomeNet Feedback Form**

Please use the form below to send your question or comment to KEGG and GenomeNet. Please enter information in all fields.  
(Japanese characters accepted)

Name:

Email address:   
(a copy will be sent to you as well)

Affiliation:

Category:

<input type="radio"/> KEGG PATHWAY	<input type="radio"/> KEGG MEDICUS	<input type="radio"/> DBGET/LinkDB
<input type="radio"/> KEGG BRITE	<input type="radio"/> KEGG API	<input type="radio"/> Copyright permission
<input type="radio"/> KEGG GENES	<input type="radio"/> KAAS	<input type="radio"/> KEGG license
<input type="radio"/> KEGG LIGAND	<input type="radio"/> GenomeNet tools	<input type="radio"/> Other

Comments:

KEGGデータベースや  
GenomeNetに関する質問  
やコメントなど受け付け  
ています  
日本語でOK