

KEGG/GenomeNetの Webサービスの紹介

ライフサイエンス統合データベースセンター (DBCLS)

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統合データベース講習会：AJACS岩手 2014/12/5

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）
 - ・ GENES, ORTHOLOGY(KO), OC, KAAS, MAPLE …
- ・ ケミカル情報（化合物と反応データ）
 - ・ LIGAND
- ・ システム情報（パスウェイと階層分類）
 - ・ PATHWAY, BRITE, MODULE, KEGG mapper …

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の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:** Located at the top right, showing "Search 統合データベース for [redacted]".
- Logo:** A circular logo featuring stylized letters T, G, C, and S.
- Navigation Links:** On the left sidebar, links include "ゲノムネット", "統合データベース", "医薬品データベース", "KEGG", "varDB", "研究支援データベース", "計算ツール", "FTP", and "フィードバック".
- Highlighted Sections:**
 - ゲノムネットデータベースリソース**: Circled in red, this section lists "ゲノムネット統合データベース", "KEGG MEDICUS: 疾患・医薬品統合リソース", "KEGG: 生命システム情報統合データベース", and various KEGG sub-databases like PATHWAY, BRITE, Organisms, GENES, LIGAND, and REACTION.
 - ゲノムネット計算ツール**: Circled in red, this section lists "配列解析" tools like BLAST, FASTA, MOTIF, CLUSTALW, MAFFT, PRRN, and "ゲノム情報解析" tools like OC Viewer, REST services, and KAAS.
- Right Sidebar:** Includes links to "KEGG パスウェイ一覧", "BRITE 機能階層 (日本語)", "KEGG 生物種一覧", "メタゲノム", and "ドラフトゲノム".
- Diagram:** A complex diagram titled "データベース間のリンク" (Links between databases) showing the interconnected nature of the KEGG network.
- Graph:** A line graph titled "データベース増加図" (Database Increase Graph) showing the growth of various KEGG 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 on the left containing links to various databases and tools, and a main content area on the right with an introduction and a list of entry points.

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ール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

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

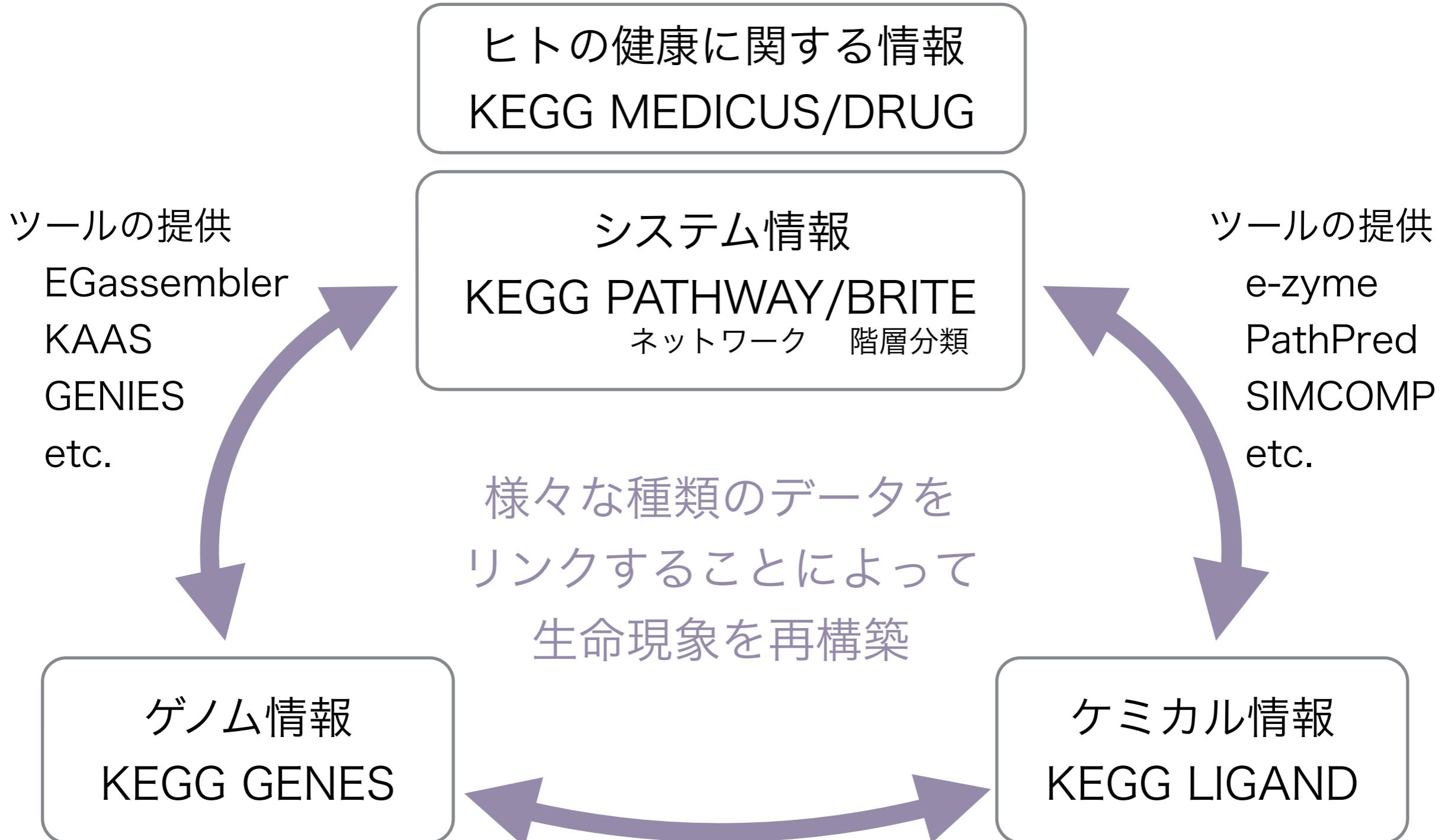
KEGG MEDICUS ゲノムと疾患・医薬品の統合リソース (日本語) [お薬手帳]

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 Enc



KEGG: Kyoto Encyclopedia of Genes and Genomes

KEGG Home
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利用申し込み

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Feedback

Kanehisa Labs

KEGG2

データタイプごとのエントリーポイント

KEGG PATHWAY
KEGG BRITE
KEGG MODULE
KEGG DISEASE
KEGG DRUG
KEGG ENVIRON
KEGG MEDICUS
KEGG ORTHOLOGY
KEGG GENES
KEGG GENOME
KEGG Organisms
KEGG LIGAND
KEGG COMPOUND
KEGG GLYCAN
KEGG REACTION
Reaction Modules
一般向けのエントリーポイント
KEGG MEDICUS
生物種ごとのエントリーポイント
KEGG Organisms
解析ツール



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	KEGG PATHWAY KEGG BRITE KEGG MODULE KEGG Mapper KEGG Atlas	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
	KEGG DISEASE KEGG DRUG KEGG ENVIRON KEGG MEDICUS	New drug maps Update history	Human diseases Infectious diseases ATC drug classification	DISEASE DRUG ENVIRON
	KEGG ORTHOLOGY		KEGG Orthology (KO)	ORTHOLOGY
Genomic information	KEGG GENES KEGG GENOME KEGG Organisms	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 MGENOME†
Chemical information	KEGG LIGAND KEGG COMPOUND KEGG GLYCAN KEGG REACTION 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.

KEGG で提供している
データベース

KEGG/GenoNet で
提供しているツール

Select Organism Go Clear (examples) hsa mmu sce eco bsu syn

KEGGにあるデータ、ないデータ

	ある	ない
ゲノム	遺伝子配列 アノテーション	制御領域 バリエーション タンパク質立体構造
パスウェイ	代謝、制御マップ 病気、薬開発マップ	シミュレーション用の パラメータ
化合物	二次元構造 薬、代謝物、反応 反応パターン	物性、立体構造 反応速度定数

データ間のリンク

外部データベースへのリンク

ゲノム情報

配列データ

KEGG GENES

KEGG – Table of Contents



Kyoto Encyclopedia of Genes and Genomes

KEGG – Table of Contents

KEGG2 PATHWAY BRITE MODULE DISEASE DRUG KO GENOME GENES LIGAND DBGET

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	KEGG DISEASE KEGG DRUG KEGG ENVIRON KEGG MEDICUS	New drug maps Update history	Human diseases Infectious diseases ATC drug classification	DISEASE DRUG ENVIRON	
	KEGG ORTHOLOGY		KEGG Orthology (KO)	ORTHOLOGY	
	Genomic information	KEGG GENES KEGG GENOME KEGG Organisms	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 EGENOME† MGENOME†
		KEGG LIGAND KEGG COMPOUND KEGG GLYCAN KEGG REACTION 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 GENES

- ・遺伝子・タンパク質配列を集めたデータベース

The screenshot shows the KEGG GENES homepage. At the top, there is a navigation bar with links to KEGG2, PATHWAY, BRITE, MODULE, KO, GENOME, GENES (which is bolded), SSDB, and Organisms. Below the navigation bar is a search bar with the placeholder "Enter org:gene (Example) syn:ssr3451". Below the search bar are several buttons: Entry, Gene cluster, Ortholog, Paralog, Motif, and Clear. A red box highlights the "Entry" button.

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 is a supplementary collection of gene catalogs for eukaryotic draft genomes, which are given automatic KO assignment by KAAS with GENES used as a reference data set. KEGG MGENES contains gene catalogs for metagenomes of environmental samples (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	Draft genomes with automatic (KAAS) annotation
MGENES	Metagenomes	Metagenomes with automatic (KAAS) annotation
VGENES	Viruses	No annotation; available only in DBGET

Below the table, there are several search and filter options. A red box highlights the "bfind mode" radio button. To the right, a sidebar provides information on annotation methods:

- マニュアル
- KOALA : 自動 (SSEARCH)
- KAAS : 自動 (BLAST)

生物種、サンプルリスト

- KEGGに登録されている生物種、サンプルのリスト



KEGG Organisms: Complete Genomes

Eukaryotes: 299 Bacteria: 2989 Archaea: 175

[Genomes | Species | Genus | Draft | Meta]

Eukaryotes 系統分類 生物種コード 種名 データソース

Category	Organisms	Source
	hsa Homo sapiens (human)	RefSeq
	pu Pan troglodytes (chimpanzee)	RefSeq
	pps Pan paniscus (bonobo)	RefSeq
	ggo Gorilla gorilla gorilla (western lowland gorilla)	RefSeq
	pon Pongo abelii (Sumatran orangutan)	RefSeq
	nle Nomascus leucogenys (northern white-cheeked gibbon)	RefSeq
	mcc Macaca mulatta (rhesus monkey)	RefSeq
	mcf Macaca fascicularis (crab-eating macaque)	RefSeq
	cjc Callithrix jacchus (white-tufted-ear marmoset)	RefSeq
	mmu Mus musculus (mouse)	RefSeq
	rno Rattus norvegicus (rat)	RefSeq
	cge Cricetus griseus (Chinese hamster)	RefSeq
	ngi Nannospalax galili (Upper Galilee mountains blind mole rat)	RefSeq
	hgl Heterocephalus glaber (naked mole rat)	RefSeq
	ocu Oryctolagus cuniculus (rabbit)	RefSeq
	tup Tupai chinensis (Chinese tree shrew)	RefSeq
	cfa Canis familiaris (dog)	RefSeq
Mammals	aml Ailuropoda melanoleuca (giant panda)	RefSeq
	umr Ursus maritimus (polar bear)	RefSeq
	fca Felis catus (domestic cat)	RefSeq
	ptg Panthera tigris altaica (Amur tiger)	RefSeq
	bta Bos taurus (cow)	RefSeq
	bom Bos mutus (wild yak)	RefSeq
	phd Pantholops hodgsonii (chiru)	RefSeq
	chx Capra hircus (goat)	RefSeq
	oas Ovis aries (sheep)	RefSeq
	ssc Sus scrofa (pig)	RefSeq
	cfr Camelus ferus (Wild Bactrian camel)	RefSeq
	bacu Balaenoptera acutorostrata scammoni (minke whale)	RefSeq
	lve Lipotes vexillifer (Yangtze River dolphin)	RefSeq
Vertebrates	ecb Equus caballus (horse)	RefSeq

生物種、サンプルリスト

- KEGGに登録されている生物種、サンプルのリスト

ID				
Category			Organisms	Source
Animals	Vertebrates	Mammals	T10035 Saimiri boliviensis boliviensis (Bolivian squirrel monkey)	GenBank
			T10034 Loxodonta africana (African savanna elephant)	GenBank
		Fishes	T10005 Tetraodon nigroviridis (spotted green pufferfish)	GenBank
	Arthropods	Insects	T10030 Danaus plexippus (monarch butterfly)	MonarchBase
			T10031 Heliconius melpomene (postman butterfly)	Heliconius Genome Project
			T10014 Acyrthosiphon pisum (pea aphid) (AphidBase)	AphidBase
		Crustaceans	T10016 Pediculus humanus (human body louse) (VectorBase)	VectorBase
	Nematodes		T10017 Daphnia pulex (water flea)	JGI
			T10022 Dirofilaria immitis (dog heartworm nematode)	U Basel / U Edinburgh
	Cnidarians		T10026 Acropora digitifera (stony coral)	OIST

Category	Project	Source
Ocean	T30001 Planktonic microbial communities from North Pacific Subtropical Gyre.	NCBI
	T30002 Planktonic microbial communities from Monterey Bay, CA.	NCBI
	T30718 GS000a GS000a - Sargasso Station 13 / 11	CAMERA/GOS
	T30719 GS000b GS000b - Sargasso Station 13 / 11	CAMERA/GOS
	T30720 GS000c GS000c - Sargasso Stations 3	CAMERA/GOS
	T30721 GS000d GS000d - Sargasso Station 13	CAMERA/GOS
	T30722 GS001a GS001a - Hydrostation S	CAMERA/GOS
	T30723 GS001b GS001b - Hydrostation S	CAMERA/GOS
	T30724 GS001c GS001c - Hydrostation S	CAMERA/GOS
	T30725 GS002 GS002 - Gulf of Maine	CAMERA/GOS
MGENES	T30726 GS003 GS003 - Browns Bank, Gulf of Maine	CAMERA/GOS
	T30727 GS004 GS004 - Outside Halifax, Nova Scotia	CAMERA/GOS
	T30728 GS005 GS005 - Bedford Basin, Nova Scotia	CAMERA/GOS

生物種、サンプルエントリー

- 生物種やサンプルのデータソース、文献、系統などの詳細情報

KEGG GENOME: Homo sapiens (human)

Kegg **Homo sapiens (human)**

Genome info Pathway map Brite hierarchy Module Genome map Blast

Search genes: Go Clear 遺伝子のキーワード検索

Genome information

T number	T01001
Org code	hsa
Aliases	HUMAN, 9606
Full name	Homo sapiens (human)
Definition	Homo sapiens (human)
Annotation	manual
Taxonomy	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

bfind/bget: キーワード、エントリー検索

ヒットしたエントリのリスト

Database: GENES - Search term: histidine (1 - 1000) Next	
hsa:727896	cysteine and histidine-rich domain (CHORD) containing 1 pseudogene
hsa:644844	PHGR1; proline/histidine/glycine-rich 1
hsa:26973	CHORDC1, CHP1; cysteine and histidine-rich domain (CHORD) containing 1; K16729 cysteine and histidine-rich domain-containing protein 1
hsa:1801	DPH1, DPH2L, DPH2L1, OVCA1; diphthamide biosynthesis 1; K07561 2-(3-amino-3-carboxypropyl)imidazolidine-2,4-dione synthase [EC:2.5.1.108]
hsa:3094	HINT1, HINT, NMNAT, PKCI-1, PRKCNH1; histidine triad nucleotide binding protein 1; K02120 (HIT) family protein
hsa:121260	SLC15A4, PHT1, PTR4; solute carrier family 15 (oligopeptide transporter), member 4; K16729 family 15 (peptide/histidine transporter), member 3/4
hsa:135114	HINT3, HINT4; histidine triad nucleotide binding protein 3 (EC:3.4.2.1)
hsa:3273	HRG, HPRG, HRGP, THPH11; histidine-rich glycoprotein
hsa:3067	HDC; histidine decarboxylase (EC:4.1.1.22); K01590 histidine decarboxylase [EC:4.1.1.22]
hsa:2272	FHIT, AP3Aase, FRA3B; fragile histidine triad (EC:3.6.1.29); K01522 bis(5'-adenosyl)-triphosphate kinase [EC:3.6.1.29]
hsa:646962	HRCT1, LGLL338, PRO537, UNQ338; histidine rich carboxyl terminus 1
hsa:84681	

“histidine”で bfind
(キーワード検索)



GENESエントリ

KF
Escherichia coli K-12 MG1655: b4139

Entry	b4139	CDS	T00007
Gene name	aspA		
Definition	aspartate ammonia-lyase (EC:4.3.1.1)		
Orthology	K01744	aspartate ammonia-lyase [EC:4.3.1.1]	
Organism	eco	Escherichia coli K-12 MG1655	
Pathway	eco00250	Alanine, aspartate and glutamate metabolism	
	eco01100	Metabolic pathways	
Brite	KEGG Orthology (KO) [BR:eco00001]		
	Metabolism		
	Amino acid metabolism		
	00250 Alanine, aspartate and glutamate metabolism		
	b4139 (aspA)		
	Enzymes [BR:eco01000]		
	4. Lyases		
	4.3 Carbon-nitrogen lyases		
	4.3.1 Ammonia-lyases		
	4.3.1.1 aspartate ammonia-lyase		
	b4139 (aspA)		
	BRITE hierarchy		
SSDB	Ortholog	Paralog	Gene cluster
Motif	Pfam: Lyase_1 FumaraseC_C		Motif
Other DBs	NCBI-GI: 90111690		

“eco:b4139”で bget
(エントリー検索)



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

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

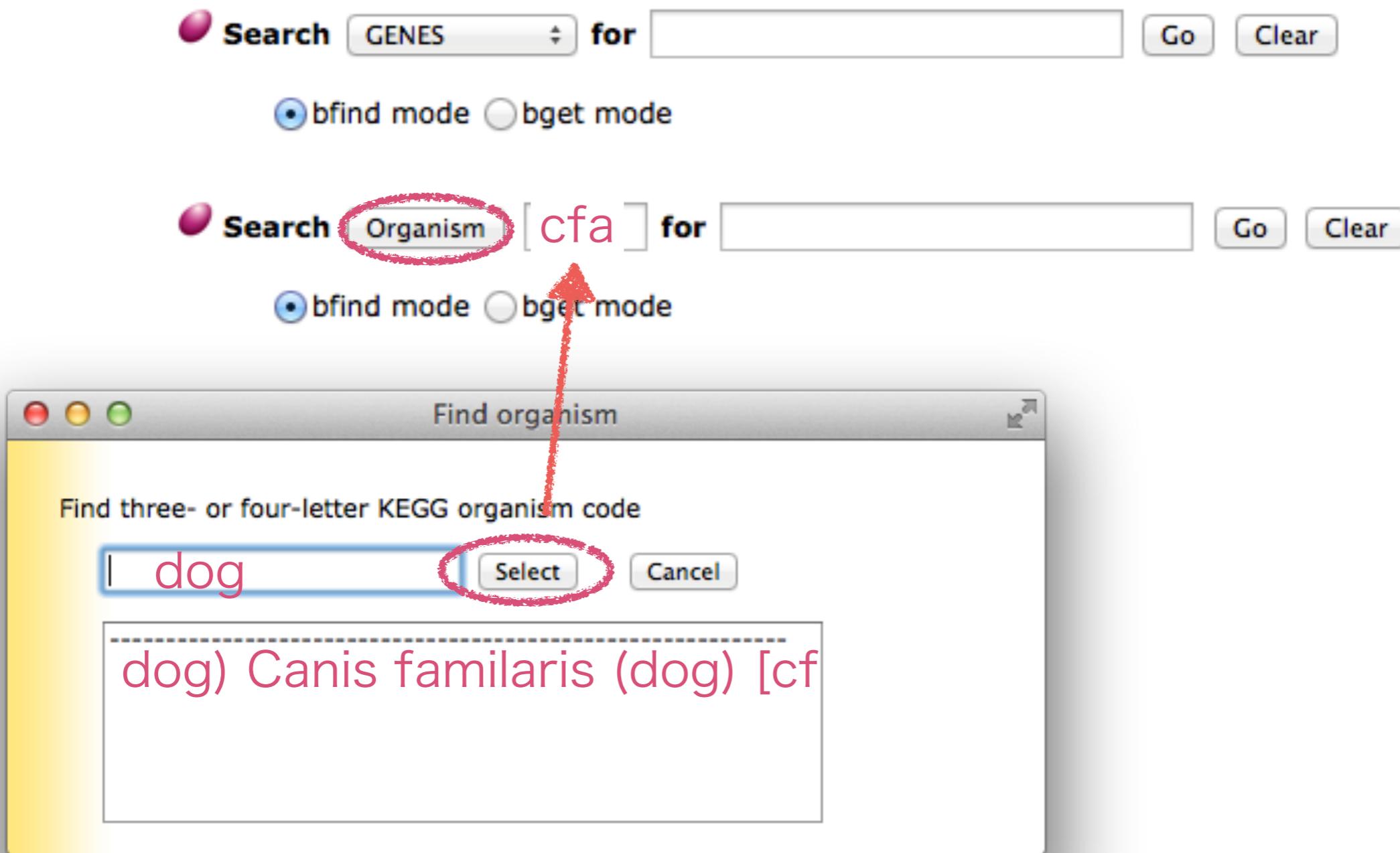
Gene Annotation

The annotation of KEGG GENES involves assignment of KO identifiers (K numbers). Internally, this is done using the KOALA and GFIT annotation tools based on the SSDB database (see: [Ortholog Annotation in KEGG](#)). The annotation of KEGG DGENES and EGENES is done automatically using the KAAS program, and EGENES is generated from EST datasets by the EGassembler program. Both of these programs are made publicly available.

Annotate genomes using KEGG

bfind/bget: キーワード、エントリー検索

- 生物種コードの検索



KEGG GENES エントリの IDへの変換

- NCBI gi, NCBI GeneID, UniProtなどのIDからKEGG GENES エントリIDへの変換が可能

KEGG GENES ページ

Gene Name Conversion

KEGG GENES can be retrieved by giving identifiers of outside databases, such as NCBI-GeneID (Entrez Gene ID), NCBI-gi, and UniProt accession numbers. Cross-reference lists are available at the FTP site.

 **Search GENES for**

bget mode

Last updated: April 1, 2014

KEGG

GenomeNet

Kanehisa Laboratories

KEGG Objects ページ

Enter outside DB accession numbers to convert to KEGG GENES entries:

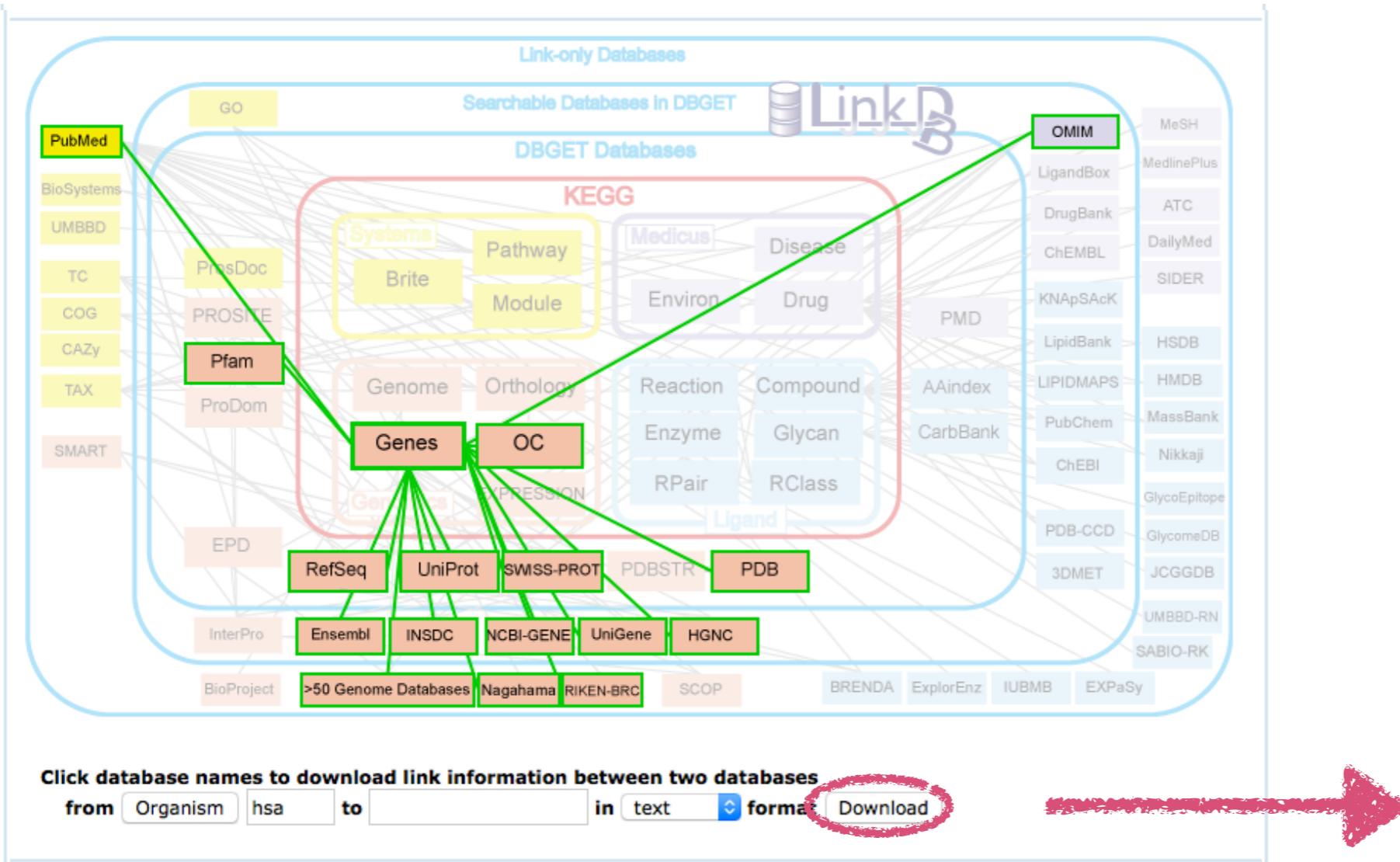
NCBI GeneID NCBI gi UniProt

(Example) 3775638 3737440 3743551 3897645 3902295

Last updated: July 25, 2014

KEGG GENES エントリの IDへの変換

LinkDB



生物種ごとの遺伝子IDの対応表が取得できる

hsa:1	up:P04217	equivalent
hsa:1	up:V9HWD8	equivalent
hsa:10	up:A4Z6T7	equivalent
hsa:10	up:P11245	equivalent
hsa:100	up:F5GWI4	equivalent
hsa:100	up:P00813	equivalent
hsa:1000	up:A8MWK3	reverse
hsa:1000	up:P19022	equivalent
hsa:10000	up:Q9Y243	equivalent
hsa:100008586	up:076087	equivalent
hsa:100008586	up:P0CL80	equivalent
hsa:100008586	up:P0CL81	equivalent
hsa:100008586	up:P0CL82	equivalent
hsa:10001	up:075586	equivalent
hsa:10002	up:F1D8Q9	equivalent
hsa:10002	up:Q9Y5X4	equivalent
hsa:10003	up:Q9Y3Q0	equivalent
hsa:100037417	up:A6NH4	equivalent
hsa:100037417	up:B4DJQ7	equivalent
hsa:100037417	up:B7Z522	reverse
hsa:100038246	up:P0CAT3	equivalent
hsa:10004	up:Q9UQ01	equivalent
hsa:100049587	up:Q08ET2	equivalent
hsa:10005	up:E9PRD4	reverse
hsa:10005	up:014734	equivalent
hsa:10006	up:B6VEX3	equivalent
hsa:10006	up:B6VEX4	equivalent
hsa:10006	up:B6VEX5	equivalent
hsa:10006	up:Q8IZP0	equivalent
hsa:10007	up:B7Z3X4	reverse
hsa:10007	up:E7EVU7	reverse
hsa:10007	up:P46926	equivalent
hsa:10008	up:Q6IAE6	equivalent
hsa:10008	up:Q9Y6H6	equivalent
hsa:10000	up:Q96T34	equivalent

GENES エントリ

例：eco:b4139

- 例：eco:b4139でbget

Gene Catalogs

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DGENES	Draft genomes	Draft genomes with automatic (KAAS) annotation
MGENES	Metagenomes	Metagenomes with automatic (KAAS) annotation
VGENES	Viruses	No annotation; available only in DBGET

Search GENES for eco:b4139 Go Clear

bfind mode bget mode

Search Organism for Go Clear

bfind mode bget mode

GENES エントリ

例：eco:b4139

- 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 :

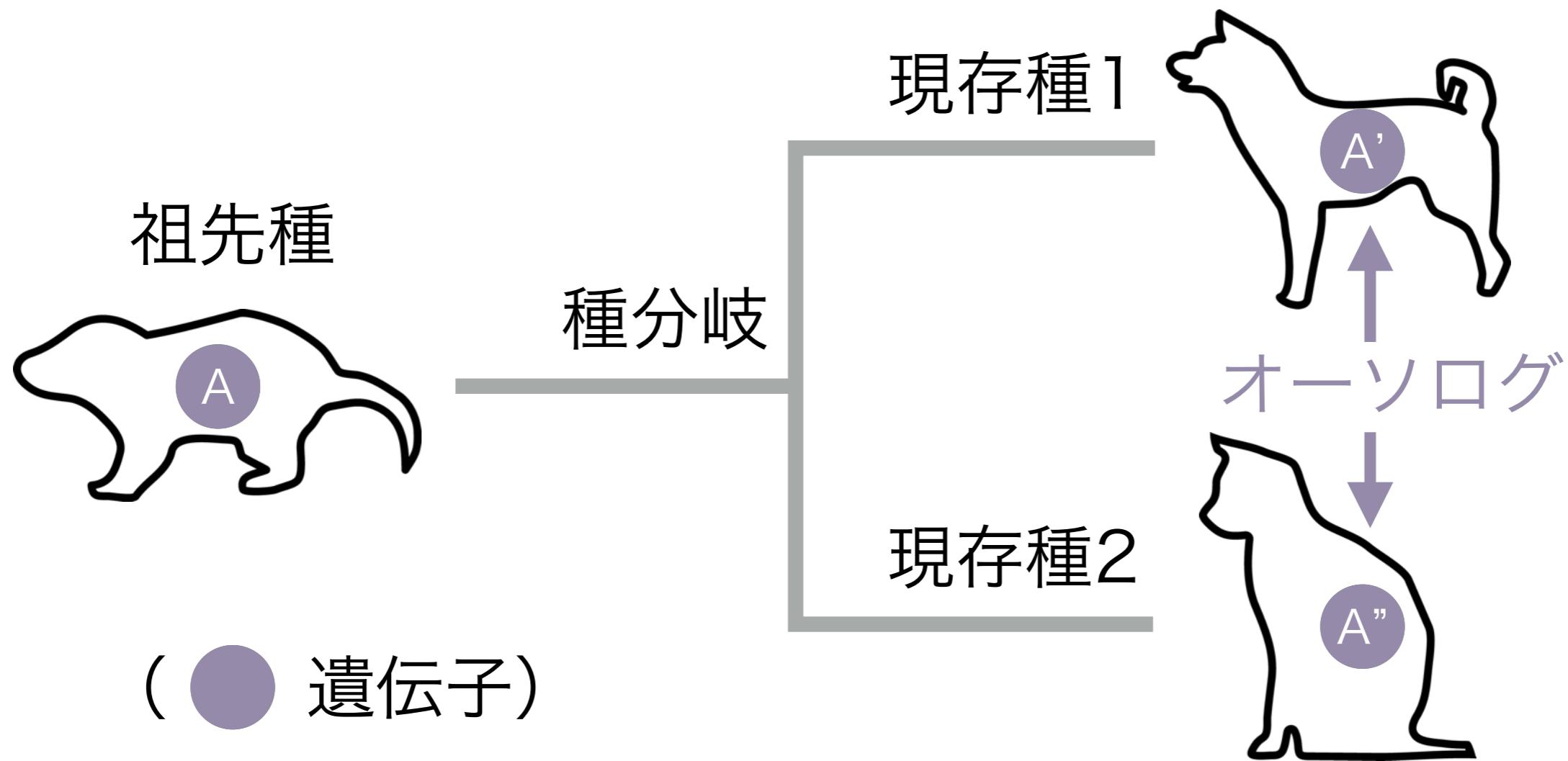
オリジナルサイトでの記述

Orthology :

KEGGでつけられたアノテーション (KO)

KEGG Escherichia coli K-12 MG1655: b4139		
Entry	b4139	CDS T00007
Gene name	aspA	
Definition	aspartate ammonia-lyase (EC:4.3.1.1)	
Orthology	K01744 aspartate ammonia-lyase [EC:4.3.1.1]	
Organism	eco Escherichia coli K-12 MG1655	
Pathway	eco00250 Alanine, aspartate and glutamate metabolism eco01100 Metabolic pathways	
Brite	KEGG Orthology (KO) [BR:eco00001] Metabolism Amino acid metabolism 00250 Alanine, aspartate and glutamate metabolism b4139 (aspA) Enzymes [BR:eco01000] 4. Lyases 4.3 Carbon-nitrogen lyases 4.3.1 Ammonia-lyases 4.3.1.1 aspartate ammonia-lyase b4139 (aspA)	
	BRITE hierarchy	
SSDB	Ortholog Paralog Gene cluster GFIT	
Motif	Pfam: Lyase_1 FumaraseC_C Motif	
Other DBs	NCBI-GI: 90111690 NCBI-GeneID: 948658 Pasteur: aspA EcoGene: EG10095 ECOCYC: EG10095 ASAP: ABE-0013551 UniProt: P0AC38	
Structure	PDB: 1JSW Thumbnail Jmol	
Position	complement(4366891..4368327) Genome map	
AA seq	478 aa AA seq DB search MSNNIRIEEDLLGTREVPADAYYGVHTLRAIENFYISNNKISDIPEFVRGMVMVKAAAM ANKELQTIPKSANIAAACDEVLNNNGKCMDQFPVDVYQGGAGTSVNMTNEVLANIGLE LMGHQKGEYQYLNPNDHVNKCSTNDAYPTGFRIAVYSSLIKLVDAINQLREGFERKAVE	

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

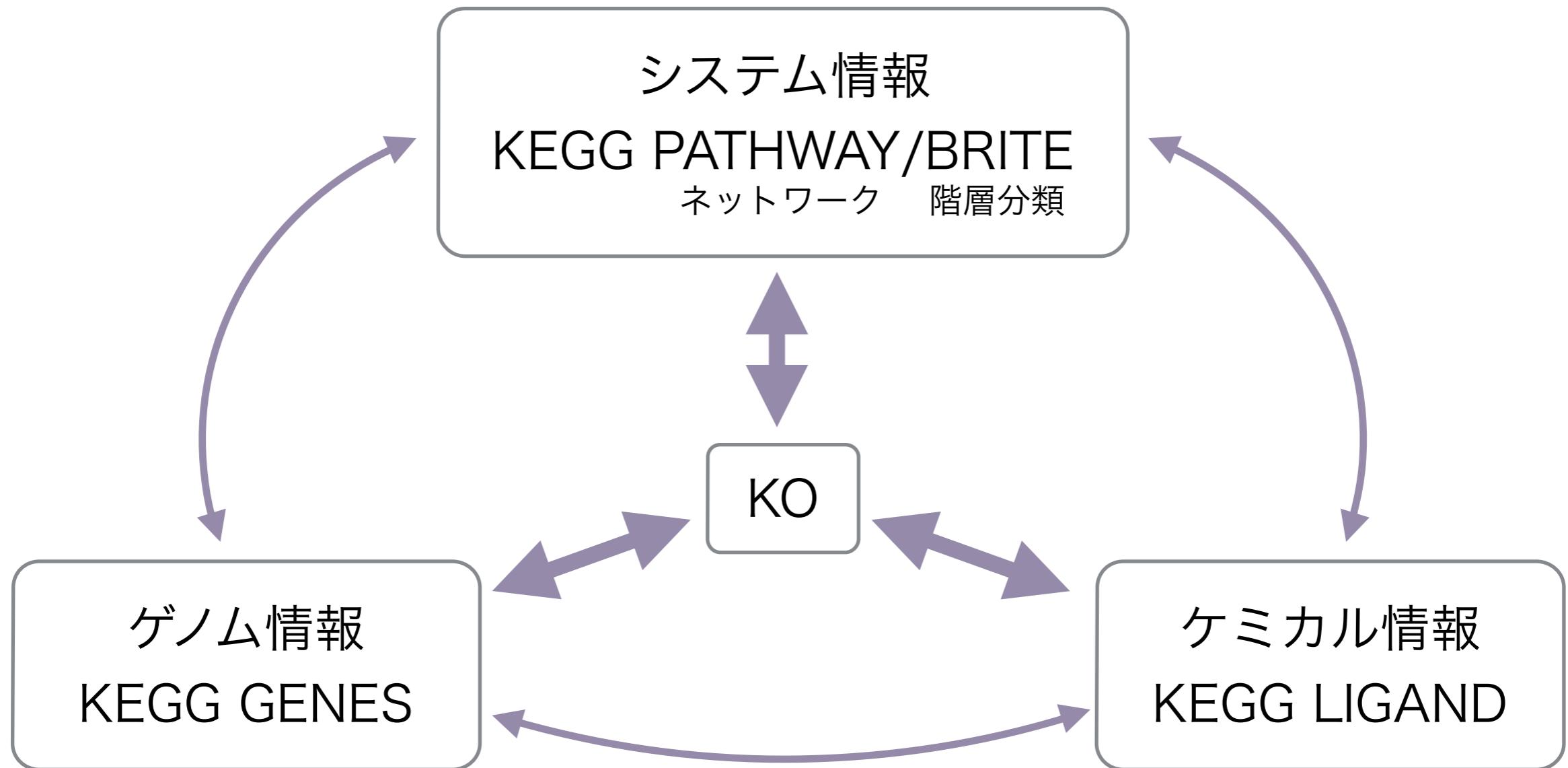
KEGG ORTHOLOGY (KO) エントリ

- 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: K01744 Help

Entry	K01744	K0
Name	aspA	
Definition	aspartate ammonia-lyase [EC:4.3.1.1]	
Pathway	ko00250 Alanine, aspartate and glutamate metabolism	
Brite	KEGG Orthology (KO) [BR:ko00001] Metabolism Amino acid metabolism 00250 Alanine, aspartate and glutamate metabolism K01744 aspA; aspartate ammonia-lyase Enzymes [BR:ko01000] 4. Lyases 4.3 Carbon-nitrogen lyases 4.3.1 Ammonia-lyases 4.3.1.1 aspartate ammonia-lyase K01744 aspA; aspartate ammonia-lyase	BRITE hierarchy
Other DBs	RN: R00490 COG: COG1027 GO: 0008797	
Genes	ECO: b4139(aspA) ECJ: Y75_p4026(aspA) ECD: ECDH10B_4332(aspA) EBW: BWG_3852(aspA) ECOK: ECMDS42_3579(aspA) ECE: Z5744(aspA) ECS: ECs5120(aspA) ECF: ECH74115_5655(aspA) ETW: ECSP_5239(aspA) ELX: CDC0157_4805(aspA) » show all	Taxonomy KOALA UniProt
Reference	PMID:3541901	
Authors	Woods SA, Miles JS, Roberts RE, Guest JR	
Title	Structural and functional relationships between fumarase and aspartase. Nucleotide sequences of the fumarase (fumC) and aspartase (aspA) genes of Escherichia coli K12.	
Journal	Biochem J 237:547-57 (1986)	

KOと各データベースとの関係



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

ゲノム情報解析ツール

GenomeNet

KEGG KEGG2 PATHWAY BRITE MEDICUS DBGET LinkDB

[English | Japanese]



Search 統合データベース

for

Go

Clear

ゲノムネット

ゲノムネットとは
お知らせ
謝辞

統合データベース

統合DBの概要
DBGETの概要
リリース情報

医薬品データベース

KEGG

varDB

研究支援データベース

計算ツール その他のツール

FTP

フィードバック

ゲノムネットデータベースリソース

ゲノムネット統合データベース

DBGET search
LinkDB search SPARQL エンドポイント *New!*

KEGG: 生命システム情報統合データベース

KEGG2 - 目次のページ
KEGG PATHWAY - システム情報: パスウェイ
KEGG BRITE - システム情報: オントロジー
KEGG Organisms - 生物種ごとの入口
KEGG GENES - ゲノム情報
KEGG LIGAND - ケミカル情報
KEGG MEDICUS - 疾患・医薬品情報

Reaction Ontology: 反応パターンと分類

varDB: 抗原変異データベース

研究支援データベース

CYORF - シアノバクテリア
BSORF - 枯草菌
EXPRESSION - 遺伝子発現プロファイル

ゲノムネット計算ツール

配列解析

BLAST / FASTA - ホモロジー検索
リボソーム RNA データベース追加 *Updated!*
MOTIF - モチーフ検索

CLUSTALW / MAFFT / PRRN - 複数アライメント

ゲノム情報解析

OC Viewer - オーソログクラスタ *Updated!*
REST サービス
KAAS - KEGG自動アノテーションサーバー
MAPLE - 代謝・生理機能評価サーバー
EGassembler - ESTコンティング作成
GENIES - 遺伝子ネットワーク予測
DINIES - 医薬品-標的のネットワーク予測

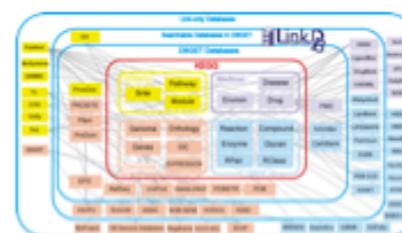
BRITE 機能階層 (日本語)

KEGG パスウェイマップ
KEGG 生物種

生物種ごとのゲノム一覧

完全 (KEGG GENES)
ドラフト (KEGG DGENES)
メタ (KEGG MGENES)
ウイルス (KEGG VGENES)
EST (EGENES)

オーソログクラスタ (OC)



データベース間のリンク



自動アノテーション
ネットワーク予測
ノード増加図

KAAS

- KEGG自動アノテーションサーバー

- 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

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

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

Query gene : KO assignment

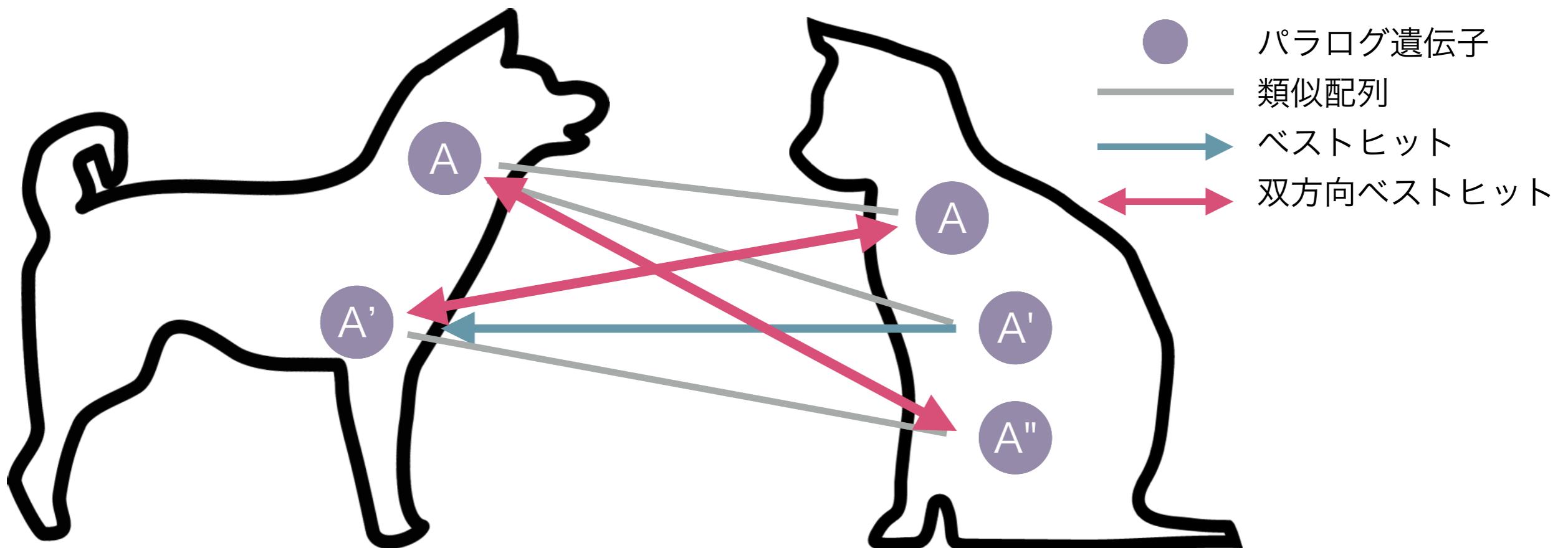
test070411

- query_0001
- query_0002 K00003
- query_0003 K00872
- query_0004 K01733
- query_0005
- query_0006
- query_0007 K03310
- query_0008 K00516
- query_0009 K03831
- query_0010 K07034
- query_0011
- query_0012
- query_0013
- query_0014 K04043
- query_0015 K03586
- 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、双向性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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for ortholog assignment and pathway mapping

Request Help

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Example of Results

KO assignment

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

Query gene : KO assignment

test070411

- query_0001
- query_0002 K00903
- query_0003 K00872
- query_0004 K01733
- query_0005
- query_0006
- query_0007 K03310
- query_0008 K00516
- query_0009 K03831
- query_0010 K07034
- query_0011
- query_0012
- query_0013
- query_0014 K04043
- query_0015 K03586
- query_0016

KEGG pathway mapping

GLYCOLYSIS

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  
MAALTRDPQFQKLQQWYREHRSENLRR  
LFDANKDRFNHFSLTLNTNHGHILVDYSKN  
>Query02
```

File upload (Nucleotide)

Query name 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) データベース側の生物種の選択

Representative set

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)

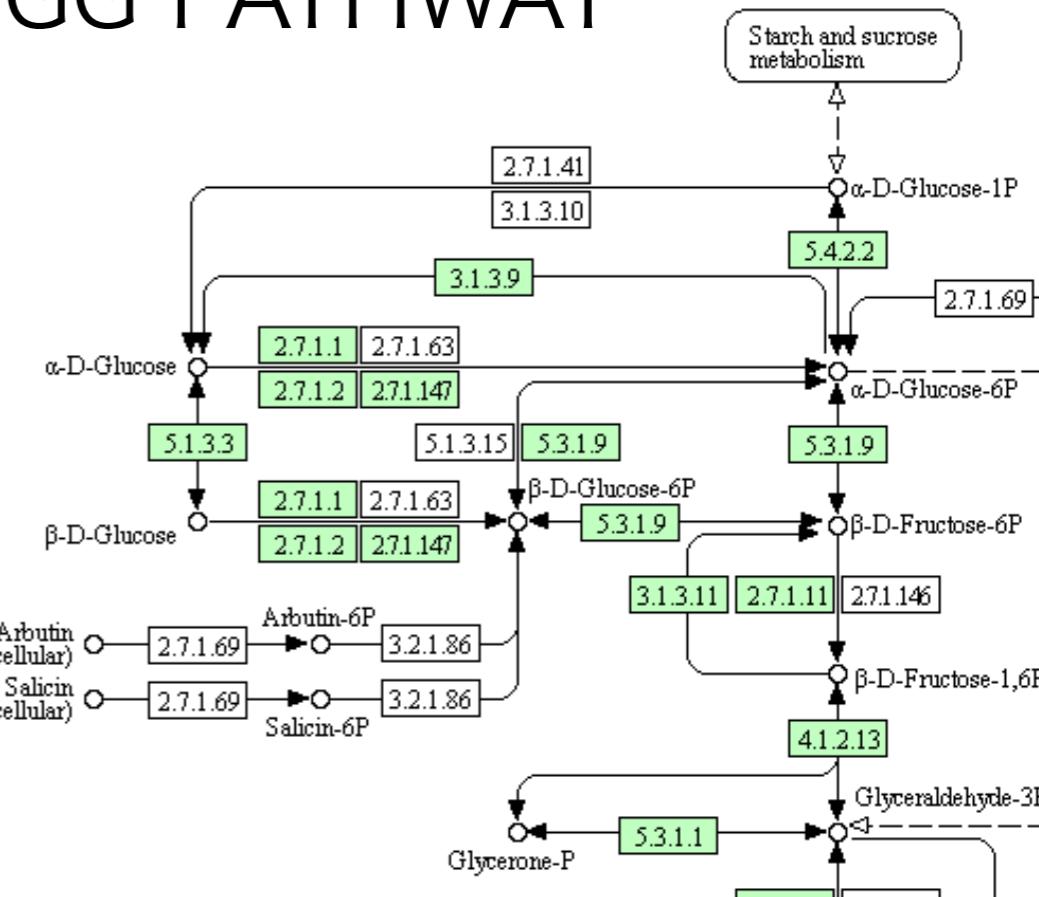
KAAS

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
マッピング

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:3.4.23.4]
- 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 E3.4.23.42; yapsin 2 [EC:3.4.23.42]

MAPLE

- 機能モジュール (KEGG Module)へのマッピング
- KAASを利用して、KOをアサイン



MAPLE - Metabolic And Physiological potential Evaluator

for gene mapping to the KEGG functional modules and calculation of module completion ratio (MCR)

Home Request

About MAPLE

Metabolic and physiological potential evaluator (MAPLE) is an automatic system for mapping genes in the individual genome and metagenome to the functional modules defined by KEGG and for calculating the module completion ratio (MCR), the percentage of a module component filled with the input genes. It first assigns KEGG Orthology (KO) to the query genes using KEGG Automatic Annotation Server (KAAS), then maps the KO-assigned genes to the KEGG functional modules, and finally calculates MCR of each functional module. The MAPLE system provides a user-friendly web interface for submitting genomic and metagenomic data and viewing the mapping pattern and MCR results.

- [MAPLE Help](#)

Metagenome or Partial Genome Sequences

KO assignment to short-read sequences (400-500nt) produced by a high throughput DNA sequencer is performed by KAAS by single-directional best hit (SBH) method. Query sequences must be translated into amino acid (aa) sequences before submission, and sequences longer than 100aa are recommended for accurate KO assignment.

- [MAPLE job request \(SBH method\)](#)

Complete or Draft Genome Sequences

KO assignment for the complete gene sets identified in the complete genome or contigs is performed by KAAS by the bi-directional best hit (BBH) method.

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

Comparison of User's Results

Comparison of MCR results and mapping patterns to each KEGG module from multiple jobs is possible. A user can compare the results between user's jobs (metagenomic samples and individual organisms), in addition to the comparison between the user's results and the KEGG annotated genomes. The comparison results are displayed side by side in parallel.

Example of Results

Mapping genes to the modules

Summary of module completion
KAAS BLAST top
100.0% 100.0%

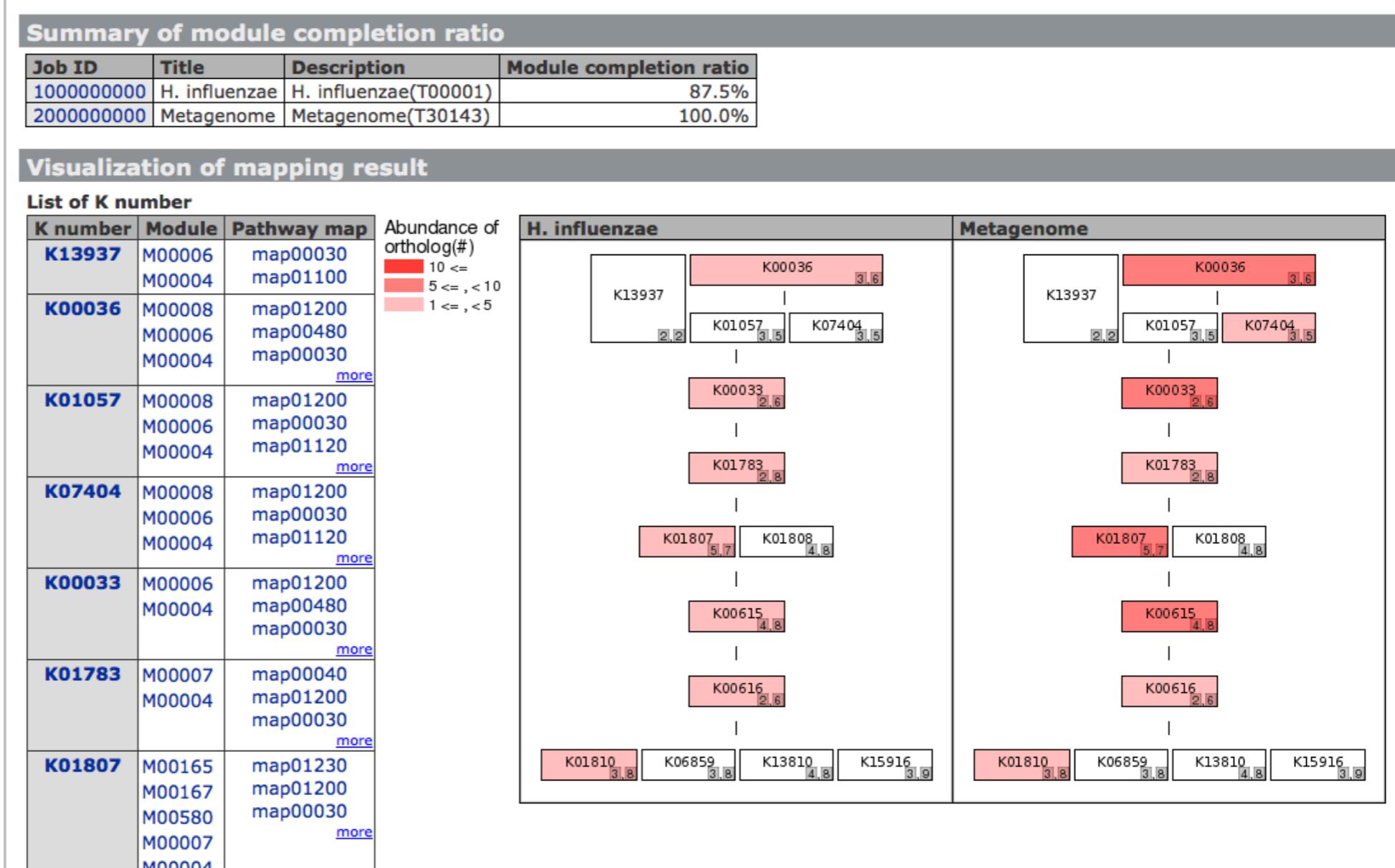
ID	Type	Pathway map
K00036	M00008 (66.7%)	map01200 map00480 map00293
K01057	M00008 (66.7%) M00006 (100.0%) M00004 (100.0%)	map01200 map00293 map01120 map00293
K00033	M00006 (100.0%) M00004 (100.0%)	map01200 map00480 map00293
K01783	M00007 (100.0%) M00004 (100.0%)	map00040 map01200 map00293 map00293
K01800	M00165 (81.8%) M00167 (75.0%) M00007 (100.0%) M00004 (100.0%)	map01200 map00030 map01110 map00293
K00615	M00165 (81.8%) M00167 (75.0%) M00007 (100.0%) M00004 (100.0%)	map01200 map00030 map01051 map00293
K00616	M00007 (100.0%) M00004 (100.0%)	map01200 map00293 map00293
K13810	M00001 (100.0%)	map00520

MCR calculation of each pathway module

ID	Type	Value
M00001	Pathway module	100.0%
M00002	Pathway module	100.0%
M00003	Pathway module	100.0%
M00004	Pathway module	100.0%
M00005	Pathway module	100.0%
M00006	Pathway module	100.0%
M00007	Pathway module	100.0%
M00008	Pathway module	100.0%
M00009	Pathway module	100.0%
M00010	Pathway module	100.0%
M00011	Pathway module	100.0%
M00012	Pathway module	100.0%
M00013	Pathway module	100.0%
M00014	Pathway module	100.0%
M00015	Pathway module	100.0%
M00016	Pathway module	100.0%
M00017	Pathway module	100.0%
M00018	Pathway module	100.0%
M00019	Pathway module	100.0%
M00020	Pathway module	100.0%
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M00080	Pathway module	100.0%
M00081	Pathway module	100.0%
M00082	Pathway module	100.0%
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M00100	Pathway module	100.0%
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M00110	Pathway module	100.0%
M00111	Pathway module	100.0%
M00112	Pathway module	100.0%
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M00167	Pathway module	100.0%
M00168	Pathway module	100.0%
M00169	Pathway module	100.0%
M00170	Pathway module	100.0%
M00171	Pathway module	100.0%
M00172	Pathway module	100.0%
M00173	Pathway module	100.0%
M00174	Pathway module	100.0%
M00175	Pathway module	100.0%
M00176	Pathway module	100.0%
M00177	Pathway module	100.0%
M00178	Pathway module	100.0%
M00179	Pathway module	100.0%
M00180	Pathway module	100.0%
M00181	Pathway module	100.0%
M00182	Pathway module	100.0%
M00183	Pathway module	100.0%
M00184	Pathway module	100.0%
M00185	Pathway module	100.0%
M00186	Pathway module	100.0%
M00187	Pathway module	100.0%
M00188	Pathway module	100.0%
M00189	Pathway module	100.0%
M00190	Pathway module	100.0%
M00191	Pathway module	100.0%
M00192	Pathway module	100.0%
M00193	Pathway module	100.0%
M00194	Pathway module	100.0%
M00195	Pathway module	100.0%
M00196	Pathway module	100.0%
M00197	Pathway module	100.0%
M00198	Pathway module	100.0%
M00199	Pathway module	100.0%
M00200	Pathway module	100.0%
M00201	Pathway module	100.0%
M00202	Pathway module	100.0%
M00203	Pathway module	100.0%
M00204	Pathway module	100.0%
M00205	Pathway module	100.0%
M00206	Pathway module	100.0%
M00207	Pathway module	100.0%
M00208	Pathway module	100.0%
M00209	Pathway module	100.0%
M00210	Pathway module	100.0%
M00211	Pathway module	100.0%
M00212	Pathway module	100.0%
M00213	Pathway module	100.0%
M00214	Pathway module	100.0%
M00215	Pathway module	100.0%
M00216	Pathway module	100.0%
M00217	Pathway module	100.0%
M00218	Pathway module	100.0%
M00219	Pathway module	100.0%
M00220	Pathway module	100.0%
M00221	Pathway module	100.0

MAPLE

- Pathwayより小さな生物学的な機能単位 (Module)
- Moduleの埋まり具合で、機能を持っているかどうかを判断できる



BlastKOALA



BlastKOALA

Query Data Input

KEGG
New service by KEGG
for genome annotation

- KAASのsingle-bestに近い
- reference databaseを絞っているため、ある程度早く、網羅的にKOをアサインできる

KOALA (KEGG Orthology And Links Annotation) is KEGG's internal annotation tool for **K number** assignment of KEGG GENES using SSEARCH computation results in KEGG SSDB (see brief description [here](#)). BlastKOALA accepts users' sequence data and assigns K numbers by the same algorithm after the BLAST search against a nonredundant set of KEGG GENES. See [Step-by-step Instructions](#)

Upload a fasta-format amino acid sequence file

Help

ファイルが選択されていません。

Your query data consisting of multiple amino acid sequences will be given K numbers by BlastKOALA.

Enter taxonomy group of your genome

Not known Prokaryotes Bacteria Archaea
 Eukaryotes Animals Plants Fungi Protists
 Taxonomy ID

Taxonomy group information is used in the scoring scheme for K number assignment. Enter NCBI taxonomy ID of your genome, if known, at the species, genus, family or any other level, which will be converted to an appropriate KEGG taxonomy group currently defined. Alternatively, just select a more generic group name shown.

Enter KEGG GENES database file to be searched

family_eukaryotes
 genus_eukaryotes
 genus_prokaryotes
 species_prokaryotes
 family_eukaryotes + genus_prokaryotes

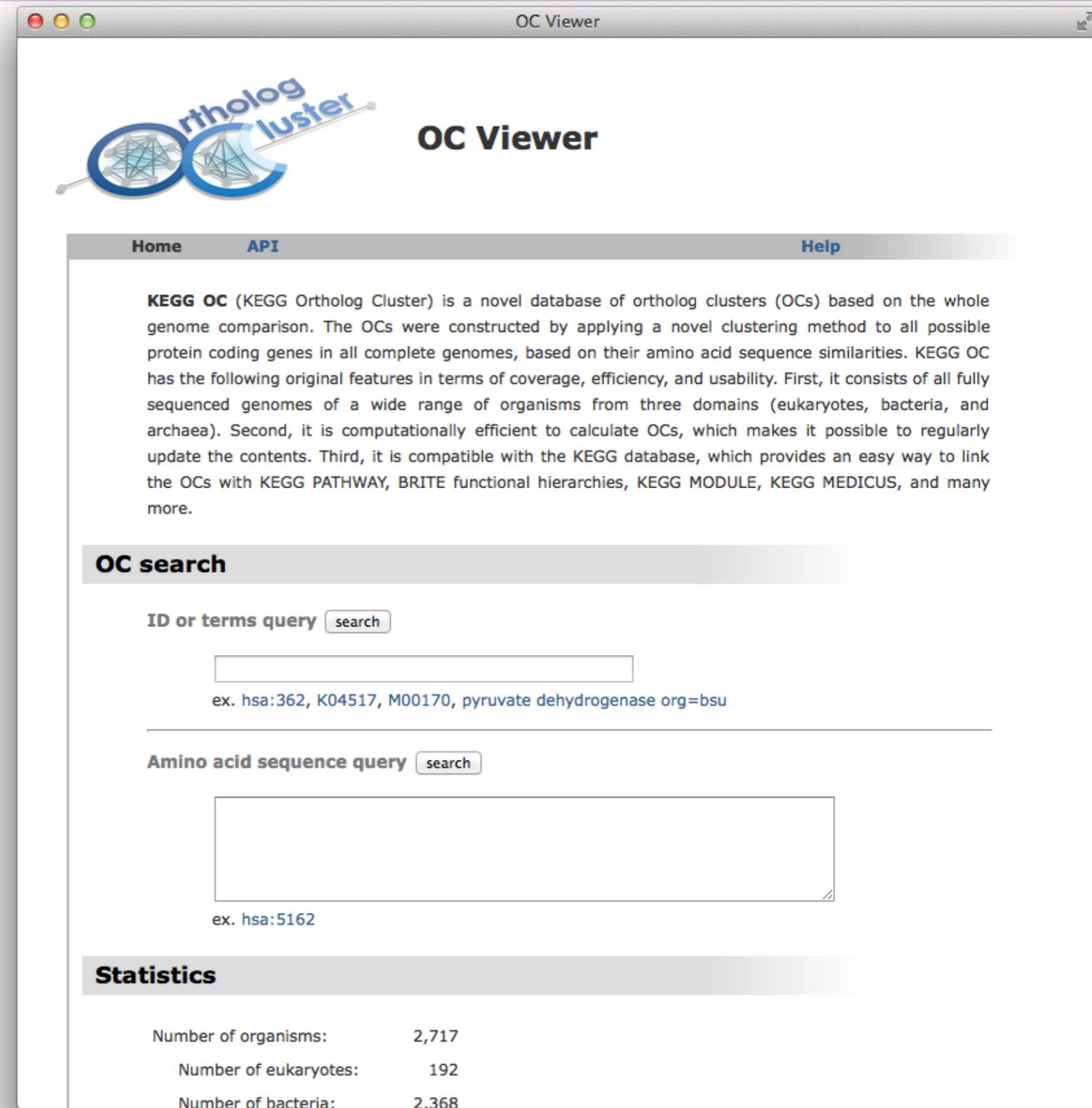
DB size (2014/11/19) and query data limit

	eukaryotes	prokaryotes
organism	4285661	-
species	4129625	-
genus	3475358	7500
family	2631384	10000
family_euk + genus_prok	5084043	5000

The database files are generated from KEGG GENES as a collection of representative genomes by

KEGG OC (Ortholog Cluster)

- KOでは文献情報を基にして、機能の判っている遺伝子の分類を行っている
- 機能の判らない遺伝子はKOを作つておらず、そういう遺伝子はまだ多い
- そこで、全遺伝子の配列類似性を基にした自動クラスタリングを行うことで、オーソロググループを推定
- 3000生物種の1270万配列



The screenshot shows the OC Viewer interface. At the top, there is a logo for "Ortholog Cluster" featuring two overlapping blue circles with a network graph inside. The title "OC Viewer" is displayed in the top right corner. Below the title, there is a navigation bar with links for "Home", "API", and "Help". The main content area contains a detailed description of the KEGG OC database, highlighting its features such as coverage, efficiency, and compatibility with other KEGG databases. Below this description, there are two search input fields: "OC search" and "Amino acid sequence query", each with a "search" button. The "OC search" field includes an example entry: "ex. hsa:362, K04517, M00170, pyruvate dehydrogenase org=bsu". The "Amino acid sequence query" field also includes an example entry: "ex. hsa:5162". At the bottom of the interface, there is a "Statistics" section providing summary data:

Number of organisms:	2,717
Number of eukaryotes:	192
Number of bacteria:	2,368

KEGG OC (Ortholog Cluster)

OC Viewer

ID or terms query **search**

OC.231838 (43 sequences)

OC Root	2nd	3rd	4th	5th	PC	Gene/Definition
OC.231838	Archaea	Euryarchaeota	Methanocaldococcus		mja.676	mja: MJ_0612 prephenate dehydrogenase (EC:1.3.1.12); K04517 prephenate dehydrogenase
OC.231838	Archaea	Euryarchaeota	Methanocaldococcus		mfe.216	mfe: Mefer_0217 prephenate dehydrogenase; K04517 prephenate dehydrogenase
OC.231838	Archaea	Euryarchaeota	Methanocaldococcus		mvu.1158	mvu: Metvu_1180 prephenate dehydrogenase; K04517 prephenate dehydrogenase
OC.231838	Archaea	Euryarchaeota	Methanocaldococcus		mfs.1548	mfs: MFS40622_1593 Prephenate dehydrogenase; K04517 prephenate dehydrogenase
OC.231838	Archaea	Euryarchaeota	Methanocaldococcus		mif.202	mif: Metin_0196 Prephenate dehydrogenase; K04517 prephenate dehydrogenase
OC.231838	Archaea	Euryarchaeota			mig.137	mig: Metig_0107 chorismate mutase; K04517 prephenate dehydrogenase [EC:1.3.1.12]; K04517 prephenate dehydrogenase
OC.231838	Archaea	Euryarchaeota	Methanococcus	Methanococcus_1550	mmp.1514	mmp: MMP1514 tyrA; prephenate dehydrogenase (EC:1.3.1.12); K04517 prephenate dehydrogenase
OC.231838	Archaea	Euryarchaeota	Methanococcus	Methanococcus_maripaludis.697	mmq.74	mmq: MmarC5_0061 prephenate dehydrogenase (EC:1.3.1.12); K04517 prephenate dehydrogenase
OC.231838	Archaea	Euryarchaeota	Methanococcus	Methanococcus_1550	mmx.1134	mmx: MmarC6_1158 prephenate dehydrogenase; K04517 prephenate dehydrogenase
OC.231838	Archaea	Euryarchaeota	Methanococcus	Methanococcus_maripaludis.697	mmz.760	mmz: MmarC7_0760 prephenate dehydrogenase (EC:1.3.1.12); K04517 prephenate dehydrogenase
OC.231838	Archaea	Euryarchaeota	Methanococcus	Methanococcus_maripaludis.697	mmd.1635	mmd: GYY_08410 prephenate dehydrogenase (EC:1.3.1.12); K04517 prephenate dehydrogenase

(plain text of OC.231838) (previous ver.)

Refinement of cluster
OC depth

KOs in cluster
K04517 (42) prephenate dehydrogenase (EC:1.3.1.12)
> Pathway search
> BRITE search

Organism selection

- Eukaryotes
- Prokaryotes
- Bacteria
- Archaea
 - Euryarchaeota
 - Methanocaldococcus
 - mja: Methanocaldococcus jannaschii
 - mfe: Methanocaldococcus fervens
 - mvu: Methanocaldococcus vulcanius
 - mfs: Methanocaldococcus sp. FS406-22
 - mif: Methanocaldococcus infernus
 - Methanoterris
 - mig: Methanoterris igneus
 - Methanococcus

Distribution of taxonomic categories

Methanococcus	Methanococcoides
Methanocaldococcus	Methanothermococcus
Methanosaeta	Methanothermus
Methanobrevibacter	Methanobacterium
Methanocella	Methanosaeta
Methanobacterium	Methanothermobacter
Methanospirillum	Methanospira
Methanobacter	Methanobacter
Methanomethylovorans	Methanobacter
Methanohalophilus	Methanobacter
Methanopyrus	Methanobacter
Methanosaliculum	Methanobacter
Methanotorris	Methanobacter

Neighbor clusters

- OC.231828-231832
- OC.231833 (16)
- OC.231834 (366)
- OC.231835 (27)
- OC.231836 (2)
- OC.231837 (1)
- OC.231838 (43)**
- OC.231839 (8)
- OC.231840 (2)
- OC.231841 (6)
- OC.231842 (1)

遺伝子リスト

階層的オーソログクラスタ

KOとの対応

系統の頻度

隣接クラスタ

ケミカル情報

化合物・反応データ

KEGG LIGAND

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	KEGG PATHWAY KEGG BRITE KEGG MODULE KEGG Mapper KEGG Atlas	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	
	KEGG DISEASE KEGG DRUG KEGG ENVIRON KEGG MEDICUS	New drug maps Update history	Human diseases Infectious diseases ATC drug classification	DISEASE DRUG ENVIRON	
		KEGG ORTHOLOGY	KEGG Orthology (KO)	ORTHOLOGY	
	Genomic information	KEGG GENES KEGG GENOME KEGG Organisms	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 EGENOME† MGENOME†
Chemical information	KEGG LIGAND KEGG COMPOUND KEGG GLYCAN KEGG REACTION 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 LIGAND

- KEGGにおける“Chem(o)-“の部分、すなわち生化学的情報全般

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

KEGG2 PATHWAY BRITE MODULE LIGAND COMPOUND GLYCAN REACTION RMODULE

Enter C/G/R/RP/RC numbers (Example) C00389 C05903 C06562 C08650 C09727 C09762

Filter Pathway mapping Brite mapping Get title Get entry Clear

Chemical Substances and Reactions

KEGG LIGAND contains our knowledge on the universe of chemical substances and reactions that are relevant to life. It is a composite database consisting of COMPOUND, GLYCAN, REACTION, RPAIR, RCLASS, and ENZYME databases, whose entries are identified by C, G, R, RP, RC, and EC numbers, derived from the IUBMB/IUPAC Enzyme Nomenclature, but the others are maintained.

サブカテゴリ

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

ID番号のIdentifierと各DBに含まれるデータの説明

化合物、糖鎖、反応に特化した入り口

ケミカル情報のキーワード、エントリ検索

- KEGG独自のIDのほか、名前、名前や組成式、質量などから検索できる

KEGG LIGAND Database

	Database	Identifier	Content	Specialized entry point
LIGAND	COMPOUND	C number	Chemical compound structures	KEGG COMPOUND
	GLYCAN	G number	Glycan structures	KEGG GLYCAN
	REACTION	R number	Biochemical reactions	KEGG REACTION
	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 generated 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

Search GLYCAN
Glycan ID example) G10596 Go Clear

Search REACTION
Reaction ID example) R00259 Go Clear

Search RPAIR
Rpair ID example) RP00010 Go Clear

Chemical Structure Search

Search similar compound structures

KEGG LIGAND

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

Name Go Clear

Search GLYCAN

Glycan ID Go

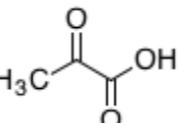
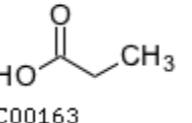
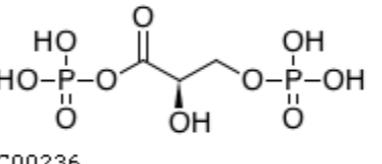
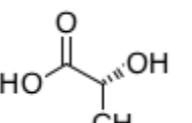
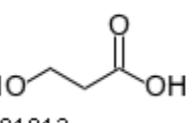
Search REACTION

Reaction ID Go

Search RPAIR

Rpair ID Go

Page : 1 Go of 2 Items : 1 - 20 of 27 Top Previous Next Bottom

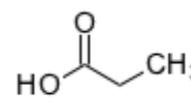
No	Entry	Structure	Name	Formula
1	C00022	 C00022	Pyruvate Pyruvic acid 2-Oxopropanoate 2-Oxo propanoic acid Pyroracemic acid	C ₃ H ₄ O ₃
2	C00163	 C00163	Propanoate Propionate Propanoic acid Propionic acid	C ₃ H ₆ O ₂
3	C00236	 C00236	3-Phospho-D-glyceroyl phosphate 1,3-Bisphospho-D-glycerate (R)-2-Hydroxy-3-(phosphonoxy)-1-monoanhydride with phosphoric propanoic acid D-Glycerate 1,3-diphosphate	C ₃ H ₈ O ₁₀ P ₂
4	C00256	 C00256	(R)-Lactate D-Lactate D-Lactic acid D-2-Hydroxy propanoic acid D-2-Hydroxypropionic acid	C ₃ H ₆ O ₃
5	C01013	 C01013	3-Hydroxypropanoate 3-Hydroxy propanoic acid 3-Hydroxypropionate 3-Hydroxypropionic acid Hydracrylic acid	C ₃ H ₆ O ₃

KEGG 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独自のKCFフォーマット

KEGG COMPOUND: C00163

COMPOUND: C00163

Entry	C00163	Compound
Name	Propanoate; Propionate; Propanoic acid; Propionic acid	
Formula	C ₃ H ₆ O ₂	
Exact mass	74.0368	
Mol weight	74.0785	
Structure	 C00163	
	Mol file KCF file DB search Jmol KegDraw	
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 4.1.3.32 2.7.2.15 6.2.1.1 2.8.3.1 6.2.1.13 3.7.1.- 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 BRITE hierarchy	
Other DBs	CAS: 79-09-4 PubChem: 3463 ChEBI: 30768	

KCFフォーマットとKEGG atom type

ENTRY	C00163	Compound			
ATOM	5	KEGG Atom Types			
	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	0999	V2000										
24.7142		24.7142		-18.7600		0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
25.9258		25.9258		-19.4624		0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
23.5027		23.5027		-19.4624		0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
24.7142		24.7142		-17.3612		0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
27.1373		27.1373		-18.7600		0.0000	C	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																		

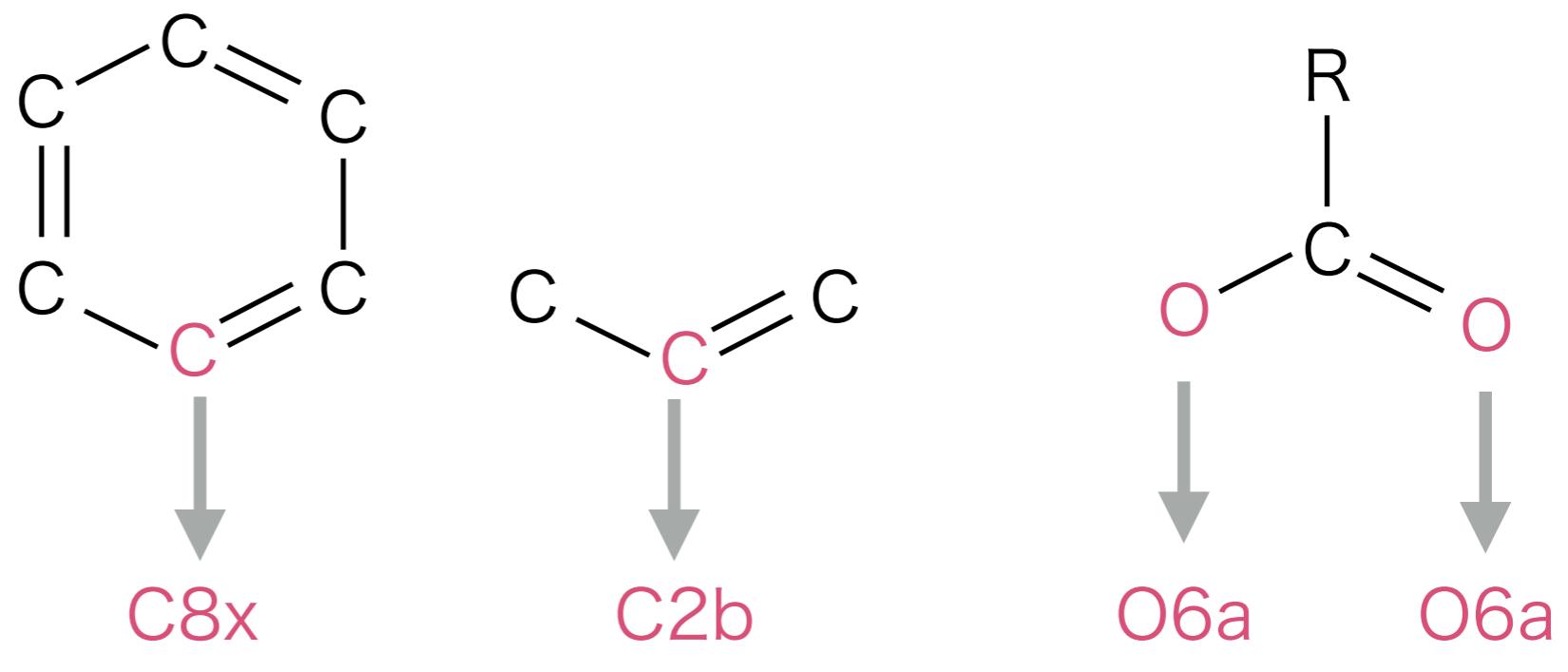
mol

KCFフォーマットとKEGG atom type

KEGG atom types

Atom	Functional group	Atom type	Description	Frequency
C	Alkane	C1a	R-CH3	16473
		C1b	R-CH2-R	20193
		C1c	R-CH(-R)-R	4964
		C1d	R-C(-R)2-R	698
	Cyclic alkane	C1x	ring-CH2-ring	14010
		C1y	ring-CH(-R)-ring	27376
		C1z	ring-C(-R)2-ring	4463
	Alkene	C2a	R=CH2	634
		C2b	R=CH-R	3965
		C2c	R=C(-R)2	1914
N	Cyclic alkene	C2x	ring-CH=ring	2964
		C2y	ring-C(-R)=ring or ring-C(=R)-ring	3722
	Alkyne	C3a	R≡CH	43
		C3b	R≡C-R	282
	Aldehyde	C4a	R-CH=O	350
	Ketone	C5a	R-C(=O)-R	3595
	Cyclic ketone	C5x	ring-C(=O)-ring	2257
	Carboxylic acid	C6a	R-C(=O)-OH	3190
	Carboxylic ester	C7a	R-C(=O)-O-R	1691
	Aromatic ring	C7x	ring-C(=O)-O-R	1691
O	Undefined C	C8x	ring-C(=O)-O-R	1691
		C8y	ring-C(=O)-O-R	1691
		C0		
	Amine	N1a	R-NH2	16473
		N1b	R-NH-R	20193
		N1c	R-N(R)2	4964
		N1d	R-N(R)(R')2	698
	Cyclic amine	N1x	ring-NH2	16473
		N1y	ring-NH-R	20193
	Imine	N2a	R-C(=O)NH2	16473
P	Cyclic imine	N2b	R-C(=O)NH-R	20193
		N2x	ring-C(=O)NH2	4964
		N2y	ring-C(=O)NH-R	698
	Cyan	N3a	R-C≡N	16473
		N4x	ring-C≡N	20193
		N4y	ring-C≡N	4964
		N5x	ring-C≡N	698
		N5y	ring-C≡N	1691
	Aromatic ring	N0		
	Undefined N	O1a	R-OH	16473
S	Hydroxy	O1b	N-OH	20193
		O1c	P-OH	4964
		150		3111

代謝化合物に多い炭素、窒素、酸素、硫黄、リンとハロゲン元素などを、結合パターン、周辺原子の種類、リング、芳香性によって68のタイプに分類



KEGG GLYCAN エントリ

- ・ G番号
 - ・ 糖鎖分子の構造を収録したデータベース
 - ・ 構造は二次元のツリーグラフとして持つ
 - ・ データ形式はKEGG独自のKCFフォーマット (Compound/Drugとの互換性はない)

GLYCAN: G10596		Help
Entry	G10596	Glycan
Composition	(GlcNAc)2 (Man)7 (PP-Dol)1	
Mass	1541.4 (PP-Dol)	
Structure	 Man _{a1} —2 Man _{a1} —3 Man _{a1} —6 Man _{b1} —4 GlcNAc _{b1} —4 GlcNAc _{a1} —PP-Dol Man _{a1} —2 Man _{a1} —2 Man _{a1} G10596	
	KCF file KCaM KegDraw	
Class	Glycoprotein; N-Glycan BRITE hierarchy	
Reaction	R06259 R06260	
Pathway	map00510 N-Glycan biosynthesis map01100 Metabolic pathways	
Module	M00055 N-glycan precursor biosynthesis	
Enzyme	2.4.1.259 2.4.1.260	
Other DBs	CCSDB: 6177 6178 6179 27485 GlycomeDB: 10116 JCGGDB: JCGG-STR000133	
LinkDB	All DBs	
KCF data	Show	

KEGG 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

Help

Entry	R01353	Reaction
Name	ATP:propanoate phosphotransferase	
Definition	ATP + Propanoate \leftrightarrow ADP + Propanoyl phosphate	
Equation	$C00002 + C00163 \leftrightarrow C00008 + C02876$	
RPair	RP00003 C00002 C00008 main RP01451 C00163 C02876 main RP06540 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 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

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

KEGG RPAIR: RP01451

KCF data																																																																														
	<input type="button" value="Hide"/>																																																																													
ALIGN	<pre> 5 1 1:C6a 6:C7a #M1 2 2:C1b 7:C1b 3 3:O6a 2:O7a #R1 4 4:O6a 8:O6a 5 5:C1a 9:C1a - * 1:P1b #D1 </pre>																																																																													
ENTRY1	<p>COMPOUND C00163</p> <p>ATOM 5</p> <table> <tbody> <tr><td>1</td><td>C6a</td><td>C</td><td>-0.2862</td><td>0.0000</td></tr> <tr><td>2</td><td>C1b</td><td>C</td><td>0.4276</td><td>-0.4138</td></tr> <tr><td>3</td><td>O6a</td><td>O</td><td>-1.0000</td><td>-0.4138</td></tr> <tr><td>4</td><td>O6a</td><td>O</td><td>-0.2862</td><td>0.8241</td></tr> <tr><td>5</td><td>C1a</td><td>C</td><td>1.1414</td><td>0.0000</td></tr> </tbody> </table> <p>BOND 4</p> <table> <tbody> <tr><td>1</td><td>1</td><td>2</td><td>1</td></tr> <tr><td>2</td><td>1</td><td>3</td><td>1</td></tr> <tr><td>3</td><td>1</td><td>4</td><td>2</td></tr> <tr><td>4</td><td>2</td><td>5</td><td>1</td></tr> </tbody> </table>	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	1	1	2	1	2	1	3	1	3	1	4	2	4	2	5	1																																				
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3	1	4	2																																																																											
4	2	5	1																																																																											
ENTRY2	<p>COMPOUND C02876</p> <p>ATOM 9</p> <table> <tbody> <tr><td>1</td><td>P1b</td><td>P</td><td>20.2552</td><td>-14.4472</td></tr> <tr><td>2</td><td>O7a</td><td>O</td><td>18.8576</td><td>-14.4535</td></tr> <tr><td>3</td><td>O1c</td><td>O</td><td>21.6530</td><td>-14.4472</td></tr> <tr><td>4</td><td>O1c</td><td>O</td><td>20.2488</td><td>-13.0428</td></tr> <tr><td>5</td><td>O1c</td><td>O</td><td>20.2552</td><td>-15.8448</td></tr> <tr><td>6</td><td>C7a</td><td>C</td><td>17.6466</td><td>-15.1557</td></tr> <tr><td>7</td><td>C1b</td><td>C</td><td>16.4292</td><td>-14.4535</td></tr> <tr><td>8</td><td>O6a</td><td>O</td><td>17.6466</td><td>-16.5533</td></tr> <tr><td>9</td><td>C1a</td><td>C</td><td>15.2182</td><td>-15.1557</td></tr> </tbody> </table> <p>BOND 8</p> <table> <tbody> <tr><td>1</td><td>1</td><td>2</td><td>1</td></tr> <tr><td>2</td><td>1</td><td>3</td><td>1</td></tr> <tr><td>3</td><td>1</td><td>4</td><td>1</td></tr> <tr><td>4</td><td>1</td><td>5</td><td>2</td></tr> <tr><td>5</td><td>2</td><td>6</td><td>1</td></tr> <tr><td>6</td><td>6</td><td>7</td><td>1</td></tr> <tr><td>7</td><td>6</td><td>8</td><td>2</td></tr> <tr><td>8</td><td>7</td><td>9</td><td>1</td></tr> </tbody> </table>	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	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
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7	6	8	2																																																																											
8	7	9	1																																																																											

アラインメント

化合物 1

化合物 2

RCLASSとRDM

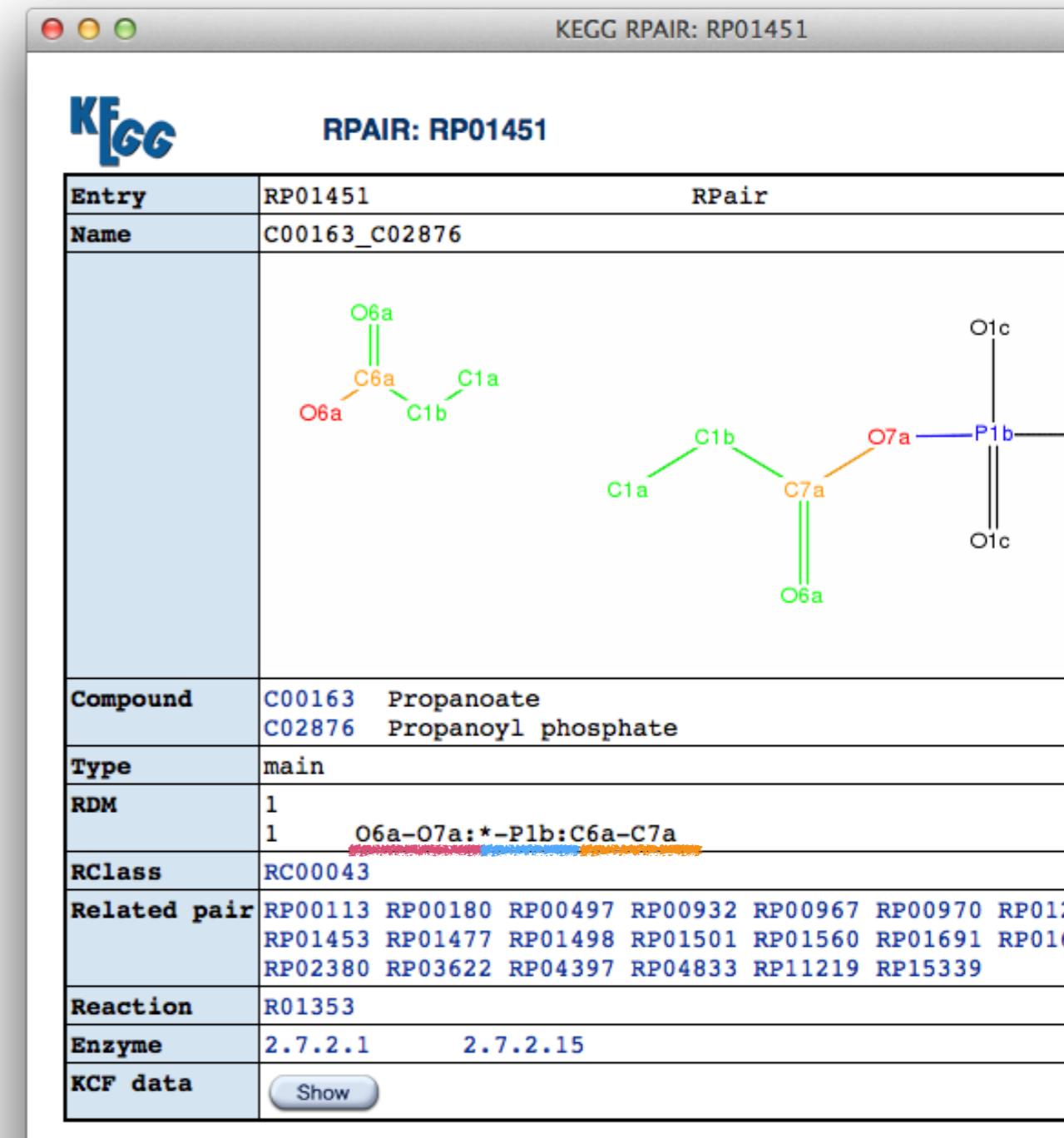
- 反応の前後の変化した部分だけを記述したものがRDMパターン
- O6a-O7a:*-P1b:C6a-C7a

- 同一のDRMパターンを持つものでRPAIRを分類したものがRCLASS

KEGG RPAIR: RP01451

RPAIR: RP01451

Entry	RP01451	RPair
Name	C00163_C02876	
Compound	C00163 Propanoate C02876 Propanoyl phosphate	
Type	main	
RDM	1 1 O6a-O7a:*-P1b:C6a-C7a	
RClass	RC00043	
Related pair	RP00113 RP00180 RP00497 RP00932 RP00967 RP00970 RP01133 RP01453 RP01477 RP01498 RP01501 RP01560 RP01691 RP01700 RP02380 RP03622 RP04397 RP04833 RP11219 RP15339	
Reaction	R01353	
Enzyme	2.7.2.1 2.7.2.15	
KCF data	Show	



KEGG 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

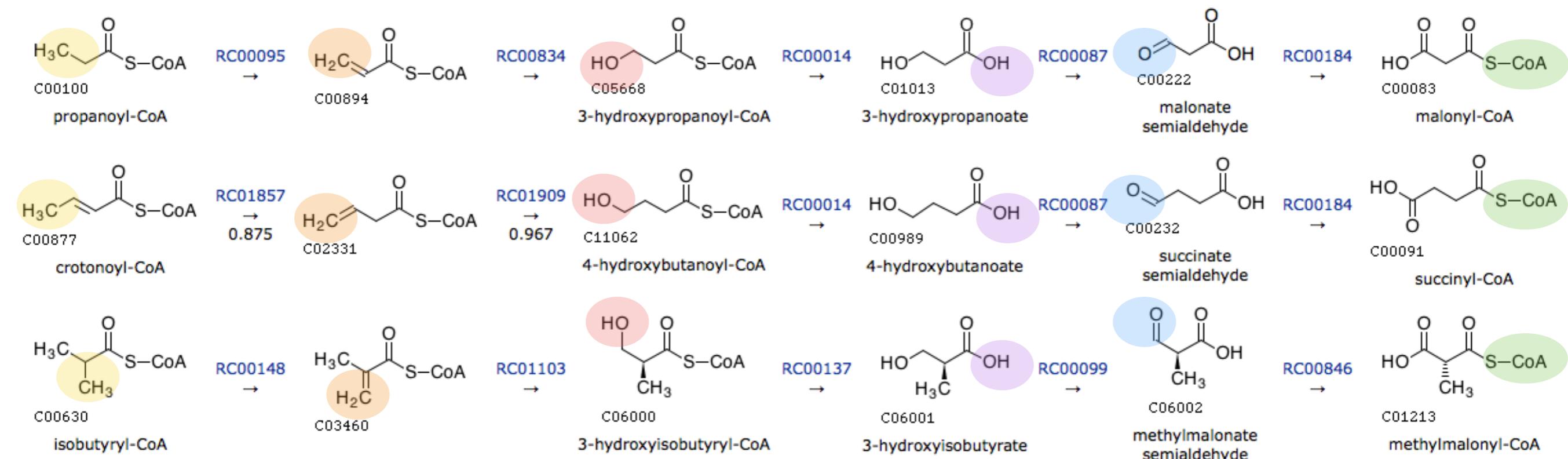
KEGG RCLASS: RC00043

RCLASS: RC00043

Entry	RC00043	RClass		
Definition	06a-O7a:*-P1b:C6a-C7a			
RPair	RP00113 RP00180 RP00497 RP00932 RP00967 RP00970 RP01282 RP01453 RP01477 RP01498 RP01501 RP01560 RP01691 RP01694 RP03622 RP04397 RP04833 RP11219 RP15339	<input type="button" value="DB search"/>		
Related class	<input type="button" value="DB search"/>			
Reaction	R00239 R00315 R00316 R00317 R00320 R00322 R00480 R00539 R00542 R01074 R01353 R01354 R01395 R01421 R01423 R01504 R01512 R01515 R01517 R01660 R01688 R01690 R02188 R02649 R03098 R03841 R04002 R07770 R08404 R08405 R08406 R08407 R09776			
Enzyme	1.2.1.31 2.7.2.2 2.7.2.8 2.7.2.14 2.7.7.58 6.2.1.1 6.3.4.10	2.7.1.61 2.7.2.3 2.7.2.10 2.7.2.15 2.7.7.63 6.2.1.11 6.3.4.11	2.7.1.106 2.7.2.4 2.7.2.11 2.7.2.- 3.6.1.7 6.2.1.17 6.3.4.15	2.7.2.1 2.7.2.7 2.7.2.12 2.7.4.17 3.6.1.20 6.3.4.9
Pathway	rn00010 Glycolysis / Gluconeogenesis rn00260 Glycine, serine and threonine metabolism rn00270 Cysteine and methionine metabolism rn00300 Lysine biosynthesis			

KEGG 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
連続反応をReaction Moduleとしてデータベースに蓄積

ケミカル情報解析ツール

お知らせ
謝辞

統合データベース
統合DBの概要
DBGETの概要
リリース情報

医薬品データベース

KEGG

varDB

研究支援データベース

計算ツール
その他のツール

FTP

フィードバック

ゲノムネット統合データベース

DBGET search
LinkDB search SPARQL エンドポイント *New!*

KEGG: 生命システム情報統合データベース

KEGG2 - 目次のページ
KEGG PATHWAY - システム情報: パスウェイ
KEGG BRITE - システム情報: オントロジー
KEGG Organisms - 生物種ごとの入口
KEGG GENES - ゲノム情報
KEGG LIGAND - ケミカル情報
KEGG MEDICUS - 疾患・医薬品情報

Reaction Ontology: 反応パターンと分類

varDB: 抗原変異データベース

研究支援データベース

CYORF - シアノバクテリア
BSORF - 枯草菌
EXPRESSION - 遺伝子発現プロファイル

ゲノムネット計算ツール

配列解析

BLAST / FASTA - ホモロジー検索
リボソーム RNA データベース追加 *Updated!*
MOTIF - モチーフ検索
CLUSTALW / MAFFT / PRRN - 複数アライメント

ゲノム情報解析

OC Viewer - オーソログクラスタ *Updated!*
REST サービス
KAAS - KEGG自動アノテーションサーバー
MAPLE - 代謝・生理機能評価サーバー
EGassembler - ESTコンティング作成
GENIES - 遺伝子ネットワーク予測
DINIES - 医薬品-標的ネットワーク予測

ケミカル情報解析

SIMCOMP / SUBCOMP - 化合物構造検索
REST サービス
KCaM - 糖鎖構造検索
PathComp - 可能な反応経路の計算
PathSearch - 類似反応経路検索
PathPred - 分解・合成反応経路予測
E-zyme - 化合物間の酵素反応予測

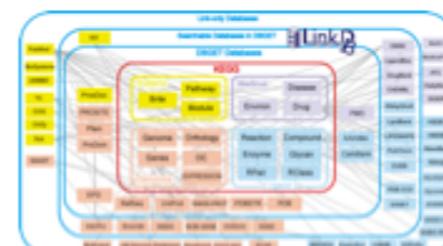
BRITE 機能階層 (日本語)

KEGG パスウェイマップ
KEGG 生物種

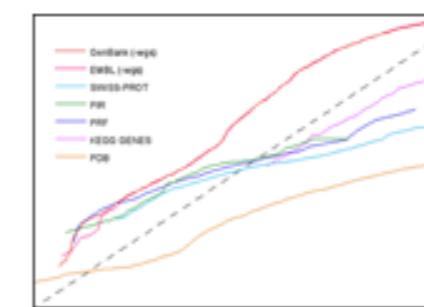
生物種ごとのゲノム一覧

完全 (KEGG GENES)
ドラフト (KEGG DGENES)
メタ (KEGG MGENES)
ウイルス (KEGG VGENES)
EST (EGENES)

オーソログクラスタ (OC)



データベース間のリンク

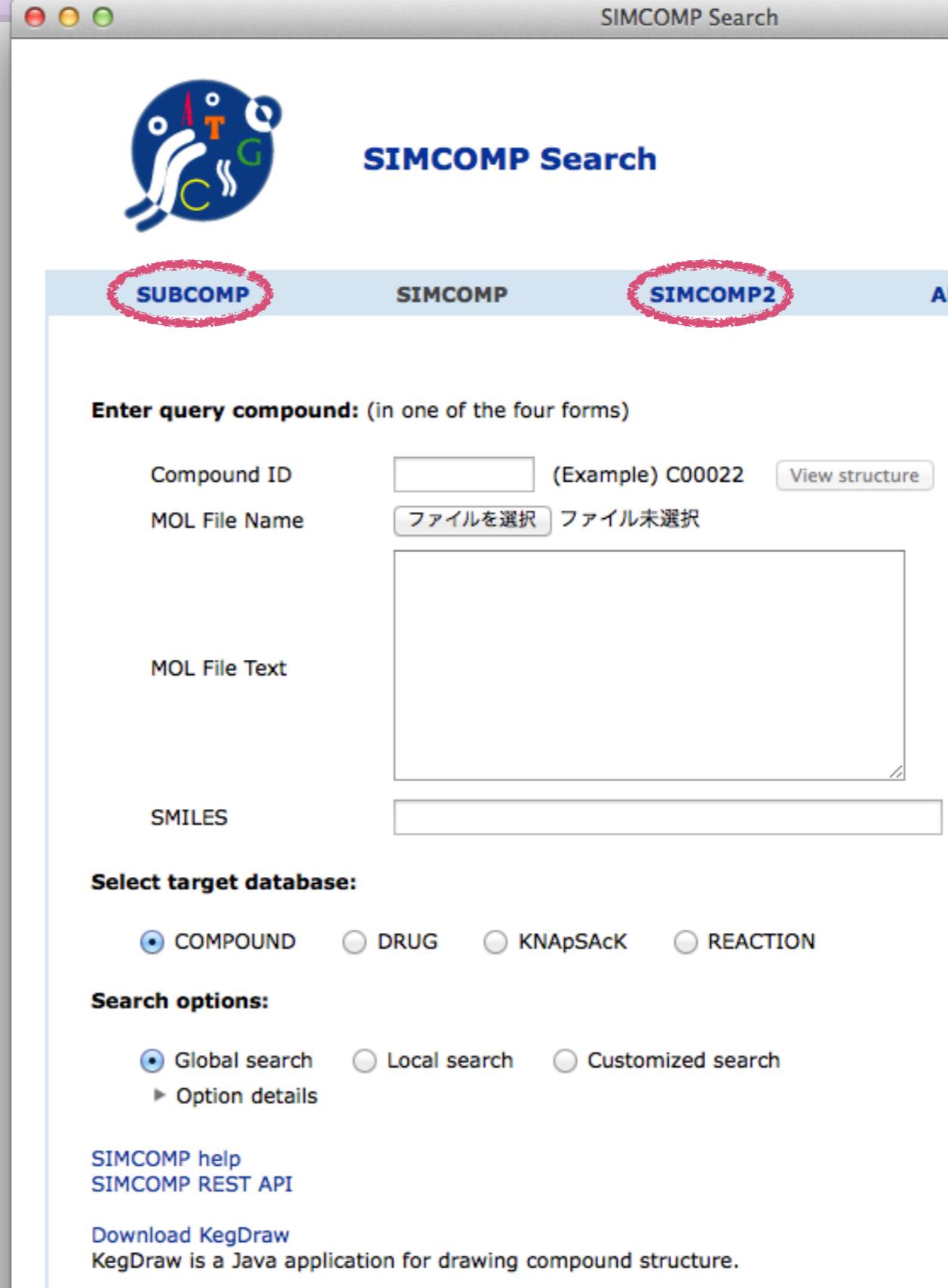


データベース増加図

化学構造比較
パスウェイ予測

SIMCOMP/SUBCOMP

- 化合物の構造類似性検索
- 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



The screenshot shows the SIMCOMP Search interface. At the top, there's a logo with letters T, G, C and the text "SIMCOMP Search". Below the logo, there's a navigation bar with tabs: "SUBCOMP" (highlighted with a red circle), "SIMCOMP", "SIMCOMP2" (highlighted with a red circle), "API", and "KEGG".

The main search area has four input fields:

- "Enter query compound: (in one of the four forms)" with sub-fields for "Compound ID" (with an example value "C00022" and a "View structure" button), "MOL File Name" (with "ファイルを選択" and "ファイル未選択" buttons), "MOL File Text" (a large text input area), and "SMILES" (a text input area).

Below these fields is a section titled "Select target database:" with radio buttons for "COMPOUND" (selected), "DRUG", "KNAPSAcK", and "REACTION".

Under "Search options:", there are three radio buttons: "Global search" (selected), "Local search", and "Customized search". There's also a link "Option details".

At the bottom, there are links for "SIMCOMP help", "SIMCOMP REST API", "Download KegDraw" (described as "KegDraw is a Java application for drawing compound structure"), and "KEGG".

オプションのGlobalは不連続なものも含めた全てのグラフマッチで、Localは連続した最大グラフマッチを行う

SIMCOMP/SUBCOMP

SIMCOMP Search

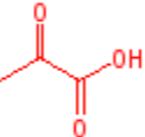
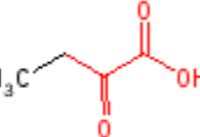
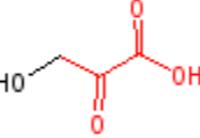
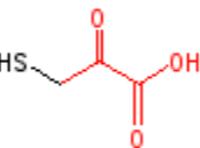
 **SIMCOMP Search Result**

Database : KEGG COMPOUND

Number of entries in a page Hide structure

Page : Go of 5 Items : 1 - 20 of 85 Top Previous Next Bottom

Top 10 Clear Select operation Exec

No	Entry	Structure	Name
<input checked="" type="checkbox"/> 1	C00022		Pyruvate Pyruvic acid 2-Oxopropanoate 2-Oxopropanoic acid Pyroracemic acid
<input checked="" type="checkbox"/> 2	C00109		2-Oxobutanoate 2-Ketobutyric acid 2-Oxobutyric acid 2-Oxobutyrate 2-Oxobutanoic acid alpha-Ketobutyric acid alpha-Ketobutyrate
<input checked="" type="checkbox"/> 3	C00168		Hydroxypyruvate Hydroxypyruvic acid 3-Hydroxypyruvate 3-Hydroxypyruvic acid
<input checked="" type="checkbox"/> 4	C00957		Mercaptopyruvate 3-Mercaptopyruvic acid 3-Mercaptopyruvate

E-zyme 2

- ・ 基質と生成物の二次元構造の情報から、代謝を担う酵素の酵素番号、酵素遺伝子を推定

www.genome.jp/tools/e-zyme2/

E-zyme 2 for prediction of enzymatic reactions

enter pair

KEGG Compound ID

MOL File Name

MOL File Text

E-zyme 2 for prediction of enzymatic reactions

alignment [KCF]

C00077

C00327

[edit alignment](#)

RDM pattern

N1a-N1b:
* -C5a:C1b-C1b

[search similar RCLASS](#)

prediction

[E-zyme 2](#) [E-zyme 1](#)

KO assignments

- select organism : in checked OCs
- select taxon : in checked OCs

types	eukaryotic	prokaryotic	both	UniProt KO

KO	score	ortholog clusters containing the KO	references
K00611	1.000	OC.20310 OC.25702 OC.20511 OC.65668 OC.22891 ...	117 OCs <input checked="" type="checkbox"/> 1 RPs
K09065	0.793	OC.197998	1 OCs <input type="checkbox"/> 1 RPs
K13043	0.706	OC.197998	1 OCs <input type="checkbox"/> 1 RPs
K12251	0.573	OC.170205 OC.170204 OC.170191 OC.170209 OC.170197 ...	45 OCs <input type="checkbox"/> 1 RPs
		OC.103146 OC.59924 OC.53035 OC.53030	77 -

システム情報

分子の相互作用ネットワーク

KEGG PATHWAY/BRITE …

- PATHWAY
 - ・ パスウェイマップDB
- BRITE
 - ・ 機能階層・オントロジーDB
- MODULE
 - ・ 機能ユニットDB
- Mapper
 - ・ PATHWAY/BRITE/MODULEへのマッピングツール
- Atlas
 - ・ KEGG global mapのViewer

 **KEGG - Table of Contents**

KEGG2 PATHWAY BRITE MODULE KO GENOME GENES LIGAND DISEASE DRUG DBGET

Search for

Category	Entry Point	Search & Compute	DBGET Search
Systems information	KEGG PATHWAY KEGG BRITE KEGG MODULE KEGG Mapper KEGG Atlas	Search Pathway Search Brite Reconstruct Module Map Taxonomy	PATHWAY BRITE MODULE
Genomic information	KEGG ORTHOLOGY KEGG Annotation	BlastKOALA <i>New!</i> KO system	ORTHOLOGY
	KEGG GENOME KEGG GENES KEGG Organisms [Species Genus]	SSDB search OC viewer† BLAST† / FASTA† KAAS†	GENOME GENES DGENES MGENOME† MGENEST†
Chemical information	KEGG LIGAND KEGG COMPOUND KEGG GLYCAN KEGG REACTION Reaction Modules	SIMCOMP† / SUBCOMP† KCaMt PathSearch† PathCompt† PathPred† E-zyme†	COMPOUND GLYCAN REACTION RPAIR RCLASS ENZYME
Health information	KEGG DISEASE KEGG DRUG KEGG ENVIRON KEGG MEDICUS	MEDICUS search Drug interaction checker Human diseases Infectious diseases ATC drug classification	DISEASE DRUG DGROUP ENVIRON

KEGG is developed by Kanehisa Laboratories. See [Kanehisa et al. \(2014\)](#) for updates of KEGG.
† Developed and maintained by Kyoto University Bioinformatics Center as part of its GenomeNet service.

KEGG PATHWAY

- 生体内（外）の分子間ネットワーク図
- 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

Pathway Maps

KEGG PATHWAY is a collection of manually drawn pathway maps representing our knowledge on 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:

7. Drug Development

Pathway Mapping

KEGG PATHWAY mapping is the process to map molecular datasets, especially large-scale datasets from 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

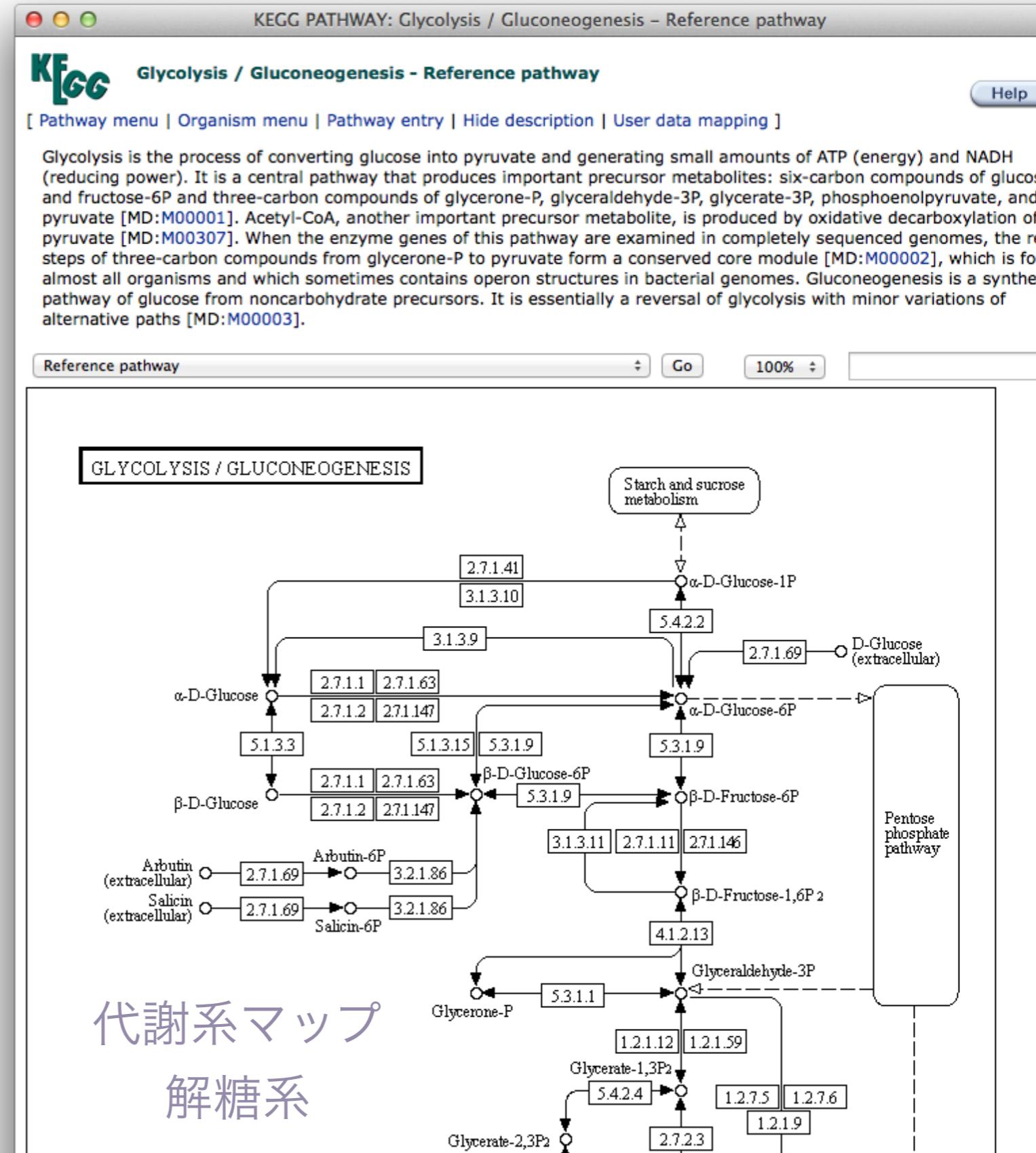
Metabolic pathways	[KEGG Atlas]	KEGG modules
Biosynthesis of secondary metabolites	[KEGG Atlas]	KEGG reaction modules
Microbial metabolism in diverse environments	[KEGG Atlas]	
Carbon metabolism	[KEGG Atlas]	
2-Oxocarboxylic acid metabolism	[KEGG Atlas]	
Fatty acid metabolism	[KEGG Atlas]	
Biosynthesis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

1.1 Carbohydrate metabolism

Glycolysis / Gluconeogenesis	Enzymes
Citrate cycle (TCA cycle)	Compounds with biological roles
Pentose phosphate pathway	
Pentose and glucuronate interconversions	

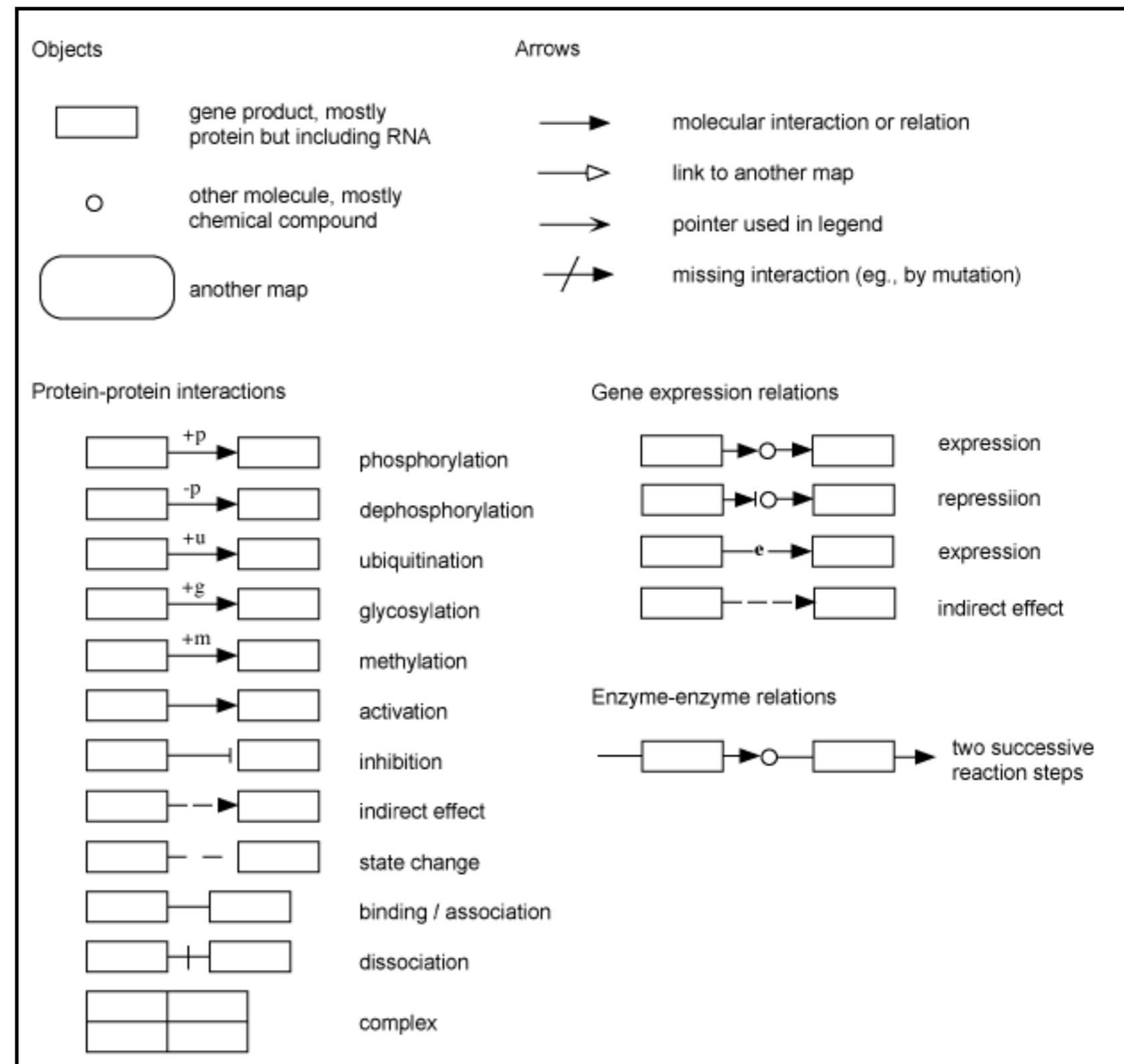
KEGG PATHWAY

- 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



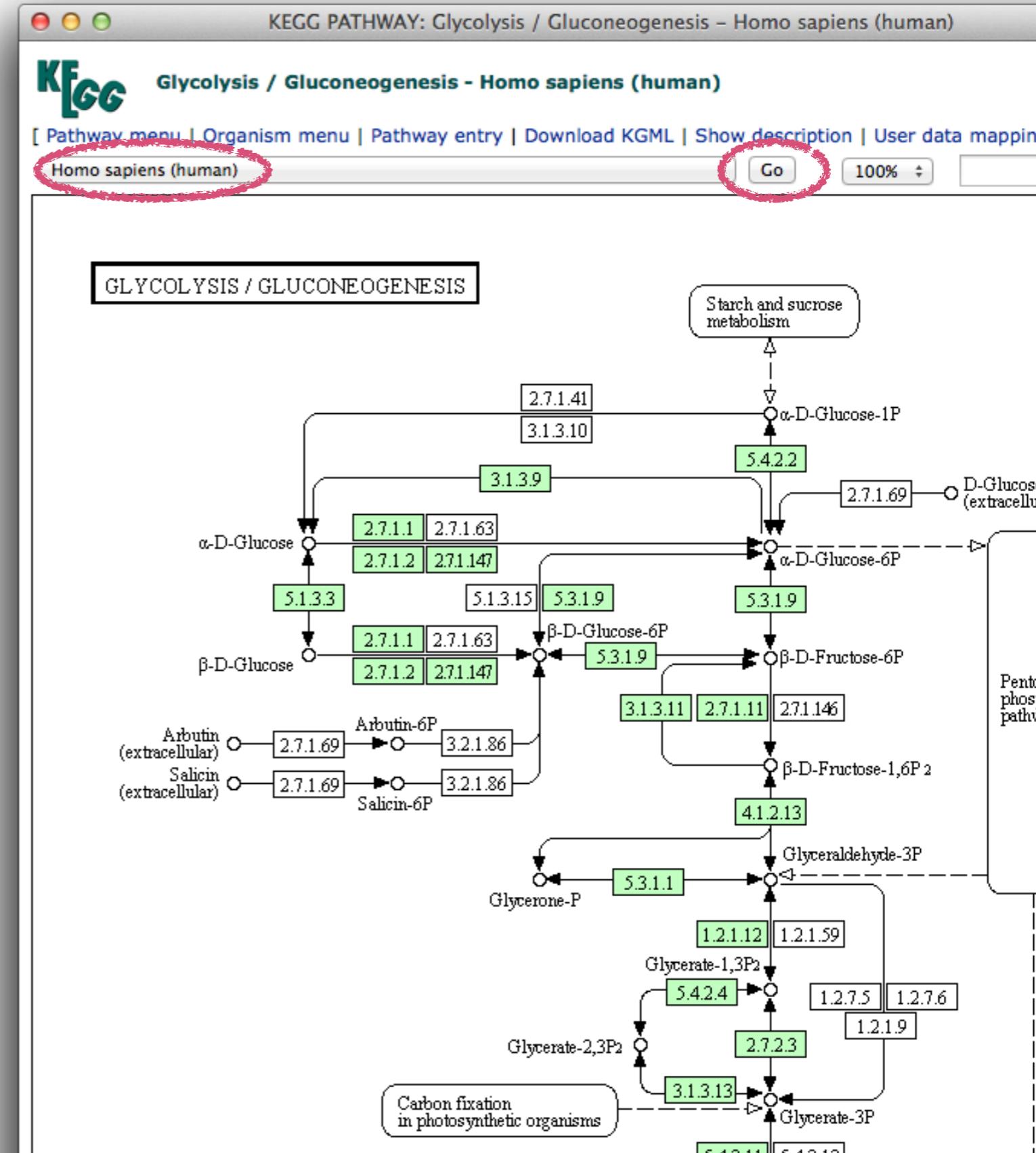
KEGG PATHWAY

- 矢印には代謝反応、リン酸化、脱リン酸化、キチン化、活性化、抑制など様々なタイプ、意味がある
- リヌビ

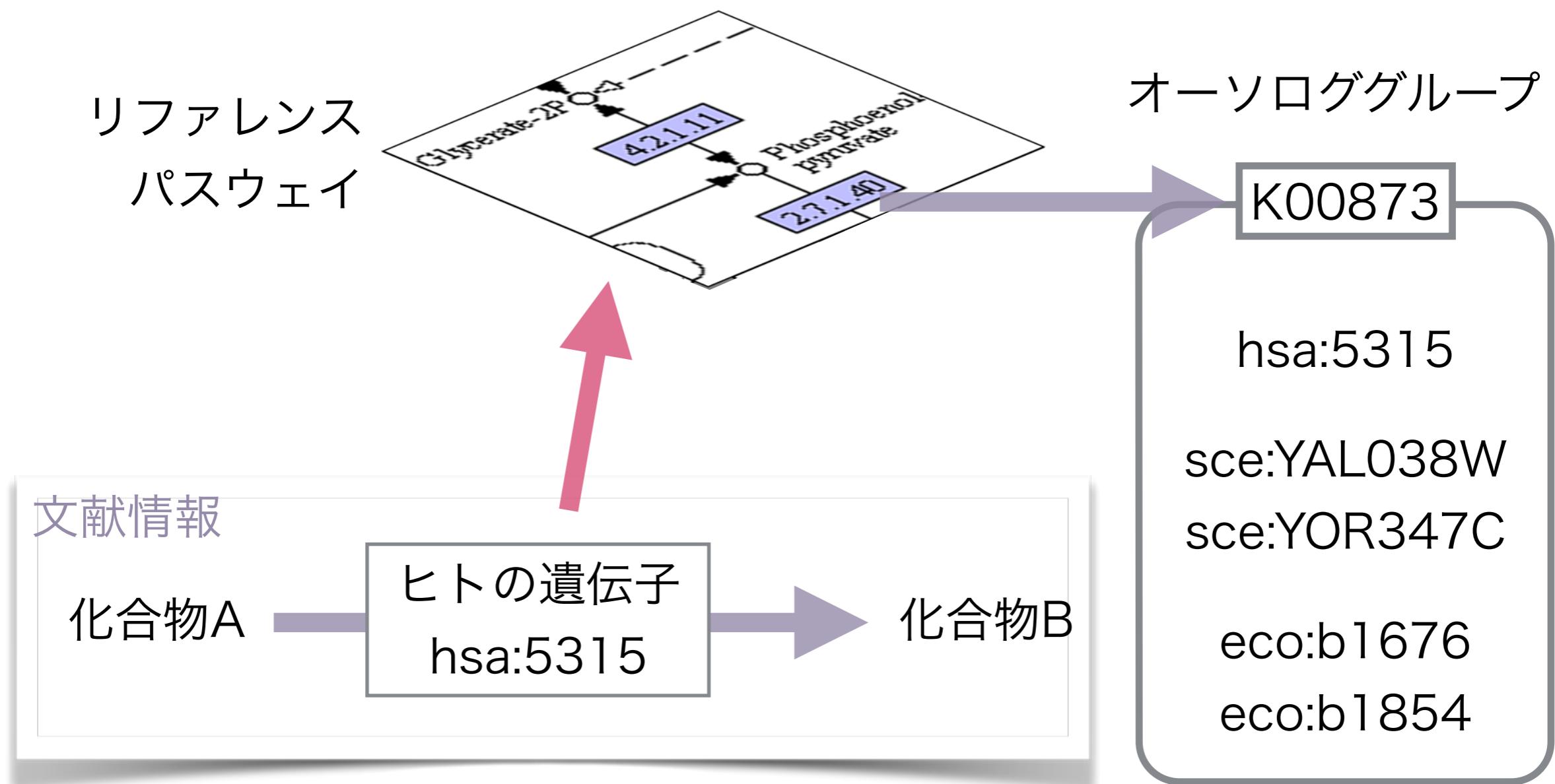


KEGG PATHWAY

- Reference Pathway (KO)
 - 対応するオーソログ(KO)エントリのある箱に色付け
- Reference Pathway (EC)
 - 対応する酵素(ENZYME)エントリのある箱に色付け
- Reference Pathway (Reaction)
 - 対応する反応(REACTION)エントリのある箱に色付け
- 生物種名
 - 遺伝子と対応するKOのある箱に色付け

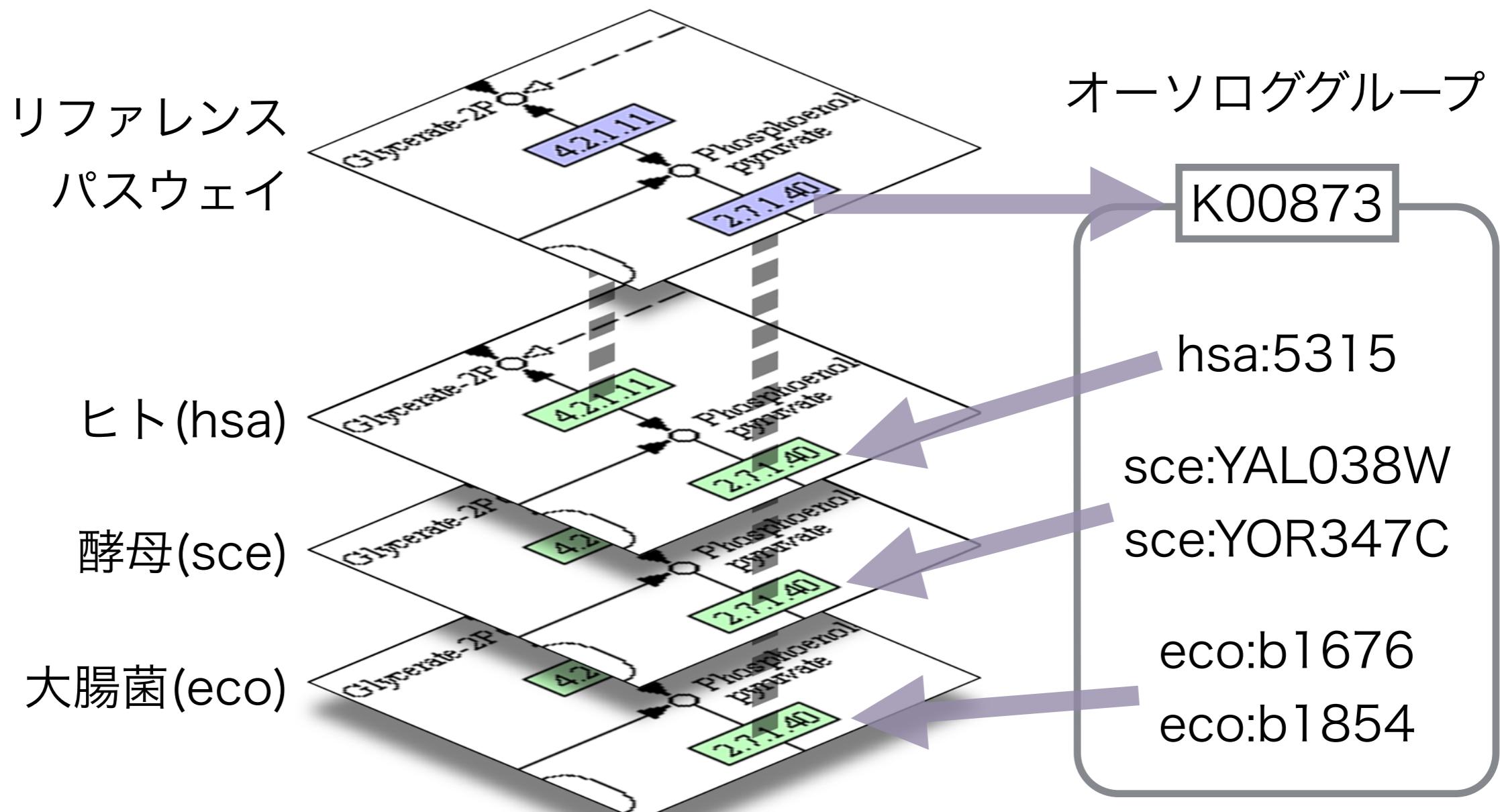


KEGG PATHWAY



文献情報からリファレンスパスウェイが作成される

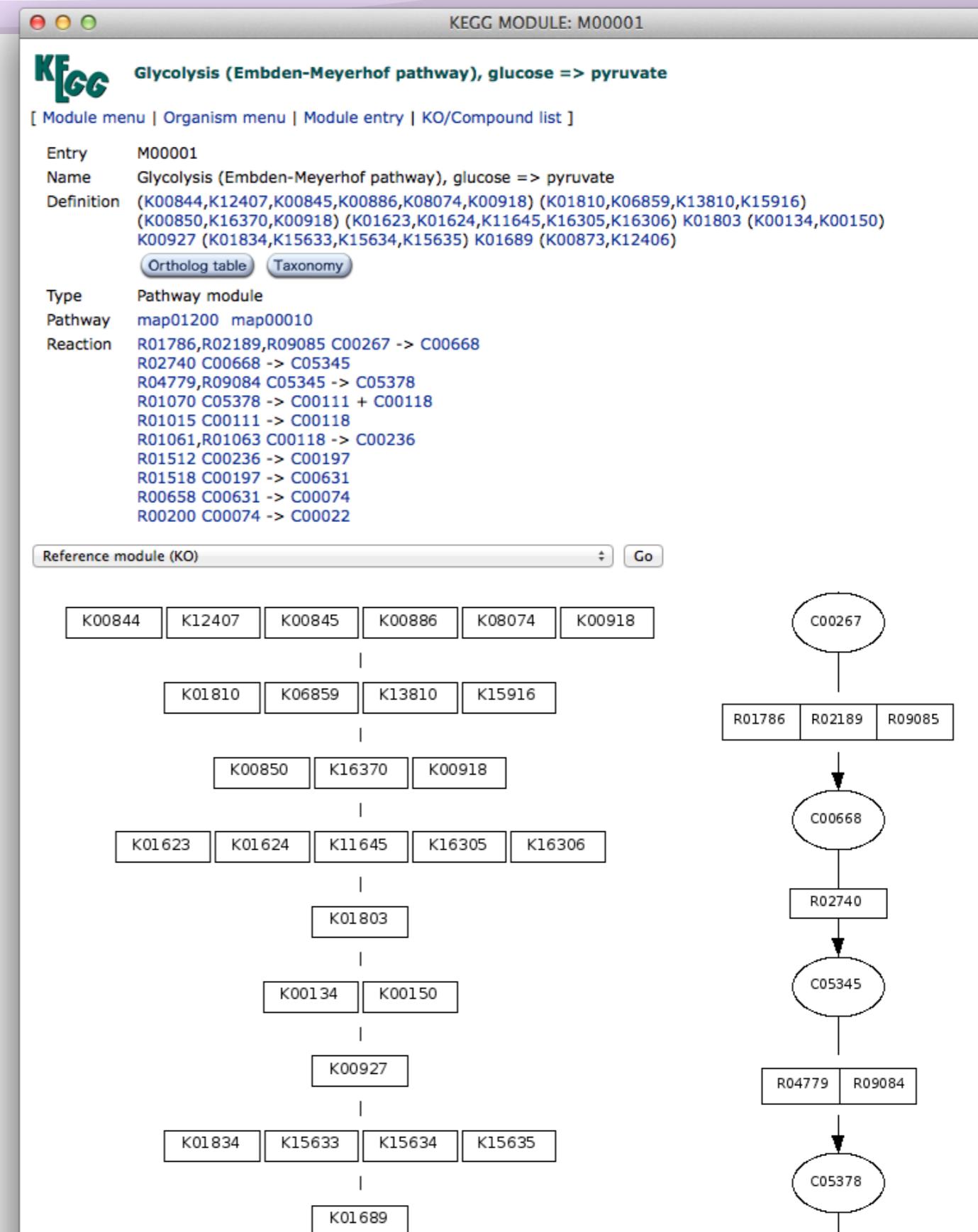
KEGG PATHWAY



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

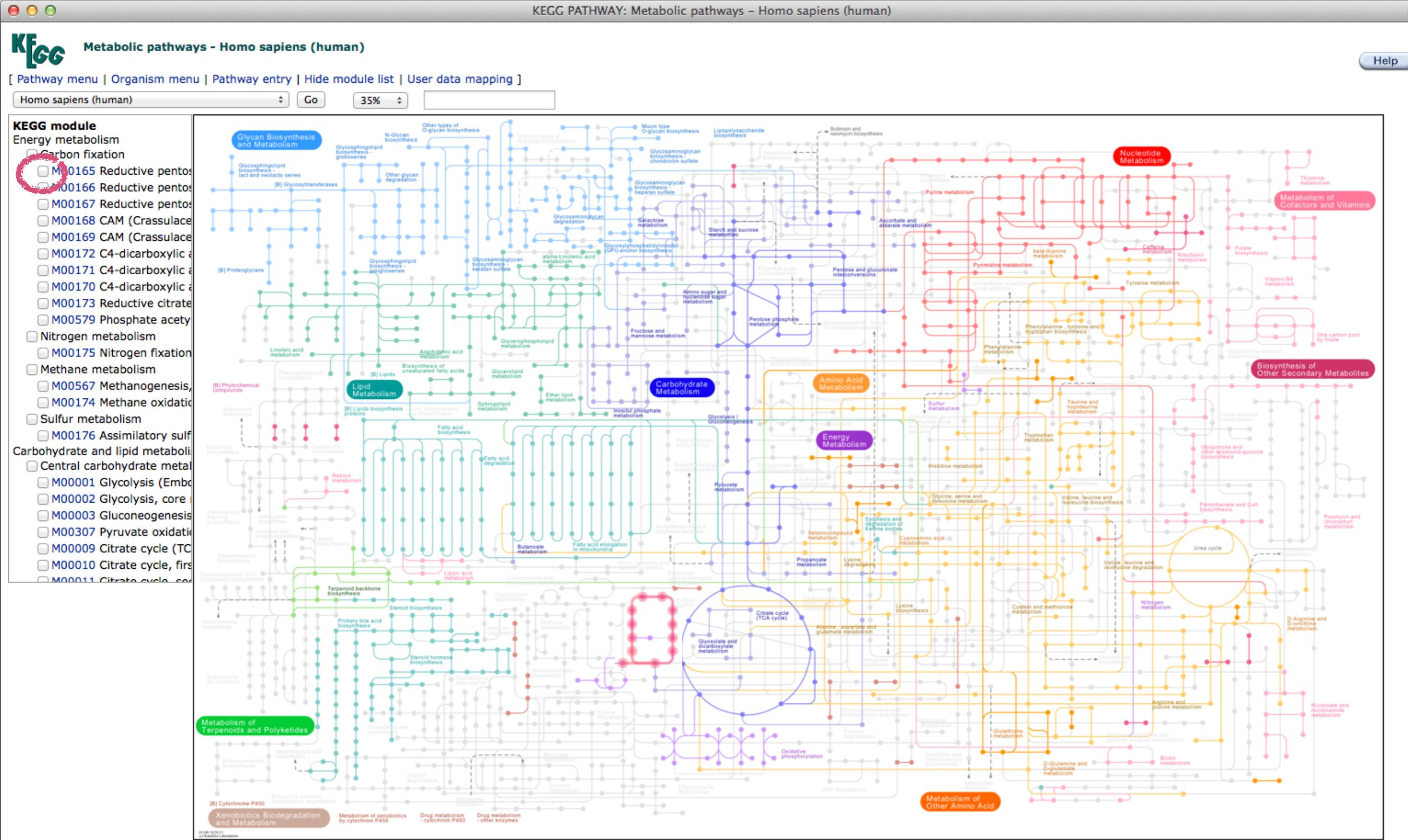
KEGG MODULE

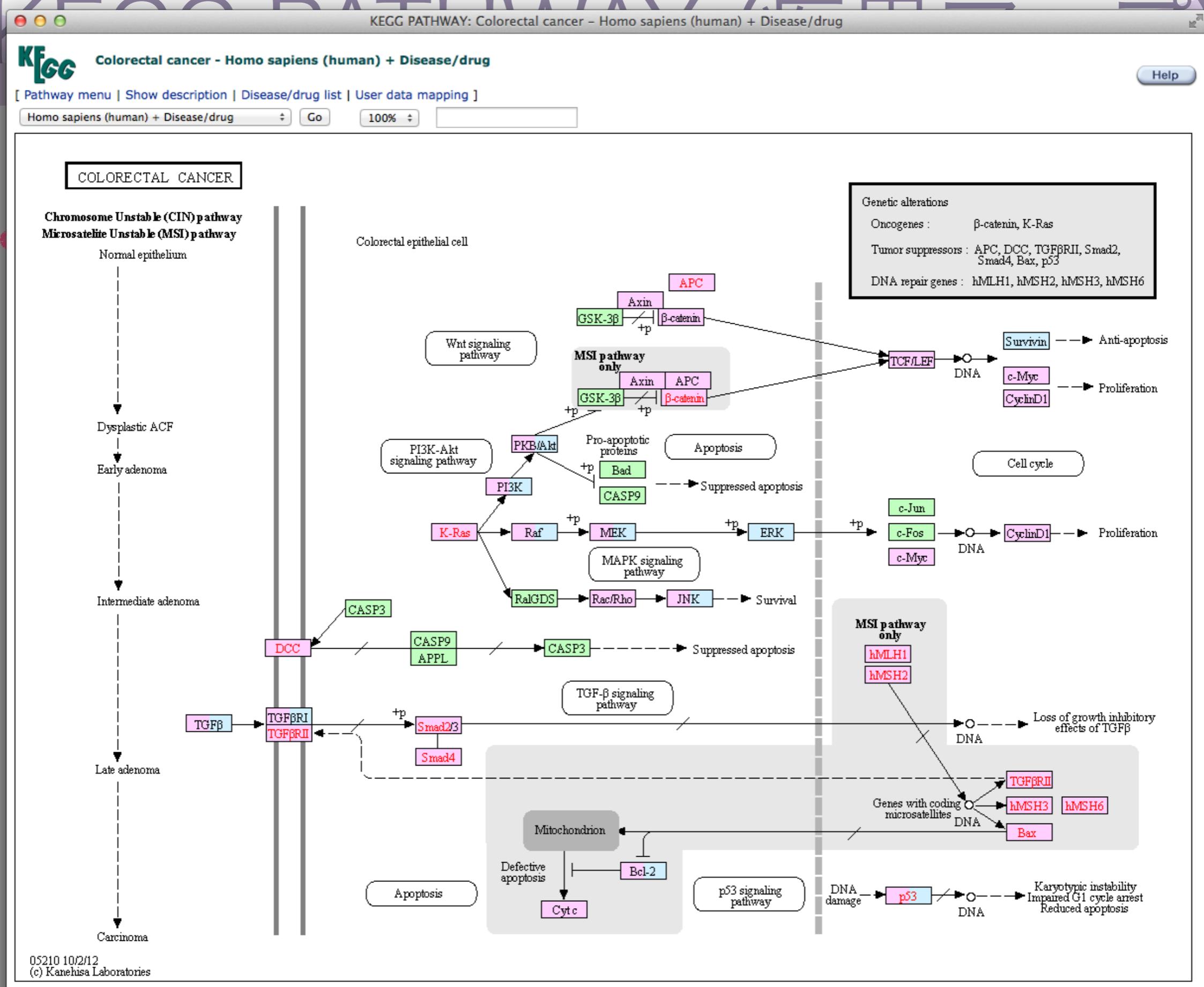
- M番号
- PATHWAYマップより小さい単位
- 生物種間での保存度合い、複合体の形成、オペロンなどを考慮した機能単位
- オーソロググループ (KO) の組み合わせで表現



KEGG global map

KEGG PATHWAY: Metabolic pathways – Homo sapiens (human)



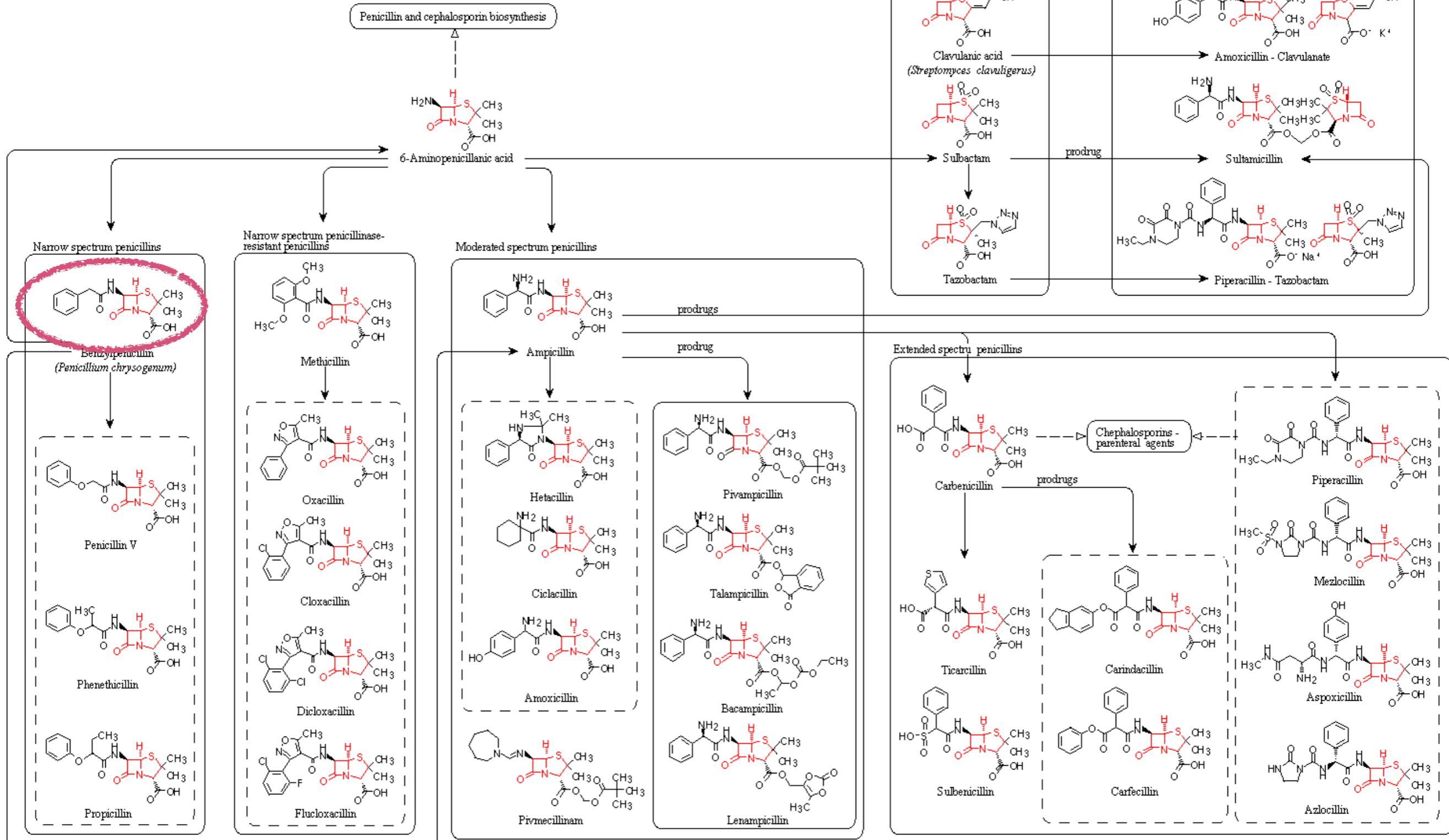


KEGG PATHWAY (薬の開発)

KEGG PATHWAY Database

PENICILLINS

ペニシリン系抗生物質



KEGG Mapper

- ・キーワード検索
 - ・Entry, Name, Description及びマップ内のオブジェクト（遺伝子、オーソログ、反応、化合物など）に対しキーワード検索
- ・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

The screenshot shows the KEGG PATHWAY Database homepage. At the top, there's a logo for "Kyoto Encyclopedia of Genes and Genomes" and the text "KEGG PATHWAY Database". Below that, a banner says "Wiring diagrams of molecular interactions, reactions, and relations". A navigation bar at the top has tabs: KEGG2, PATHWAY, BRITE, MODULE, DISEASE, DRUG, KO, GENOME, GENES, LIGAND, and DBG. Below the navigation bar is a search interface with fields for "Select prefix" (with options "map" and "Organism") and "Enter keywords", a "Go" button, and a "Help" link. A red box highlights this search area. The main content area is titled "Pathway Maps" and contains text about KEGG PATHWAY being a collection of manually drawn pathway maps representing knowledge on molecular interaction and reaction networks. It lists categories: 1. Metabolism, 2. Genetic Information Processing, 3. Environmental Information Processing, 4. Cellular Processes, 5. Organismal Systems, 6. Human Diseases, and 7. Drug Development. It also mentions KEGG drug structure maps. Another red box highlights the "Pathway Mapping" section. This section describes the process of mapping molecular datasets to KEGG pathway maps for biological interpretation. It lists three tools: Search Pathway (basic), Search&Color Pathway (advanced), and Color Pathway (selected pathway map coloring tool). A third red box highlights the "1. Metabolism" section, which provides links to various metabolic pathway atlases. At the bottom right, there are links for KEGG modules and KEGG reaction modules.

KEGG PATHWAY Database

Kyoto Encyclopedia of Genes and Genomes

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

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:

7. Drug Development

Pathway Mapping

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]	

Search & Color Pathway

KEGG PATHWAY: Glycolysis / Gluconeogenesis

Search PATHWAY KEGG PATHWAY: Glycolysis / Gluconeogenesis

Glycolysis / Gluconeogenesis

[Pathway menu | Organism menu | Pathway entry | Download KGML | Show description | User data mapping]

Reference pathway (KO) Go 100%

Pathway Search Result

Sort by the pathway list

Show all objects

- ko01200 Carbon metabolism
- ko00562 Inositol phosphate
- ko00010 Glycolysis / Gluconeogenesis
- ko00051 Fructose and mannose metabolism
- ko01100 Metabolic pathways
- ko00710 Carbon fixation in photosynthetic organisms
- ko01230 Biosynthesis of amino acids
- ko01110 Biosynthesis of secondary metabolites
- ko01120 Microbial metabolism in diverse environments
- ko00900 Terpenoid backbone biosynthesis
- ko00730 Thiamine metabolism
- ko00052 Galactose metabolism
- ko00030 Pentose phosphate pathway
- ko00750 Vitamin B6 metabolism
- ko00331 Clavulanic acid biosynthesis
- ko00680 Methane metabolism

GLYCOLYSIS / GLUCONEOGENESIS

The diagram illustrates the Glycolysis / Gluconeogenesis pathway. Key components include:

- Metabolites:** α-D-Glucose, β-D-Glucose, α-D-Glucose-1P, α-D-Glucose-6P, β-D-Glucose-6P, β-D-Fructose-6P, β-D-Fructose-1,6P₂, Glyceraldehyde-3P, Glycerone-P, Glycerate-1,3P₂, Glycerate-2,3P₂, Glycerate-3P.
- Enzymes:** 2.7.1.41, 3.1.3.10, 5.4.2.2, 2.7.1.69, 3.1.3.9, 2.7.1.1, 2.7.1.63, 2.7.1.2, 27.1.147, 5.1.3.3, 5.1.3.15, 5.3.1.9, 3.1.3.11, 2.7.1.11, 27.1.146, 4.1.2.13, 5.3.1.1, 1.2.1.12, 1.2.1.59, 5.4.2.4, 1.2.7.5, 1.2.7.6, 2.7.2.3, 3.1.3.13, 5.4.2.11, 5.4.2.12.
- Pathways connected:** Starch and sucrose metabolism, Pentose phosphate pathway, Carbon fixation in photosynthetic organisms.

A red circle highlights the enzyme **5.3.1.1**.

Search &Color Pathway

- ・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 and UniProt IDs may be used for organism-specific pathways

Enter object ID by bgcolor, fgcolor:

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

474487 #f0e68c,red

Alternatively, enter the file name containing the data:

ファイル未選択

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)

00140 Steroid hormone biosynthesis
00561 Glycerolipid metabolism
00564 Glycerophospholipid metabolism
00565 Ether lipid metabolism
00600 Sphingolipid metabolism
00590 Arachidonic acid metabolism
00591 Linoleic acid metabolism
00592 alpha-Linolenic acid metabolism
01040 Biosynthesis of unsaturated fatty acids

Nucleotide metabolism

00230 Purine metabolism
00240 Pyrimidine metabolism

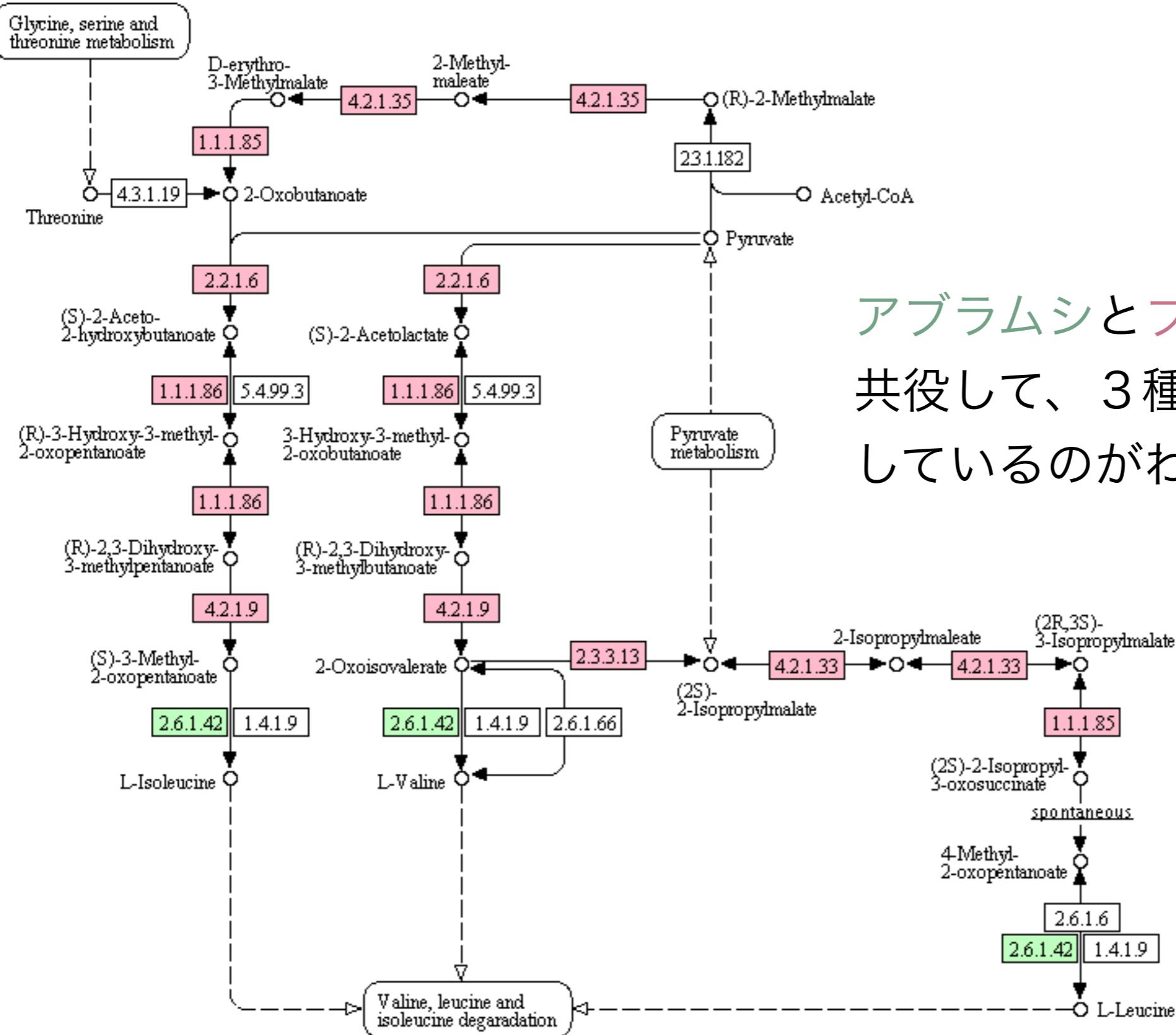
Amino acid metabolism

00250 Alanine, aspartate and glutamate metabolism
00260 Glycine, serine and threonine metabolism
00270 Cysteine and methionine metabolism
00280 Valine, leucine and isoleucine degradation
00290 Valine, leucine and isoleucine biosynthesis
00300 Lysine biosynthesis
00310 Lysine degradation
00330 Arginine and proline metabolism
00340 Histidine metabolism
00350 Tyrosine metabolism
00360 Phenylalanine metabolism
00380 Tryptophan metabolism
00400 Phenylalanine, tyrosine and tryptophan biosynthesis

Metabolism of other amino acids

00410 beta-Alanine metabolism
00430 Taurine and hypotaurine metabolism
00440 Phosphonate and phosphinate metabolism
00450 Selenocompound metabolism
00460 Cyanoamino acid metabolism

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

- ・ 共生関係
- ・ 寄生関係
- ・ ヒトと腸内細菌叢の
関係

Reconstruct Pathway

- ・自分のデータでの複数の生物種のマッピング

データ形式

```
# organism1
gene1    K02874
gene4    K00416
gene7    K12864
gene10   K03695
gene11   K11836
gene12 ...
# organism2
gene2798 K11649
gene2799 K12816
gene2800 ...
# organism3
gene5398 K03627
gene5399 K02893
gene5400 ...
```

KEGG Mapper – Reconstruct Pathway

About KEGG Mapper

[Search Pathway](#)
[Search&Color Pathway](#)
[Color Pathway](#)
[Color Pathway WebGL](#)

[Search Brite](#)
[Search&Color Brite](#)
[Join Brite](#)

[Search Module](#)
[Search&Color Module](#)

[Reconstruct Pathway](#)
[Reconstruct Brite](#)
[Reconstruct Module](#)
[Map Taxonomy](#)

Enter gene list with KO annotation:

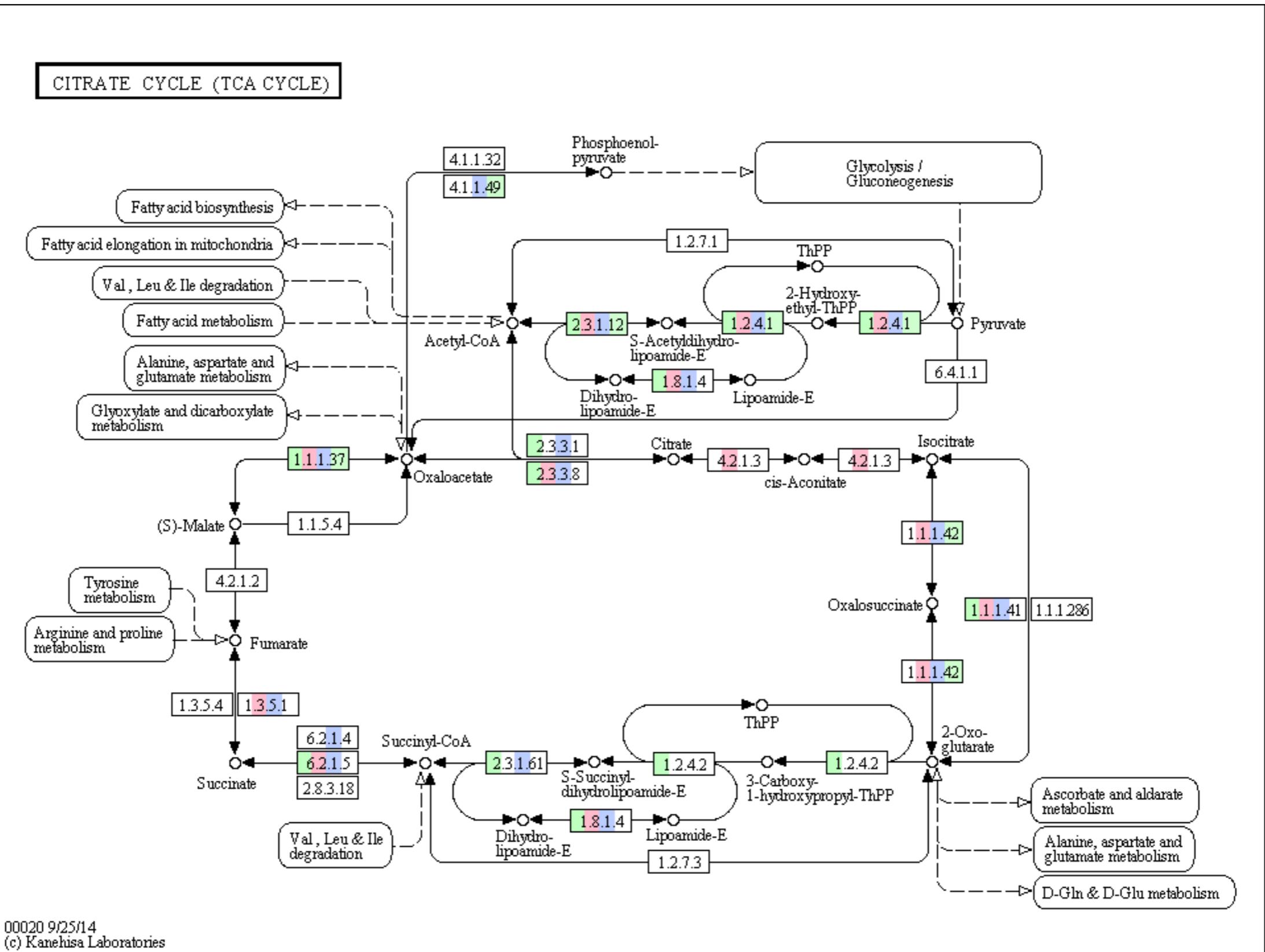
Exar
ge
ge

Alternatively, enter the file name containing the data:

ファイルが選択されていません。

Include global/overview maps

Reconstruct Pathway



KEGG BRITE

- ・機能や知識の階層分類オントロジー
- ・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

Kyoto Encyclopedia of Genes and Genomes

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
Protein kinases
Peptidases
Glycosyltransferases
LPC kinase/phosphatase

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
Therapeutic category of drugs in Japan
Topical steroids potency in Japan New!
Target-based classification of drugs
Antineoplastics

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

KEGG BRITE Database リーダー www.genome.jp/kegg/brite_ja.html

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
- Ton 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

» English

Diseases (H numbers)

- ヒト疾患 [+ 遺伝子]
- 感染症疾患 [+ ゲノム]
- 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

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 KEGG identifiers only

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- 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

KEGG MEDICUS



医薬品情報 検索 ヘルプ

» English

- 疾患、医薬品、環境物質など、医療に関わる情報を生体システム情報と統合したリソース
- 医薬品情報検索
- 医薬品相互作用チェック
- 医薬品成分検索
- 疾患情報検索

KEGG MEDICUS

医薬品検索利用法
相互作用DB利用法
成分検索利用法
KEGG お薬手帳
医薬品分類
医薬品コード

KEGG DRUG

スイッチOTC薬
ゲノムマーカー

KEGG DISEASE

がん
感染症

KEGG
ゲノムネット
Kanehisa Labs

KEGG MEDICUS

KEGG MEDICUS は疾患・医薬品・環境物質など社会的ニーズの高いデータを、ゲノム情報を基盤とした生体システム情報として統合したリソースです。とくに日本と米国の医薬品添付文書を KEGG DRUG や KEGG DISEASE と統合し、研究者コミュニティだけでなく、医療従事者や一般の人々にも有用な情報を提供しています。紹介ページもご覧ください。

KEGG MEDICUS
医薬品・疾患・ゲノム・パスウェイの統合リソース

疾患分類 (ICD-10, etc.)
KEGG DISEASE (英語・日本語)
KEGG DRUG (英語・日本語)
医薬品分類 (ATC, etc.)

MEDIS 標準病名
医薬品添付文書 (医療用・一般用)
JAPIC (日本)
DailyMed (米国)

医薬品情報検索
KEGG MEDICUS 医薬品情報は KEGG DRUG データベース、我が国の医療用医薬品添付文書と一般用医薬品添付文書、米国の医療用医薬品添付文書と一般用医薬品添付文書を統合したリソースです。詳しくは医薬品検索の利用法をご覧ください。また医薬品情報の全体像については医薬品コードもご覧ください。

医薬品情報検索画面へ

医薬品相互作用チェック
KEGG では併用禁忌や併用注意に伴う相互作用を添付文書からすべて抽出しデータベース化しています。これを利用して複数の医薬品間に相互作用がないか調べることができます。医療用医薬品と一般用第1類医薬品が対象です。詳しくは医薬品相互作用データベースの利用法をご覧ください。

医薬品相互作用チェック画面へ

医薬品成分検索
医薬品には有効成分の他に様々な添加物が含まれています。これがジェネリック製品の違いやアレルギー等の副作用にも関連します。KEGG では医療用医薬品添付文書に記載された添加物をすべて抽出してデータベース化しており、有効成分とともに検索することができます。詳しくは医薬品成分検索の利用法をご覧ください。

医薬品情報検索
医薬品相互作用チェック
医薬品成分検索
疾患情報検索

KEGGデータ取得: KEGG API

<http://www.kegg.jp/kegg/rest/keggapi.html>

KEGG API

This is a brief specification document for the REST-style KEGG API.

[[Top](#) | [KEGG API](#) | [KEGG MEDICUS API](#) | [KEGG WebLinks](#) | [KEGG Database Entry Format](#)]

General form of the URL

URL form

```
http://rest.kegg.jp/<operation>/<argument>[/<argument2>][/<option>]
```

<operation> = info | list | find | get | conv | link
<argument> = <database> | <dbentries>

Database

```
<database> = KEGG database including KEGG organism (see Table 1)
```

Table 1. KEGG database names and abbreviations

Database	Name	Abbrev	kid	Remark
KEGG PATHWAY	pathway	path	map number	
KEGG BRITE	brite	br	br number	
KEGG MODULE	module	md	M number	
KEGG ORTHOLOGY	orthology	ko	K number	
KEGG GENOME	genome	genome	T number	
KEGG GENOMES	genomes	gn	T number	Composite database: genome + egenome + mgenome
KEGG GENES	genes	-	-	Composite database: consisting of KEGG organisms
KEGG LIGAND	ligand	ligand	-	Composite database: compound + glycan + reaction + rpair
KEGG COMPOUND	compound	cpd	C number	Japanese version: compound_ja cpd_ja
KEGG GLYCAN	glycan	gl	G number	
KEGG REACTION	reaction	rn	R number	
KEGG RPAIR	rpair	rp	RP number	
KEGG RCLASS	rclass	rc	RC number	
KEGG ENZYME	enzyme	ec	-	
KEGG DISEASE	disease	ds	H number	Japanese version: disease_ja ds_ja
KEGG DRUG	drug	dr	D number	Japanese version: drug_ja dr_ja
KEGG DGROUP	dgroup	dg	DG number	Japanese version: dgroup_ja dg_ja
KEGG ENVIRON	environ	ev	E number	Japanese version: environ_ja ev_ja

Auxiliary databases, dgenes, egenes, mgenes, egenome and mgenome, may also be used.

Database entry

```
<dbentries> = <dbentry>1[+<dbentry>2...]  
<dbentry> = <db:entry> | <kid> | <org:gene>
```

KEGGデータ取得: KEGG API

- APIの例

<http://rest.kegg.jp/list/hsa>

hsa:440034	DKFZp686K1684; uncharacterized LOC440034
hsa:100287010	uncharacterized LOC100287010
hsa:100506548	uncharacterized LOC100506548
hsa:100288846	uncharacterized LOC100288846
hsa:222029	DKFZp434L192; uncharacterized protein DK
hsa:284581	uncharacterized LOC284581
hsa:100130744	uncharacterized LOC100130744
hsa:389332	uncharacterized LOC389332
hsa:146512	uncharacterized protein FLJ30679
hsa:100128288	uncharacterized LOC100128288
hsa:284648	uncharacterized LOC284648
hsa:200058	uncharacterized protein FLJ23867
hsa:100128573	uncharacterized LOC100128573
hsa:149950	uncharacterized LOC149950
hsa:100289361	uncharacterized LOC100289361
hsa:100506082	uncharacterized LOC100506082
hsa:440173	uncharacterized LOC440173
hsa:646736	uncharacterized LOC646736
hsa:645644	FLJ42627; uncharacterized LOC645644
hsa:728752	uncharacterized LOC728752
hsa:100289230	uncharacterized LOC100289230
hsa:79857	FLJ13224; uncharacterized LOC79857
hsa:644656	uncharacterized LOC644656
hsa:100128361	uncharacterized LOC100128361
hsa:149684	uncharacterized LOC149684
hsa:100192386	FLJ16779; uncharacterized LOC100192386
hsa:286189	uncharacterized LOC286189
hsa:283070	uncharacterized LOC283070

<http://rest.kegg.jp/get/hsa:10458>

ENTRY	10458	CDS	T01001
NAME	BAIAP2, BAP2, FLAF3, IRSP53		
DEFINITION	BAI1-associated protein 2		
ORTHOLOGY	K05627 BAI1-associated protein 2		
ORGANISM	hsa Homo sapiens (human)		
PATHWAY	hsa04520 Adherens junction hsa04810 Regulation of actin cytoskeleton KEGG Orthology (KO) [BR:hsa00001] Cellular Processes Cell motility 04810 Regulation of actin cytoskeleton 10458 (BAIAP2) Cellular community 04520 Adherens junction 10458 (BAIAP2)		
BRITE	17q25		
POSITION	Pfam: IMD SH3_9 SH3_2 SH3_1 RasGAP BAR		
MOTIF	NCBI-GI: 222080100		
DBLINKS	NCBI-GeneID: 10458 OMIM: 605475 HGNC: 947 HPRD: 05686 Ensembl: ENSG00000175866 Vega: OTTHUMG00000177698 UniProt: Q9UQB8 I3L4C2		
STRUCTURE	PDB: 3RNJ 4JS0 2YKT 1Y20 1WDZ		
AASEQ	534 MSLSRSEEMHRLTENVYKTIMEQFNPSLRNFIAMGKNYEKALAGVTYAAKGYFDALVKMG ELASESQGSKELGDVLFQMAEVHRQIQNQLEEMLKSFHNELLTQEQLKVELDSRYLSAAL KKYQTEQRSKGDALDKCQAELKKLRKKSGSKNPQKYSDELQYIDAISNKQGELENYVS DGYKTALTEERRFCFLVEKQCAVAKNSAAYHSKGKELLAQKLPLWQQACADPSKIPERA VQLMQQVASNGATLPSALSASKSNLVISDPIPGAKPLPVPPPELFVGRMSAQESTPIMN GVTGPDGEDYSPWADRKAAPKSLSPPQSQSKLSDSYSNTLPVRKSVPKNSYATTENKT LPRSSSMAAGLERNGRMRVKAIFSHAAGDNSTLLSFKEGLITLLVPEARPDGHYGESEK TKMRGWFPFSYTRVLSDGSDRLHMSLQQGKSSSTGNLLDKDDLAIPPPDYGAASRAFPA		

Feedback

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