



KEGG、GenomeNetの サービス・利用法

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統合データベース講習会 AJACS本郷11 2012/3/2



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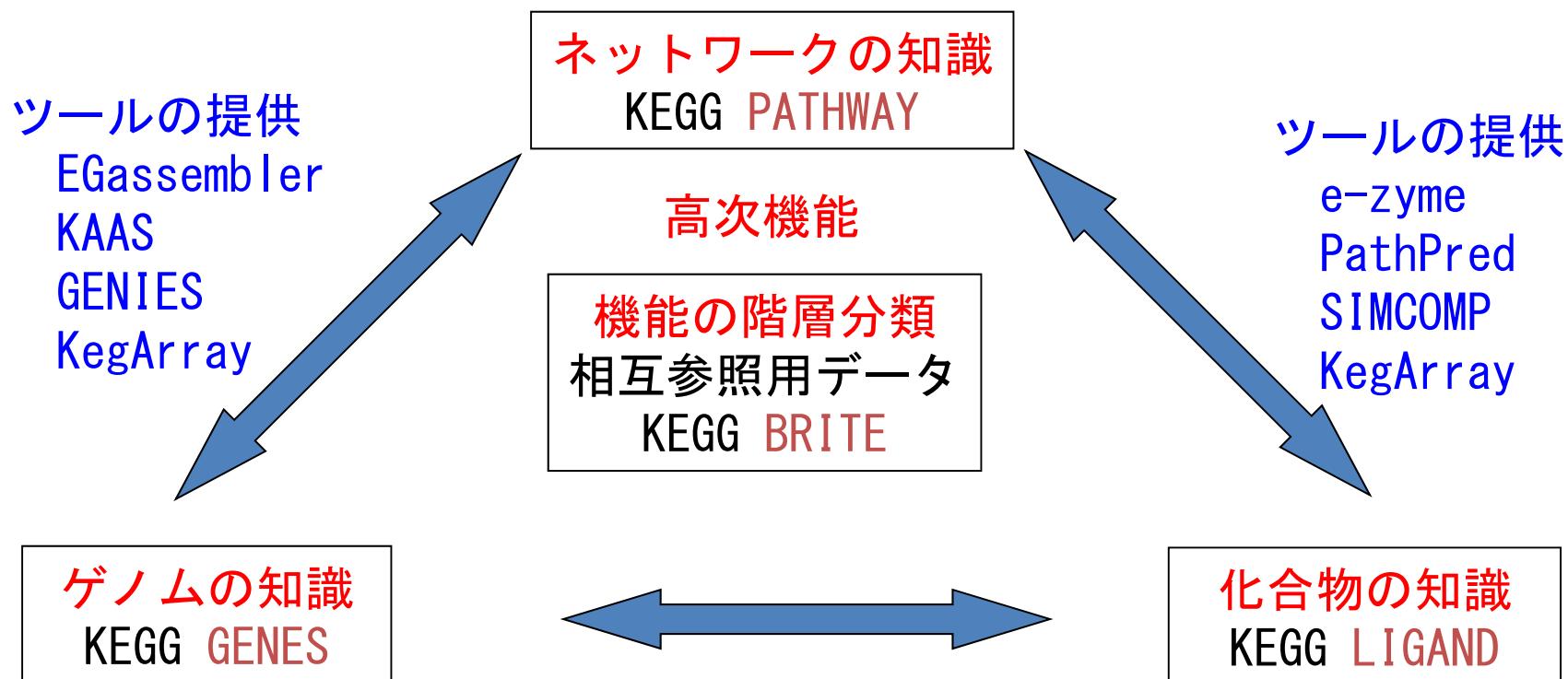
内容

- KEGGとゲノムネットの概要
- KEGG, ゲノムネットの配列データ、解析ツール
(GENES, ORTHOLOGY(KO), KAAS)
- KEGG, ゲノムネットの化合物情報、ツール
(LIGAND, SIMCOMP)
- KEGGのシステム情報、ツール
(PATHWAY, BRITE, KEGG mapper)
- そのほかのKEGGのツール群

KEGGとゲノムネットの概要

KEGG: Kyoto Encyclopedia of Genes and Genomes

様々な種類のデータを「生命現象の総体」として再構築



研究者の知識をゲノムレベルのデータと結びつける

KEGG でカバーしているデータ、いないデータ

- いる

ゲノム

遺伝子
アノテーション

パスウェイ

代謝、制御マップ
病気、薬開発マップ

化合物

2次元構造
薬、代謝物、反応
反応パターン

- いない

制御領域
バリエーション
タンパク質立体構造

シミュレーション用の
パラメータ

物性、立体構造
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

KEGG: Kyoto Encyclopedia of Genes and Genomes

The screenshot shows the KEGG homepage. At the top left is the KEGG logo. A navigation bar includes 'Search' and 'Help' buttons, and a link to 'Japanese'. On the left, a sidebar lists 'KEGG Home', 'KEGG Database', 'KEGG Objects', 'KEGG Software', 'KEGG FTP', 'GenomeNet', 'DBGET/LinkDB', 'Feedback', and 'Kanehisa Labs'. The main content area features a section titled 'Announcement' about the transition to www.kegg.jp. Below it is a 'Main entry point to the KEGG web service' section with a red box around 'KEGG2'. Other sections include 'Data-oriented entry points' (with links to Pathway, BRITE, MODULE, Disease, Drug, Orthology, Genes, and Ligand), 'Entry point for wider society' (with a link to MEDICUS), 'Organism-specific entry points' (with a link to Organisms), 'Analysis tools' (with links to Mapper, Atlas, KAAS, BLAST/Fasta, SIMCOMP, and PathPred), and a footer with copyright information.

The screenshot shows the 'KEGG - Table of Contents' page. At the top right is the KEGG logo. The main title is 'KEGG - Table of Contents'. Below it is a search bar with 'Search KEGG for' and 'Go' and 'Clear' buttons. The page is organized into several sections: 'Systems information' (KEGG PATHWAY, BRITE, MODULE, Disease, Drug, MEDICUS, Orthology), 'Genomic information' (GENES, GENOME, Organisms), and 'Chemical information' (LIGAND, COMPOUND, GLYCAN, REACTION). Each section contains links to specific databases and their update history. A note at the bottom says 'See Kanehisa et al. (2012) for the new features of KEGG.'



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<http://www.kegg.jp/kegg/>

<http://www.kegg.jp/kegg/kegg2.html>

KEGG: Kyoto Encyclopedia of Genes and Genomes

The screenshot shows the KEGG Current Statistics page. The left sidebar contains links for KEGG Home, Release notes, Current statistics (which is highlighted with a red box), Plea from KEGG, KEGG Database, KEGG Objects, KEGG Software, GenomeNet, DBGET/LinkDB, Feedback, and Kanehisa Labs. The main content area is titled 'Current Statistics' and displays 'KEGG Database as of 2012/3/1'. A large table lists various KEGG databases with their respective counts. The table is divided into three sections by red boxes: KEGG PATHWAY, KEGG ORTHOLOGY, GENOME, GENES, and MGENES; KEGG SSDB, DGENES, EGENES, and MGENES; and KEGG COMPOUND, GLYCAN, REACTION, RPAIR, RCLASS, and ENZYME.

Database	Description	Count
KEGG PATHWAY	Pathway maps, reference (total)	416 (156,646)
KEGG BRITE	Functional hierarchies, reference (total)	135 (47,455)
KEGG MODULE	KEGG modules, reference (total)	438 (96,702)
KEGG DISEASE	Human diseases	1,016
KEGG DRUG	Drugs	9,773
KEGG ENVIRON	Crude drugs and health-related substances	836
KEGG ORTHOLOGY	KEGG Orthology (KO) groups	15,524
KEGG GENOME	KEGG Organisms	1,730
KEGG GENES	Genes in high-quality genomes (154 eukaryotes, 1442 bacteria, 117 archaea)	7,505,149
KEGG SSDB	Best hit relations within GENES Bi-directional best hit relations within GENES	64,225,605,182 1,200,860,761
KEGG DGENES	Genes in draft genomes (17 eukaryotes)	356,803
KEGG EGENES	Genes as EST contigs (99 eukaryotes)	3,792,883
KEGG MGENES	Genes in metagenomes (139 samples)	14,822,267
KEGG COMPOUND	Metabolites and other small molecules	16,509
KEGG GLYCAN	Glycans	10,979
KEGG REACTION	Biochemical reactions	8,880
KEGG RPAIR	Reactant pair chemical transformations	13,342
KEGG RCLASS	Reaction class	2,449
KEGG ENZYME	Enzyme nomenclature	5,708

システムの知識
KEGG PATHWAY
KEGG BRITE
KEGG MEDICUS

ゲノムの知識
KEGG GENES

化合物の知識
KEGG LIGAND

<http://www.kegg.jp/kegg/>

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KEGG Objects Identifier

The screenshot shows a Firefox browser window displaying the KEGG Objects Identifier page at www.kegg.jp/kegg/kegg3.html. The page has a green sidebar on the left containing links to various KEGG services. The main content area is titled "KEGG Objects" and describes what KEGG objects are. It then focuses on the "KEGG Object Identifier", explaining its general form as "db:entry" and providing a detailed explanation of the prefix system. A table lists the database names, object types, prefixes, and examples for each. A red box highlights the "KEGG Objects" link in the sidebar, and a red box also highlights the "Prefix" column in the table. A large red text overlay at the bottom right of the page reads "基本は Prefix + 5桁の数字".

KEGG Objects

KEGG Objects are biological entities from molecular to higher levels that are represented as database entries in KEGG, such as genes and protein, small molecules, reactions, pathways, diseases and drugs.

KEGG Object Identifier

The identifier of each database entry is generally in the form of
db:entry

where "db" is the database name and "entry" is the entry name or the accession number (see [DBGET](#) for the list of database names and abbreviations). However, "db" may be omitted in thirteen of the fifteen databases shown below, because the entry name, called the **KEGG object identifier** consisting of a database-dependent prefix and a five-digit number, is unique across the databases. The KEGG object identifiers are often called D numbers, K numbers, C numbers, etc. The D number example shown below D01441 is thus equivalent to dr:D01441 or drug:D01441.

Database	Object	Prefix	Example
KEGG PATHWAY	Pathway map	map, ko, ec, rn, (org)	hsa04930
KEGG BRITE	Functional hierarchy	br, jp, ko, (org)	ko01003
KEGG MODULE	KEGG module	M, (org)_M	M00010
KEGG DISEASE	Human disease	H	H00004
KEGG DRUG	Drug	D	D01441
KEGG ENVIRON	Crude drug, etc.	E	E00048
KEGG ORTHOLOGY	KO group	K	K04527
KEGG GENOME	KEGG organism	T	T01001 (hsa)
KEGG GENES	Gene / protein		hsa:3643
KEGG COMPOUND	Small molecule	C	C00031
KEGG GLYCAN	Glycan	G	G00109
KEGG REACTION	Reaction	R	R00259
KEGG RPAIR	Reactant pair	RP	RP04458
KEGG RCLASS	Reaction class	RC	RC00046
KEGG ENZYME	Enzyme		ec:2.7.10.1

(org) represents three-, four-, or five-letter organism code

The thirteen databases are all manually created by KEGG. The remaining two databases, KEGG GENES derived from RefSeq and KEGG ENZYME derived from ExplorEnz, are also given KEGG-original annotations.

ゲノムネット

Firefox ▾

ゲノムネット www.genome.jp/ja/ Google

GenomeNet KEGG KEGG2 PATHWAY BRITE MEDICUS DBGET 環境設定 ヘルプ [English | Japanese]

Search 統合データベース for Go Clear

データベース検索システム : DBGET/LinkDB
KEGGと国内外の様々なデータベースを統合的に検索するシステム

ゲノムネット統合データベース
DBGET search
LinkDB search

ゲノムネット医薬品データベース
JAPIC 医療用医薬品
JAPIC 一般用医薬品
おくすり手帖

KEGG MEDICUS - 患者・医薬品統合リソース
医薬品検索
疾患検索

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

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

KEGG パスウェイ一覧
BRITE 機能階層(日本語)一覧
KEGG 生物種一覧

ゲノムネット医薬品データベース

データベース増加図

その他のプロジェクトデータベース

The screenshot shows the GenomeNet homepage in a Firefox browser. The main content area features a large red box highlighting the 'ゲノムネット医薬品データベース' (GenomeNet Medicine Database) section, which includes links for JAPIC medical and general medicine databases, and Oksuri Techo (medicine handbook). Below this, another red box highlights the 'varDB' section, listing databases for antigen variants, research support, CYORF (cyanobacteria), BSORF (Bacillus subtilis), and EXPRESSION (expression profile). To the right, there's a chart titled 'データベース増加図' (Database Increase Diagram) showing growth over time. The top navigation bar includes links for KEGG, KEGG2, PATHWAY, BRITE, MEDICUS, DBGET, and search functions. The left sidebar lists categories like 'ゲノムネット' (GenomeNet), '統合データベース' (Integrated Database), '医薬品データベース' (Medicine Database), 'KEGG', 'varDB', '研究支援データベース' (Research Support Database), '計算ツール' (Calculators), and 'フィードバック' (Feedback).

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

ゲノムネット計算ツール

Firefox ▾

GenomeNet

www.genome.jp

LinkDB search
KEGG: Kyoto Encyclopedia of Genes and Genomes
KEGG2 - Table of contents
KEGG PATHWAY - Systems information: pathways
KEGG BRITE - Systems information: ontologies
KEGG Organisms - Organism-specific entry points
KEGG GENES - Genomic information
KEGG LIGAND - Chemical information
KEGG MEDICUS: Health-related info resource
MEDICUS search
varDB: Antigenic variation database
Community Databases
CYORF - Cyanobacteria annotation database
BSORF - Bacillus subtilis genome database
EXPRESSION - Gene expression profile database

GenomeNet Bioinformatics Tools

Sequence Analysis
BLAST / FASTA - Sequence similarity search
MOTIF - Sequence motif search
CLUSTALW / MAFFT / PRRN - Multiple alignment

Genome Analysis
KAAS - KEGG automatic annotation server
EGassembler - EST consensus contigs
GENIES - Gene network prediction

Chemical Analysis
SIMCOMP / SUBCOMP - Chemical structure search
KCaM - Glycan structure search
PathComp - Possible reaction path computation
PathSearch - Similar reaction path search
PathPred - Reaction pathway prediction
E-zyme - Enzymatic reaction prediction

KEGG Organisms

DB growth curve

Kyoto University Bioinformatics Center

ホモロジー検索、モチーフ検索
マルチプルアライメント

遺伝子機能アノテーション、予測など

化学構造比較、パス予測など

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

KEGG, ゲノムネットの配列データ、解析ツール (GENES, ORTHOLOGY(KO), KAAS)

KEGG: Kyoto Encyclopedia of Genes and Genomes

Firefox

KEGG: Kyoto Encyclopedia of Genes... www.kegg.jp/kegg/ Google

KEGG Home
Release notes
Current statistics
Plea from KEGG

KEGG Database
KEGG overview
Searching KEGG
KEGG mapping
Color codes

KEGG Objects
Pathway maps
Brite hierarchies

KEGG Software
KegTools
KEGG API
KGML

KEGG FTP
Subscription

GenomeNet

DBGET/LinkDB

Feedback

Kanehisa Labs

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Firefox

GenomeNet www.genome.jp Google

KEGG KEGG2 PATHWAY BRITE MEDICUS DBGET [English | Japanese]

GenomeNet Database Resources

- DBGET: Integrated Database Retrieval System
- DBGET search
- LinkDB search
- KEGG: Kyoto Encyclopedia of Genes and Genomes
- KEGG2 - Table of contents
- KEGG PATHWAY - Systems information: pathways
- KEGG BRITE - Systems information: ontologies
- KEGG Organism - Organism-specific entry points
- KEGG GENES - Genomic information
- KEGG LIGAND - Chemical information
- KEGG MEDICUS: Health-related info resource
- MEDICUS search
- varDB: Antigenic variation database
- Community Databases
- CYORF - Cyanobacteria annotation database
- BSORF - Bacillus subtilis genome database
- EXPRESSION - Gene expression profile database

KEGG pathway maps
BRITE functional hierarchies
KEGG Organisms

KEGG Bioinformatics Tools

Sequence Analysis

- BLAST / FASTA - Sequence similarity search
- MOTIF - Sequence motif search
- CLUSTALW / MAFFT / PRRN - Multiple alignment

Genome Analysis

- KAAS - KEGG automatic annotation server
- ESTconsensus - EST consensus contigs
- GENIES - Gene network prediction

Chemical Analysis

- SIMCOMP / SUBCOMP - Chemical structure search
- KCalm - Glycan structure search
- PathComp - Possible reaction path computation
- PathSearch - Similar reaction path search
- PathPred - Reaction pathway prediction
- E-zyme - Enzymatic reaction prediction

Kyoto University Bioinformatics Center

KEGG GENES データベース

KEGG GENESの
サブカテゴリ

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

登録データの一覧表へのリンク
生物種単位、サンプル単位

配列の種類
アノテーションの種類
(manual, KOALA, KAAS)

KEGG Organisms

- GENES, DGENESに登録されている生物種 -



KEGG Organisms: Complete Genomes

Eukaryotes: 154 + 17(draft) Bacteria: 1442 Archaea: 117

[Genomes | ESTs | Meta | Pan]

Eukaryotes

分類

生物種コード

生物種名

データソース

Category		Species	Source
Vertebrates	Mammals	hsa Homo sapiens (human)	RefSeq
		ptr Pan troglodytes (chimpanzee)	RefSeq
		pon Pongo abelii (Sumatran orangutan)	RefSeq
		mcc Macaca mulatta (rhesus monkey)	RefSeq
		mmu Mus musculus (mouse)	RefSeq
		rno Rattus norvegicus (rat)	RefSeq
		cfa Canis familiaris (dog)	RefSeq
		aml Ailuropoda melanoleuca (giant panda)	RefSeq
		bta Bos taurus (cow)	RefSeq
		ssc Sus scrofa (pig)	RefSeq
Birds	Birds	ecb Equus caballus (horse)	RefSeq
		mdo Monodelphis domestica (opossum)	RefSeq
		oaa Ornithorhynchus anatinus (platypus)	RefSeq
		gga Gallus gallus (chicken)	RefSeq
		mpg Meleagris gallopavo (turkey)	RefSeq
Reptiles	Reptiles	tgu Taeniopygia guttata (zebra finch)	RefSeq
		acs Anolis carolinensis (green anole)	RefSeq
		xla Xenopus laevis (African clawed frog)	RefSeq

KEGG Metagenomes

- MGENESに収録されているサンプル -



KEGG Metagenomes

[Genomes | ESTs | Meta | Pan]

分類 Environmental samples	生物種コード	生物種名	データソース
-----------------------------	--------	------	--------

Category	Project	Source
Ocean	T30001 Planktonic microbial communities from North Pacific Subtropical Gyre	NCBI
	T30002 Planktonic microbial communities from Monterey Bay, CA	NCBI
	T30003 Human gut metagenome collected from healthy human sample F1-S (male adult)	Metagenome.jp
	T30004 Human gut metagenome collected from healthy human sample F1-T (female adult)	Metagenome.jp
	T30005 Human gut metagenome collected from healthy human sample F1-U (infant female)	Metagenome.jp
	T30006 Human gut metagenome collected from healthy human sample F2-V (male adult)	Metagenome.jp
	T30007 Human gut metagenome collected from healthy human sample F2-W (female adult)	Metagenome.jp
	T30008 Human gut metagenome collected from healthy human sample F2-X (male child)	Metagenome.jp
	T30009 Human gut metagenome collected from healthy human sample F2-Y (female child)	Metagenome.jp
	T30010 Human gut metagenome collected from healthy human sample In-A (male adult)	Metagenome.jp
	T30011 Human gut metagenome collected from healthy human sample In-B (male infant)	Metagenome.jp
	T30012 Human gut metagenome collected from healthy human sample In-D (male adult)	Metagenome.jp
	T30013 Human gut metagenome collected from healthy human sample In-E (male infant)	Metagenome.jp
	T30014 Human gut metagenome collected from healthy human sample In-M (infant female)	Metagenome.jp
	T30015 Human gut metagenome collected from healthy human sample In-R (female adult)	Metagenome.jp
	T30016 MH0001 MetaHIT sample from healthy Danish female	MetaHIT
	T30017 MH0002 MetaHIT sample from healthy Danish female	MetaHIT

生物種のゲノム情報

- 種の系統、データソース、アノテーションレベル、文献などの詳細情報 -



Homo sapiens (human)

Genome info Pathway map Brite hierarchy Module Genome map Blast Taxonomy

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: 19761
Number of RNA genes: 1431
Reference PMID: 11237011

Authors: Lander ES et al.
Title: Initial sequencing and analysis of the human genome

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bfind/bget – ワード、エントリー検索

- データ検索、データ取得のためのシステム
 - bfind: キーワード検索
 - bget: エントリの取得

Firefox > KEGG GENES Database

www.kegg.jp/kegg/genes.html

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.

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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

「Histidine」で
GENESにbget

Firefox - DBGET Search Result: GENES histid... +

www.kegg.jp/dbget-bin/www_bfind_sub?max_hit=1000&dbke

Search GENES for histidine Go Clear

Database: GENES - Search term: histidine (1 - 1000) Next

hsa 646982
HRC1T, LQLL338, PRO537, UNQ338; histidine rich carboxyl terminus 1
hsa3034
HLA_HIS, HSTD; histidine ammonia-lyase (EC:4.3.1.3); K01745 histidine ammonia-lyase [EC:4.3.1.3]
hsa3270
HRC, MGC133326; histidine rich calcium binding protein
hsa3271
CHORDC1, CHP1, FLJ117289, cysteine and histidine-rich domain (CHORD) containing 1
hsa54974
THG1L, FLJ11601, FLJ20545, ICF45; RNA-histidine guanyltransferase 1-like (S. cerevisiae); K10761
(RNA(His) guanyltransferase [EC:2.7.7.79]
hsa2908
PHPI1, CGI-202, DKPZ554M173, HSPC141, PHF14, RP11-215L13.10, b2A15L13.10; phosphohistidine
phosphotransferase 1 (EC:3.1.3.1); K01112 [EC:3.1.3.1-]
hsa4691
HINT2, HIT-17, histidine triad nucleotide binding protein 2
hsa13514
HINT3, FLJ33125, FLJ99898, HINT4, MGC22975; histidine triad nucleotide binding protein 3 (EC:3.-.-)
hsa3094
HINT5, FLJ30414, FLJ32340, HINT, PKC1I-1, PRKCNH1; histidine triad nucleotide binding protein 1
(EC:3.1.3.1-)
hsa46077
LHPF, FLJ44848, FLJ46044, HDHD202, MGC117251, MGC142189, MGC142191; phosphosyntine
phosphotransidase inorganic pyrophosphate phosphatase (EC:3.6.1.1); K11725 phosphosyntine
phosphotransidase inorganic pyrophosphate phosphatase (EC:3.6.1.1.3.1.3.-)
hsa46444
PHD1, proline/histidine/glycine-rich 1
hsa2657
HDC, MGC183399; histidine decarboxylase (EC:4.1.1.22); K01590 histidine decarboxylase [EC:4.1.1.22]
hsa727996
cysteine and histidine-rich domain (CHORD) containing 1 pseudogene
hsa2272
FH1_AP34aspe, FRAB3; fragile histidine triad gene (EC:3.6.1.20); K01522 bis(5'-adenosyl)-triphosphatase
(EC:3.6.1.20.1)
hsa50262
CHYB1, CHRP, K1440486, MGC13010; cysteine/histidine-rich 1

「eco:b4139」
で bfind

KEGG GENESのIDを探したいときは？ - KEGG Objects -

The screenshot shows a Firefox browser window displaying the KEGG Objects page at www.genome.jp/kegg/kegg3.html. The page contains a table mapping KEGG databases to their corresponding IDs:

KEGG GENEOME	KEGG organism	I	101001 (hsa)
KEGG GENES	Gene / protein		hsa:3643
KEGG COMPOUND	Small molecule	C	C00031
KEGG GLYCAN	Glycan	G	G00109
KEGG REACTION	Reaction	R	R00259
KEGG RPAIR	Reactant pair	RP	RP04458
KEGG RCLASS	Reaction class	RC	RC00046
KEGG ENZYME	Enzyme		ec:2.7.10.1

Below the table, a note states: "The thirteen databases are all manually created by KEGG. The remaining two databases, KEGG GENES derived from RefSeq and KEGG ENZYME derived from ExplorEnz, are also given KEGG-original annotations."

KEGG Organism Code

In addition to the T number shown above, an organism in KEGG is given a three-letter KEGG organism code (with prefix "d" for automatically annotated genomes), which is treated like a database name. Therefore, individual genes in an organism can be identified in the following way:

org:gene

where "org" is the KEGG organism code and "gene" is the KEGG GENES or DGENES entry name (see below). The KEGG organism code is also used as a prefix to identify organism-specific pathway maps or BRITE functional hierarchies (see: Pathway maps and Brite hierarchies).

Links to Outside Databases

The KEGG objects are linked to numerous outside database entries with the same biological meaning, such as the same gene or protein in the same organism, enabling the user to integrate information from different sources (see the list of outside links in the GenomeNet LinkDB page).

The KEGG GENES entry names, which are usually NCBI GeneIDs or locus_tags, can be converted to/from the identifiers of the major sequence databases through the GenomeNet LinkDB system. The following interface allows conversion from NCBI or UniProt.

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

NCBI GeneID NCBI gi UniProt

3775638 3737440 3743551 3897645 3902295

(Example) 3775638 3737440 3743551 3897645 3902295

Convert Entry list Clear

Last updated: January 4, 2012

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The screenshot shows a Firefox browser window displaying the BCONV Result page at www.genome.jp/dbget-bin/www_bconv?ncbi-geneid+3775638+3737440+3. The page title is "Database: ncbi-geneid". It lists five converted database IDs:

ncbi-geneid	syf:Syncoc7942_0655	photosystem II D2 protein (photosystem q(a) protein); K02706 photosys
3775638	syd:Syncoc9605_1992	photosystem II D2 protein (photosystem q(a) protein); K02706 photosys
3737440	sey:Syncoc902_0317	photosystem II reaction centre protein FsbD/D2; K02706 photosystem II
3743551	cya:CIA_2358	pabD-1; photosystem II protein D2; K02706 photosystem II P680 reaction center
3897645	cya:CYB_0854	pabD-1; photosystem II protein D2; K02706 photosystem II P680 reaction center
3902295		

DBGET integrated database retrieval system, GenomeNet

KEGG Objectのページで、
NCBI GenID, NCBI gi, UniProt から、
KEGG GENES entry の IDに変換可能

GENESをbfindで検索

- 例: aspartate ammonia-lyase -

The screenshot shows the KEGG GENES Database search page. At the top, there's a navigation bar with links for KEGG2, PATHWAY, BRITE, MODULE, KO, GENOME, GENES, SSDB, and Organisms. Below this is a search bar with the placeholder "Enter org:gene (Example) syn:ssr3451" and buttons for Entry, Gene cluster, Ortholog, Paralog, Motif, and Clear. A "Gene Catalogs" section follows, containing a table with rows for GENES, DGENES, EGENES, MGENES, and VGENES. The VGENES row indicates "No annotation; available only in DBGET". At the bottom, there are two search boxes: one for "Search GENES for aspartate ammonia-lyase" with "bfind mode" selected, and another for "Search Organism hsa for" with "bfind mode" selected.

The screenshot shows the DBGET Search Result page for the search term "aspartate ammonia-lyase". The search bar at the top has "Search GENES for aspartate ammonia-lyase". The results list various entries, each with a code like xtr: or pop: followed by a description. One entry, "ec:04139 aspA, ECK4133, JW4099; aspartate ammonia-lyase (EC:4.3.1.1); K01744 aspartate ammonia-lyase [EC:4.3.1.1]", is highlighted with a red box.

KEGG GENES Entry (例: eco:b4139)

The figure shows a screenshot of a web browser displaying the KEGG database entry for b4139. The main content area contains tabs for 'Entry' (b4139), 'CDS' (T00007), 'Gene name' (aspa, ECK4133, JW4099), 'Definition' (aspartate ammonia-lyase (EC:4.3.1.1)), 'Orthology' (KO1744, aspartate ammonia-lyase [EC:4.3.1.1]), 'Organism' (E. coli K-12 MG1655), 'Pathway' (eco00250, Alanine, aspartate and glutamate metabolism; eco00910, Nitrogen metabolism; eco01100, Metabolic pathways), 'Class' (Metabolism; Energy Metabolism; Nitrogen metabolism [PATH:eco00910]; Metabolism; Amino Acid Metabolism; Alanine, aspartate and glutamate metabolism [PATH:eco00250]), 'SSDB' (Ortholog, Paralog, Gene cluster, GFIT), 'Motif' (Pfam: Lyase_I FumaraseC_C, PROSITE: FUMARATE_LYASES, Motif), 'Other DBs' (NCBI-GI: 90111690, NCBI-GeneID: 940858, Pasteur: aspa, RegulonDB: ECK120000091, EcoGene: EG10095, ECOCYC: EG10095, ASAP: ABE-0013551, UniProt: POAC38), and 'Structure' (PDB: 1JSW, Thumbnails, Jmol). A sidebar on the right lists 'All links' including Pathway (3), Chemical reaction (2), Orthology (1), Enzyme (1), Reaction (1), Genomic (1), Gene (7), Orthology (1), NCBI-Gene (1), NCBI-GI (1), ECOCYC (1), ECODENE (1), PASTEUR-ECO (1), REGULONDB-ECO (1), Protein sequence (2), UniProt (1), RefSeq(pep) (1), 3D Structure (1), PDB (1), Protein domain (8), Pfam (2), PROSITE (1), Others (1), ASAP (1), All databases (20), and Download RDF.

Entry: エントリ名、種類、生物種名

Gene name: 遺伝子・タンパク質名、別名

Definition: オリジナルDBの機能アノテーション

Ortholog: KEGGでアサインしたKEGG Orthology (KO) アノテーション(後述)

Pathway: エントリの遺伝子が機能するPathwayへのリンク

Class: KEGGにおける機能力テゴリBRITE(階層テキスト)
へのリンク

SSDB: SSDB (Similarity Score Database)からの情報抽出用のリンク。(Ortholog/Paralog推定、Gene Cluster)

Motif: エントリが持つドメイン・モチーフの情報

Other DBs: 他の配列DBへのリンク

Structure: PDBへのリンク

Position: エントリのゲノム上の位置(ゲノム情報がある場合)

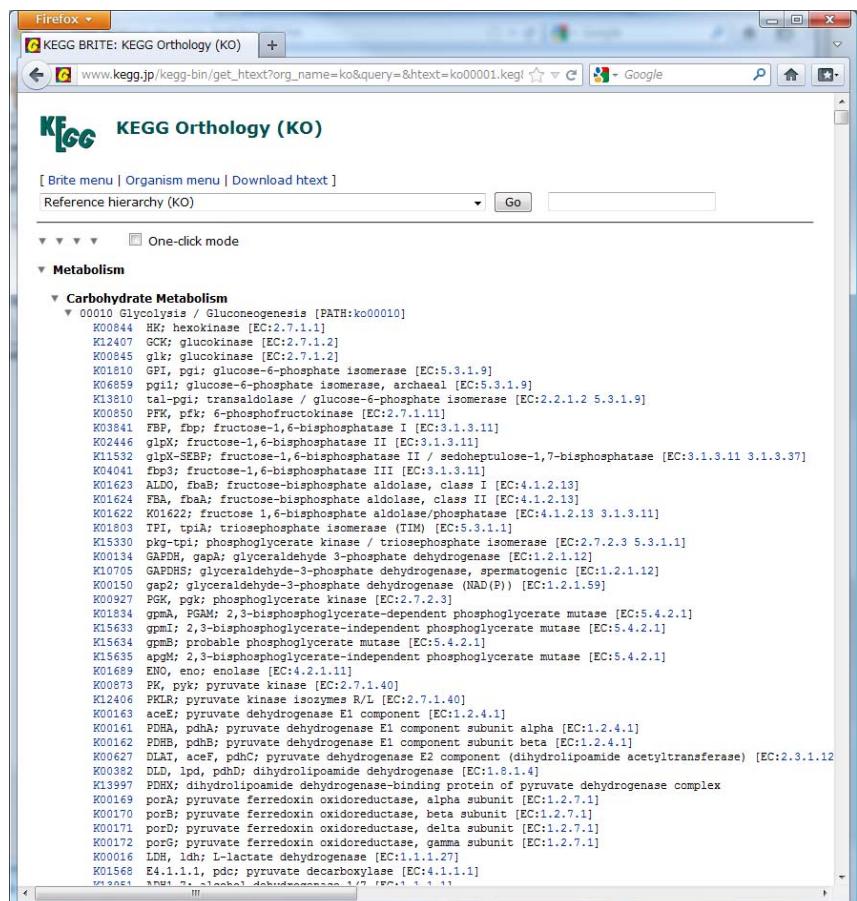
AA seq: アミノ酸配列取得、ホモロジー検索

NT seq: 塩基配列取得。

All links: LinkDBでリンクされている内部および外部DB
ソフォマティクスセンター) licensed under CC 表示 2.1 日本

KO (KEGG Orthology)

- KEGGでは同じ機能を有していると考えられるオーソログ遺伝子を集め、同一のID(K番号)をつけることでその機能を表現している
 - 新規ゲノムが新しくGenesに登録されるとき、遺伝子をオーソロググループ(KO)に追加することで、遺伝子の機能アノテーションを行っている



KO Entry



ORTHOLOGY: K01744

Help

All links

Entry	K01744	KO
Name	aspA	
Definition	aspartate ammonia-lyase [EC:4.3.1.1]	
Pathway	ko00250 Alanine, aspartate and glutamate metabolism ko00910 Nitrogen metabolism	
Class	Metabolism; Energy Metabolism; Nitrogen metabolism [PATH:ko00910] Metabolism; Amino Acid Metabolism; Alanine, aspartate and glutamate metabolism [PATH:ko00250] BRITE hierarchy	
Other DBs	RN: R00490 COG: COG1027 GO: 0008797	
Genes	ECO: b4139(aspA) ECJ: JW4099(aspA) ECO: ECDH108_4332(aspA) EBW: BWG_3852(aspA) ECE: Z5744(aspA) ECS: Ec05120(aspA) ECF: ECH74115_5655(aspA) ETW: ECSP_5239(aspA) EOJ: EC026_5305(aspA) EOI: EC0111_5074(aspA) EOH: EC0103_4934(aspA) ECG: E2348C_4465(aspA) EOK: G2583_4966(aspA) ECC: c5222(aspA) ECP: ECP_4983(aspA) ECI: UT189_C4736(aspA) ECV: APEC01_2250(aspA)	
	⋮	
	MMH: Mmah_0724 MEL: Metbo_2111 NMR: Nmar_1260 CSV: CENSVa_0942	
	Taxonomy KOALA UniProt	

DBGET integrated database retrieval system

Definition: KEGGで定義された機能アノテーション
(GENESエントリにおけるOrthologyフィールド)
Genes: 同一の機能アノテーションを付与されている遺伝子リスト

The screenshot shows a web browser window titled "Firefox" displaying the "KEGG BRITE: KEGG Organisms" page. The URL is "www.kegg.jp/kegg-bin/get_htext?htext=br08601.keg&filedir=&format=at". The page header includes the KEGG logo and navigation links for "Brite menu" and "Download htext". Below the header, there are dropdown menus for "KEGG organisms" and checkboxes for "One-click mode" and "Show matched only". The main content area is a hierarchical tree view of organisms:

- Eukaryotes (154)
 - Bacteria (1454)
 - Gammaproteobacteria (324)
 - Escherichia (32)
 - eco Escherichia coli K-12 MG1455
 - ecj Escherichia coli K-12 N3115
 - ecd Escherichia coli K-12 DH10B
 - ebw Escherichia coli K-12 MC4100(MuLac) EW2952
 - ece Escherichia coli O157:H7 EDL933 (EHEC)
 - ecs Escherichia coli O157:H7 Sakai (EHEC)
 - ecf Escherichia coli O157:H7 E2348/69 (EHEC)
 - ect Escherichia coli O157:H7 H78 (EHEC)
 - ecg Escherichia coli O26:H11 11345 (EPEC)
 - eni Escherichia coli O111:H8 11128 (EPEC)
 - eho Escherichia coli O103:H2 12009 (EHEC)
 - eog Escherichia coli O127:H6 E2348/69 (EPEC)
 - eok Escherichia coli O9:H2 CB9616 (EPEC)
 - ecc Escherichia coli O4:H5:H7 CFT079 (EPEC)
 - egy Escherichia coli O154:H4 E2348/69 (EPEC)
 - eci Escherichia coli O18:K18T UT189 (EPEC)
 - ecv Escherichia coli O1:H1:R (APEC)
 - ecx Escherichia coli O9:H8 (commensal)
 - ecw Escherichia coli O139:H2 E2437/7A (ETEC)
 - ecm Escherichia coli SH5-3-5 (environmental)
 - ecy Escherichia coli O157:H7 E2348/69 (commensal)
 - ecz Escherichia coli O8:K11:H1 (commensal)
 - eqn Escherichia coli O8:K11:H1 (commensal)
 - esk Escherichia coli S5999 (EPEC)
 - ect Escherichia coli O7:K1 IAI39 (ExPEC)
 - enum Escherichia coli O17:K5:H8 UMN026 (ExPEC)
 - ect Escherichia coli O4:H5:H7 988 (ExPEC)
 - ect Escherichia coli C ATCC 8739
 - ehr Escherichia coli RE404
 - ebd Escherichia coli BL21-Gold(DE3)pLysS AG
 - eko Escherichia coli K011FL
 - efc Escherichia fergusonii
 - Salmonella (20)
 - sty Salmonella enterica subsp. enterica serovar Typhi CT18
 - str Salmonella enterica subsp. enterica serovar Typhi Ty2
 - str Salmonella enterica subsp. enterica serovar Typhimurium LT2
 - str Salmonella enterica subsp. enterica serovar Typhimurium

KAAS

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Firefox X

KEGG GENES Database +

www.genome.jp/kegg/genes.html

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 MGENES is generated from EST datasets by the EGassembler program. Both of these programs are made publicly available.

Annotate genomes using KEGG
KAAS: automatic annotation (KO assignment) and pathway reconstruction [reference]

Generate EST consensus contigs
EGassembler: automatic assembly of ESTs to generate consensus contigs [reference]

Search similar sequences in GENES
BLAST: sequence similarity search by BLAST
FASTA: sequence similarity search by FASTA

Firefox X

GenomeNet +

www.genome.jp

GenomeNet [English | Japanese]

KEGG KEGG2 PATHWAY BRITE MEDICUS DBGET

Search All databases for Phenylalanine Go Clear

GenomeNet Database Resources

DBGET: Integrated Database Retrieval System
DBGET search
LinkDB search
KEGG: Kyoto Encyclopedia of Genes and Genomes
KEGG2 - Table of contents
KEGG PATHWAY - Systems information: pathways
KEGG BRITE - Systems information: ontologies
KEGG Organisms - Organism-specific entry points
KEGG GENES: Genomic information
KEGG LIGAND - Chemical information
KEGG MEDICUS: Health-related info resource
MEDICUS search
varDB: Antigenic variation database
Community Databases
CYORF - Cyanobacter annotation database
BSORF - Bacillus subtilis genome database
EXPRESSION - Gene expression profile database

DB growth curve

GenomeNet Bioinformatics Tools

Sequence Analysis
BLAST / FASTA - Sequence similarity search
MOTIF - Sequence motif search
CLUSTALW / MAFFT / PRRN - Multiple alignment

Genome Analysis
KAAS - KEGG automatic annotation server
EGassembler - EST consensus contigs
GENIES - Gene network prediction

Chemical Analysis
SIMCOMP / SUBCOMP - Chemical structure search
KCaM - Glycan structure search
PathComp - Possible reaction path computation
PathSearch - Similar reaction path search
PathPred - Reaction pathway prediction
E-zyme - Enzymatic reaction prediction

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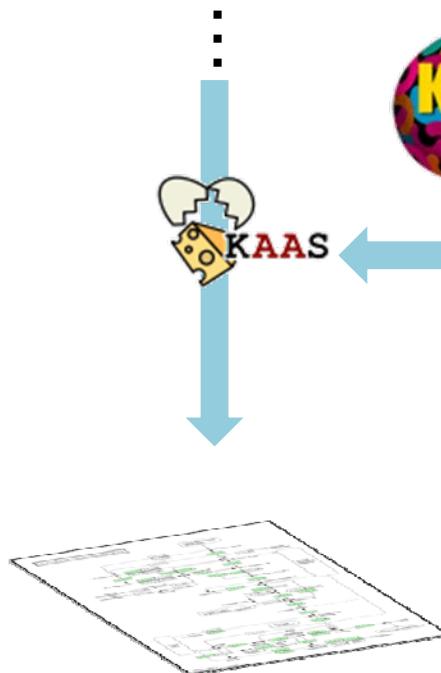
• 入力データ

- 大規模シークエンスによって得られた特定の種の大
量のアミノ酸・ヌクレオチド
配列
- ORFの配列をmulti-FASTA
形式で

```
>Os01t0102600-02 Similar to shikimate kinase family protein.+
  AMSRVRQRHDELKERYGVSDITVSVNVASQLGYSSIDSVTLEDMLVLETIYRERLIRAK+
  SMMEAAGKPF*.
>Os01t0103400-01 Hypothetical gene.+
  SSPPRAGRAAGLGSRAPPPATALLSRTTPPATAPLPSAPPATGLPSRAPAKALPSRGAPP+
  APILPLSPSRGRTAGPRPPVVARWGATGHPPSRRAVGHRPPSRRGRGPOCTSRRAAKWHPI+
  IVARPNTALEY*.
>Os01t0107400-01 Hypothetical protein.+
  LESYIEALEEEDPSFLQSYIPPPHPHLHHHHHHQHQQSLLROFPRYRVTTRRSASLRV+
  >Os01t0108700-01 Conserved hypothetical protein.+
  MGGMNLKMTONICLAAGGLLTFTEDGGGTTLAREIERLLLGSEARRRNKEAIKGEGREQQ+
  RMYCOPERRGGGGAGIGAAGERRGRPTAETETIDWVPGPGLTFSPPRKHNHPPSCRSSSW+
  AERSPISSLKRKPTVCLSLTERILVFVFLFSRRKMK+
>Os01t0109432-00 Hypothetical protein.+
  MSLTSSSVLMPRSLLAAASHAPAAATSSRSRSSAVMALISTSRIAQLA1LPLTTSRAPRCC+
  SSRVETASRRLRADSAADSSA+.
>Os01t0111300-01 Conserved hypothetical protein.+
  LSLPSAVRHSAPADVALRCLSSAPHDLDLALKVRFIEISFGSGSFVKLVFTKG+
>Os01t0111800-01 Conserved hypothetical protein.+
  MPSLRPILIAAAAAAVVSLIPAARVVADIDPSSGMPSPPATSPEPFPCPTTPAGISTQP+
  FPAEAPSPTTTTMFPQDPGFLASAACHARTALA1WIVVVVFVSAFLVFLQ+
```

• 出力結果

- KO アノテーション
- KOに基づく遺伝子の階層
分類データ(BRITE)
- PATHWAY マップ



Query
種Xの網羅的
遺伝子配列

テンプレート
GENES
KO
PATHWAY

Results
種XのPATHWAY

KAAS

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The screenshot shows the KAAS web interface. The main navigation bar includes links for Feedback, KEGG2, KEGG, GenomeNet, and Kanehisa Lab. The 'About KAAS' section provides a brief overview of the service. The 'KO assignment' section displays a table of ortholog assignments for a query gene. The 'KEGG pathway mapping' section shows a complex metabolic pathway diagram with various enzymes and metabolites. The 'ESTs' section discusses the use of ESTs for annotation. The 'Reference' section cites a paper by Moriya et al. (2007) in Nucleic Acids Research.

- Complete or Draft genome
 - 入力配列が特定の種の遺伝子で、ある程度網羅性が期待できると来、BBHを指標により精度の高いアノテーションを行う
- Partial genome
 - 入力が網羅的でないときには、Bidirectionalな意味がないので、SBH(片方向ベストヒット)を用いてアノテーションを行う
 - 入力が少量の場合、対話式に結果を得ることができる
- ESTs
 - 入力データがESTの時に用いる。又クレオチド配列を全パターン翻訳するため計算量が増える

KAAS結果

- 結果例のページ <http://bit.ly/yQUjjO>

The screenshot shows a Firefox browser window displaying the KAAS results page. The URL in the address bar is www.genome.jp/kaas-bin/kaas_main?mode=user&mail=tokimatu@kuicr.ky. The page title is "Query List". On the left, there is a logo featuring a heart and the word "KAAS". The main content area shows a table with one row of data:

ID	name	state	result	start (UTC)	end (UTC)	retry	Remove
1330588735	AJACS-sample	complete	html, text	3/1 7:58 2012	3/1 9:16 2012	<input type="checkbox"/>	<input type="button" value="Remove"/>

Below the table, there are navigation links: Feedback, KEGG2, KEGG, GenomeNet, and Kanehisa Lab.

KAAS結果

The screenshot shows a Firefox browser window displaying the KEGG Automatic Annotation Server (KAAS) results. The title bar reads "Firefox" and "KEGG Automatic Annotation Server". The address bar shows the URL "www.genome.jp/kaas-bin/kaas_main?mode=result&id=1330588735&mail=tok". The main content area is titled "KO Assignment Results" and features a small logo of a brain with gears. Below the title, there are navigation links: "Home", "Help", "[KO list]", "[BRITE hierarchies]", "[Pathway map]", "[Threshold change]", and "[Download]". A section titled "Query gene : KO assignment" contains the text "AJACS-sample" followed by a long list of KEGG Orthology (KO) identifiers:

- Os01t0102600-02
- Os01t0103400-01
- Os01t0107400-01
- Os01t0108700-01
- Os01t0109432-00
- Os01t0111300-01
- Os01t0111800-01
- Os01t0111800-02
- Os01t0112000-01
- Os01t0112600-01
- Os01t0114000-00
- Os01t0115200-00
- Os01t0115566-00
- Os01t0121600-01
- Os01t0129800-01
- Os01t0130200-00
- Os01t0130900-01
- Os01t0131600-01
- Os01t0133832-00
- Os01t0135700-01 K13448
- Os01t0135800-01
- Os01t0135900-01
- Os01t0135900-02
- Os01t0136050-00
- Os01t0136000-00
- Os01t0136300-01
- Os01t0136600-01
- Os01t0138000-00
- Os01t0139700-01
- Os01t0143900-01
- Os01t0145000-00
- Os01t0147850-00
- Os01t0149400-00
- Os01t0152300-00 K11252

KAAS結果

Firefox KEGG Automatic Annotation Server www.genome.jp/kaas-bin/kaas_main?mode=brite&id=1330588735&mail= urlエンコード

Firefox KEGG BRITE: KEGG Orthology (KO) ... www.genome.jp/kegg-bin/get_htext?org_name=ko&query=&htext=q00001.ke urlエンコード

BRITE hierarchies

Home Help

[KO list] [BRITE hierarchies] [Pathway map] [Threshold change] [Download]

Network hierarchy

[KEGG Orthology (KO)]

Protein families: metabolism

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

Protein families: genetic information processing

- 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
- recombination proteins

http://www.genome.jp/tools/kaas/

KEGG Orthology (KO)

[Brite menu | Organism menu | Download htext]

Reference hierarchy (KO) Go One-click mode

Metabolism

Carbohydrate Metabolism

- 00010 Glycolysis / Gluconeogenesis [PATH:ko00010]
 - Os01t0190400-01: KO0844 HK: hexokinase [EC:2.7.1.1]
 - Os01t0190400-02: KO0844 HK: hexokinase [EC:2.7.1.1]
 - Os01t0742500-01: KO0844 HK: hexokinase [EC:2.7.1.1]
 - Os05t0187100-01: KO0844 HK: hexokinase [EC:2.7.1.1]
 - Os05t0375100-00: KO0844 HK: hexokinase [EC:2.7.1.1]
 - Os05t0522500-01: KO0844 HK: hexokinase [EC:2.7.1.1]
 - Os07t0446800-00: KO0844 HK: hexokinase [EC:2.7.1.1]
 - Os03t0776000-01: KO1810 GPI, pgk: glucose-6-phosphate isomerase [EC:5.3.1.9]
 - Os06t0256500-01: KO1810 GPI, pgk: glucose-6-phosphate isomerase [EC:5.3.1.9]
 - Os08t0478800-01: KO1810 GPI, pgk: glucose-6-phosphate isomerase [EC:5.3.1.9]
 - Os09t0465600-01: KO1810 GPI, pgk: glucose-6-phosphate isomerase [EC:5.3.1.9]
 - Os01t0191700-01: KO0850 PFK, pfk: 6-phosphofructokinase [EC:2.7.1.11]
 - Os04t0469500-01: KO0850 PFK, pfk: 6-phosphofructokinase [EC:2.7.1.11]
 - Os05t0524400-02: KO0850 PFK, pfk: 6-phosphofructokinase [EC:2.7.1.11]
 - Os05t0524400-01: KO0850 PFK, pfk: 6-phosphofructokinase [EC:2.7.1.11]
 - Os09t0415800-01: KO0850 PFK, pfk: 6-phosphofructokinase [EC:2.7.1.11]
 - Os09t0479800-01: KO0850 PFK, pfk: 6-phosphofructokinase [EC:2.7.1.11]
 - Os10t0405600-01: KO0850 PFK, pfk: 6-phosphofructokinase [EC:2.7.1.11]
 - Os01t0866400-01: KO3841 FBP, fbp: fructose-1,6-bisphosphatase I [EC:3.1.3.11]
 - Os03t0267300-01: KO3841 FBP, fbp: fructose-1,6-bisphosphatase I [EC:3.1.3.11]
 - Os06t0664200-01: KO3841 FBP, fbp: fructose-1,6-bisphosphatase I [EC:3.1.3.11]
 - Os01t0118000-01: KO1623 ALDO, fbaB: fructose-bisphosphate aldolase, class I [EC:4.1.2.13]
 - Os01t0905800-01: KO1623 ALDO, fbaB: fructose-bisphosphate aldolase, class I [EC:4.1.2.13]
 - Os01t0905800-03: KO1623 ALDO, fbaB: fructose-bisphosphate aldolase, class I [EC:4.1.2.13]
 - Os06t0608700-01: KO1623 ALDO, fbaB: fructose-bisphosphate aldolase, class I [EC:4.1.2.13]
 - Os06t0608700-02: KO1623 ALDO, fbaB: fructose-bisphosphate aldolase, class I [EC:4.1.2.13]
 - Os08t0128000-01: KO1623 ALDO, fbaB: fructose-bisphosphate aldolase, class I [EC:4.1.2.13]
 - Os10t0163340-01: KO1623 ALDO, fbaB: fructose-bisphosphate aldolase, class I [EC:4.1.2.13]
 - Os11t0171300-01: KO1623 ALDO, fbaB: fructose-bisphosphate aldolase, class I [EC:4.1.2.13]
 - Os01t0147900-01: KO1803 TPI, tpiA: triosephosphate isomerase (TIM) [EC:5.3.1.1]
 - Os01t0841600-02: KO1803 TPI, tpiA: triosephosphate isomerase (TIM) [EC:5.3.1.1]
 - Os09t0535000-02: KO1803 TPI, tpiA: triosephosphate isomerase (TIM) [EC:5.3.1.1]
 - Os02t0171100-01: KO134 GAPDH, gapA: glyceraldehyde 3-phosphate dehydrogenase [EC:1.2.1.12]
 - Os02t0601300-01: KO134 GAPDH, gapA: glyceraldehyde 3-phosphate dehydrogenase [EC:1.2.1.12]
 - Os04t0484600-01: KO134 GAPDH, gapA: glyceraldehyde 3-phosphate dehydrogenase [EC:1.2.1.12]
 - Os06t0666600-01: KO134 GAPDH, gapA: glyceraldehyde 3-phosphate dehydrogenase [EC:1.2.1.12]
 - Os08t0126300-01: KO134 GAPDH, gapA: glyceraldehyde 3-phosphate dehydrogenase [EC:1.2.1.12]
 - Os08t0126300-02: KO134 GAPDH, gapA: glyceraldehyde 3-phosphate dehydrogenase [EC:1.2.1.12]
 - Os02t0169300-01: KO927 PGK, pgk: phosphoglycerate kinase [EC:2.7.2.3]
 - Os05t04946200-01: KO927 PGK, pgk: phosphoglycerate kinase [EC:2.7.2.3]
 - Os06t0668200-01: KO927 PGK, pgk: phosphoglycerate kinase [EC:2.7.2.3]
 - Os02t0751800-01: KO1834 PGmA, PGAM: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase [EC:5.4.2.1]
 - Os01t0817700-02: KL15633 gpmI: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase [EC:5.4.2.1]
 - Os01t0817700-01: KL15633 gpmI: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase [EC:5.4.2.1]
 - Os03t0330200-01: KL15633 gpmI: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase [EC:5.4.2.1]
 - Os05t0482700-01: KL15633 gpmI: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase [EC:5.4.2.1]
 - Os01t0237100-01: KL15634 qpmB: probable phosphoglycerate mutase [EC:5.4.2.1]

KAAS結果

The figure shows a screenshot of the KEGG Automatic Annotation Server interface. The top navigation bar includes 'Firefox', 'KEGG Automatic Annotation Server', and a search bar with the URL 'www.genome.jp/kaas-bin/kaas_main?mode=map&id=1330588735&mail=tokir'. Below the navigation is a logo for KAAS (Knowledge Acquisition System) featuring a heart and a brain.

The main content area has tabs for 'Home', 'Help', '[KO list]', '[BRITE hierarchies]', '[Pathway map]', '[Threshold change]', and '[Download]'. A section titled 'Color Objects in KEGG Pathways New ver.' allows users to set the default background color for assigned KOs (hex code #ffffbf) and change the gene background color (white). An 'Exec' button is present.

A list of pathway IDs and names is provided:

- 00010 Glycolysis / Gluconeogenesis (30)
- 00020 Citrate cycle (TCA cycle) (19)
- 00030 Pentose phosphate pathway (15)
- 00040 Pentose and glucuronate interconversions (11)
- 00051 Fructose and mannose metabolism (18)
- 00052 Galactose metabolism (14)
- 00053 Ascorbate and aldarate metabolism (12)
- 00050 Starch and sucrose metabolism (34)
- 000520 Amino sugar and nucleotide sugar metabolism (36)
- 000620 Pyruvate metabolism (29)
- 000630 Glyoxylate and dicarboxylate metabolism (15)
- 000640 Propanoate metabolism (16)
- 000650 Butanoate metabolism (13)
- 000660 C5-Branched dibasic acid metabolism (4)
- 000562 Inositol phosphate metabolism (18)
- 00190 Oxidative phosphorylation (67)
- 00195 Photosynthesis (33)
- 00196 Photosynthesis - antenna proteins (12)
- 00710 Carbon fixation in photosynthetic organisms (24)
- 00720 Carbon fixation pathways in prokaryotes (12)
- 000680 Methane metabolism (23)
- 00010 Nitrogen metabolism (10)

To the right, a detailed metabolic pathway diagram for 'GLYCOLYSIS / GLUCONEOGENESIS' is shown. The diagram illustrates the conversion of glucose to glyceraldehyde-3P, involving various enzymes (e.g., 2.7.1.41, 3.1.3.10, 5.4.22, 2.7.1.69, 5.1.33, 2.7.1.11, 2.7.1.147, 5.1.315, 5.3.19, 3.1.3.9, 27.1.11, 27.1.63, 2.7.1.2, 27.1.147, 3.1.3.11, 27.1.111, 27.1.146, 41.2.12, 5.3.11, 1.2.1.12, 1.2.1.59, 1.2.7.5, 1.2.7.6, 1.2.1.9, 2.7.2.3, 3.1.3.13, 5.4.24, 5.4.21, 4.2.1.11, 2.7.1.40, 4.1.1.32, 4.1.1.49, 1.2.7.1, 23.1.12, 1.2.4.1, 1.8.1.4, 41.1.1, 6.2.1.1, 6.2.1.13, 1.2.1.3, 1.2.1.5, 1.1.1.1, 1.1.1.2, 11.1.27, 11.2.8, 11.5, EuG), and various metabolites like α-D-Glucose, β-D-Glucose, α-D-Glucose-6P, β-D-Glucose-6P, α-D-Fructose-6P, β-D-Fructose-6P, α-D-Fructose-1,6P₂, Glycerolaldehyde-3P, Glycerone-P, Glycerate-1,3P₂, Glycerate-2,3P₂, Glycerate-3P, Glycerate-2P, Phosphoenol-pyruvate, Pyruvate, L-Lactate, Ethanol, Acetyl-CoA, Dihydro-lipoamide-E, S-Acetyl-dihydro-lipoamide-E, TPP, 2-Hydroxyethyl-TPP, Acetaldehyde, and Oxaloacetate. The diagram also includes boxes for 'Starch and sucrose metabolism', 'Pentose phosphate pathway', 'Carbon fixation in photosynthetic organisms', 'Citrate cycle', 'Pyruvate metabolism', and 'Propionate metabolism'.

GenomeNetからの遺伝子データベース一括検索機能

- 例: aspartate ammonia-lyase -

Firefox ▾

GenomeNet

www.genome.jp

GenomeNet

KEGG KEGG2 PATHWAY BRITE MEDICUS DBGET

[English | Japanese]

Search All databases for aspartate ammonia-lyase Go Clear

GenomeNet

About GenomeNet

Release notes

Acknowledgments

DBGET

Overview

DB release info

KEGG

varDB

Community DBs

Bioinformatics tools

Other tools

Feedback

GenomeNet Database Resources

DBGET: Integrated Database Retrieval System

DBGET search

LinkDB search

KEGG: Kyoto Encyclopedia of Genes and Genomes

KEGG2 - Table of contents

KEGG PATHWAY - Systems information: pathways

KEGG BRITE - Systems information: ontologies

KEGG Organisms - Organism-specific entry points

KEGG GENES - Genomic information

KEGG LIGAND - Chemical information

KEGG MEDICUS: Health-related info resource

MEDICUS search

varDB: Antigenic variation database

Community Databases

CYORF - Cyanobacteria annotation database

BSORF - *Bacillus subtilis* genome database

EXPRESSION - Gene expression profile database

GenomeNet Bioinformatics Tools

Sequence Analysis

BLAST / FASTA- Sequence similarity search

MOTIF - Sequence motif search

CLUSTALW / MAFFT / PRRN - Multiple alignment

Genome Analysis

K4AS - KEGG automatic annotation server

EGassembler - EST consensus contigs

GENIES - Gene network prediction

Chemical Analysis

SIMCOMP / SUBCOMP - Chemical structure search

KCAMP - Glycan structure search

PathComp - Possible reaction path computation

PathSearch - Similar reaction path search

PathPred - Reaction pathway prediction

E-zyme - Enzymatic reaction prediction

Kyoto University Bioinformatics Center

Firefox ▾

DBGET Search Result: All databases... +

www.genome.jp/dbget-bin/www_bfind_sub?mode=bfind&max_hit=1

L-Aspartate ammonia-lyase; L-Aspartate <=> Fumarate + NH3
R03696

L-threo-3-Methylaspartate ammonia-lyase; L-threo-3-Methylaspartate <=> Mesaconate + NH3
R05758

threo-3-hydroxy-L-aspartate ammonia-lyase; threo-3-Hydroxy-L-aspartate <=> Oxaloacetate + NH3
R09683

threo-3-hydroxy-D-aspartate ammonia-lyase (oxaloacetate-forming); threo-3-Hydroxy-D-aspartate <=> Oxaloacetate + NH3

Gene

KEGG ORTHOLOGY

K01744 aspa: aspartate ammonia-lyase [EC:4.3.1.1]

K04835 E4.3.1.2; methylaspartate ammonia-lyase [EC:4.3.1.2]

KEGG GENES

xtr:100486776 aspartate ammonia-lyase-like

xtr:100496602 threo-3-hydroxyaspartate ammonia-lyase-like

pop:POPTR_552480 aspartate ammonia-lyase (EC:4.2.1.2); K01679 fumarate hydratase, class II [EC:4.2.1.2]

ota:O118g01470 aspartate ammonia-lyase (ISS)

afm:AFUA_3G00790 methylaspartate ammonia-lyase (EC:4.3.1.2); K04835 methylaspartate ammonia-lyase [EC:4.3.1.2]

... > display all

KEGG EGENES

T20045:11947 K01744 aspartate ammonia-lyase [EC:4.3.1.1]

KEGG MGenes

T30003:id01390 F1-S_168_1_B_pred_1_+_2_271_0_C; K01744 aspartate ammonia-lyase [EC:4.3.1.1]

T30003:id06088 F1-S_1362_1_B_pred_3_+_1782_2448_0_P; K01744 aspartate ammonia-lyase [EC:4.3.1.1]

T30003:id27601 F1-S_11867_1_B_pred_1_+_117_1100_0_P; K01744 aspartate ammonia-lyase [EC:4.3.1.1]

T30003:id28159 F1-S_12171_1_B_pred_1_+_1_944_0_P; K01744 aspartate ammonia-lyase [EC:4.3.1.1]

T30003:id28161 F1-S_12173_1_B_pred_1_+_181_1044_0_C; K01744 aspartate ammonia-lyase [EC:4.3.1.1]

... > display all

NCBI-GENE

7788440 [NCBI-Gene]
aspa: aspartate ammonia-lyase

2784315 [NCBI-Gene]
aspa: aspartate ammonia-lyase

2795913 [NCBI-Gene]
DVU1766, aspartate ammonia-lyase

7172452 [NCBI-Gene]

KEGG, ゲノムネットの化合物情報、ツール (LIGAND, SIMCOMP)

KEGG: Kyoto Encyclopedia of Genes and Genomes

Firefox

KEGG: Kyoto Encyclopedia of Genes and Genomes

www.kegg.jp/kegg/

KEGG Home
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Plea from KEGG

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Kanehisa Labs

KEGG LIGAND

SIMCOMP/SUBCOMP

化合物類似構造・部分構造検索

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Firefox

GenomeNet

www.genome.jp

GenomeNet Database Resources

KEGG pathway maps
BRITE functional hierarchies
KEGG Organisms

DBGET: Integrated Database Retrieval System
DBGET search
LinkDB search

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MEDICUS search

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EGassembler - EST consensus contigs
GENIES - Gene network prediction

Chemical Analysis

SIMCOMP / SUBCOMP - Chemical structure search
KoSM - Glycan structure search
PathComp - Possible reaction path computation
PathSearch - Similar reaction path search
PathPred - Reaction pathway prediction
E-zyme - Enzymatic reaction prediction

Kyoto University Bioinformatics Center

KEGG LIGAND データベース

KEGG2 PATHWAY BRITE MODULE LIGAND COMPOUND GLYCAN REACTION

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, respectively. ENZYME is derived from the IUBMB/IUPAC Enzyme Nomenclature, but the others are internally developed and maintained.

Database	Identifier	Content	Specialized entry point
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

ID番号のIdentifierと各DBに含まれるデータの説明

化合物、糖鎖、反応に特化した入口

KEGG LIGANDのサブカテゴリ

KEGGにおける「Chem(o)-」の部分、すなわち生化学的な情報全般を扱う

KEGG COMPOUND（代謝化合物情報）

- 主に代謝化合物を収録したデータベース
 - 中心代謝、二次代謝物 etc.
- 構造は2次元のグラフとして持つ
 - ファイルフォーマットは、MDL/mol and KCF
- KCFフォーマットの特徴
 - KEGG Atom-Type による原子表記

The screenshot shows the KEGG Compound homepage within a Firefox browser window. The address bar displays 'www.kegg.jp/kegg/compound/'. The main content area features the KEGG logo and the heading 'KEGG COMPOUND'. Below this is a sub-heading 'Metabolome informatics resource integrating genomics and chemistry'. A navigation menu at the top includes links for KEGG2, PATHWAY, BRITE, MODULE, LIGAND, COMPOUND, GLYCAN, and REACTION. A search bar is present with the placeholder 'Enter C numbers' and several buttons: Filter, Pathway mapping, Brite mapping, Get title, Get entry, and Clear. The central part of the page is titled 'KEGG COMPOUND Database' and contains descriptive text about the database's purpose and structure. It also mentions 'DBGET search' and 'LIGAND relational database search'. A section titled 'Biosynthetic Codes' provides information on how structures are determined. At the bottom, a copyright notice from 2012 is visible.

KCFフォーマットとKEGG Atom type

- KCF (KEGG Chemical Function)
 - KEGGにおける化合物データのフォーマット
 - MDL/mol類似のフォーマットで、原子情報にKEGG atom typesを使用
- KEGG atom types
 - 原子の周辺環境を反映させて、68種類に原子タイプを細分類
 - 1)結合パターン
 - 2)周辺原子種
 - 3)リング、芳香性
 - SIMCOMPなどの構造比較計算に利用

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
C	Cyclic alkane	C1x ring-CH2-ring	14010
		C1y ring-CH(-R)-ring	27376
		C1z ring-(CH(-R))2-ring	4463
		C2a R=CH2	634
C	Alkene	C2b R=CH-R	3965
		C2c R=C(-R)2	1914
		C2x ring-CH=ring	2964
		C2y ring-C(-R)=ring or ring-C(=R)-ring	3722
C	Alkyne	C3a R=CH	43
		C3b R=C-R	282
		C4a R=CH=O	350
		C5a R-C(=O)-R	3595
C	Cyclic ketone	C5x ring-C(=O)-ring	2257
		C6a R-C(=O)-OH	3190
		C7a R-C(=O)-O-R	1691
		C7x ring-C(=O)-O-ring	869
C	Carboxylic acid	C8x ring-CH=ring	19905
		C8y ring-C(-R)=ring	20511
		C0	8
		N1a R-NH2	2440
N	Amine	N1b R-NH-R	3003
		N1c R-N(-R)2	374
		N1d R-(N(-R))3+	105
		N1x ring-NH-ring	806
N	Cyclic amine	N1y ring-(N(-R))-ring	1464
		N2a R=N-H	230
		N2b R=N-R	163
		N2x ring-N=ring	357
N	Imine	N2y ring-(N(-R))+=ring	14
		N3a R=N	119
		N4x ring-NH-ring	785
		N4y ring-(N(-R))-ring	840
N	Aromatic ring	N5x ring-N=ring	2131
		N5y ring-(N(-R))+=ring	59
		N0	194
		O1a R-OH	18369
O	Hydroxy	O1b N-OH	198
		O1c P-OH	3111
		O1d S-OH	332
		O2a R-O-R	4199
O	Ether	O2b P-O-R	2481
		O2c P-O-P	502

KEGG GLYCAN (糖鎖構造情報)

- 糖鎖分子の構造を収録したデータベース
 - エントリー数は、約1万1000
- 構造は2次元のグラフとして持つ
 - グラフは、実際にはツリーとなる
- ファイルフォーマットはKCF (Glycan)
 - Compound/Drugとの互換性はない

The screenshot shows the KEGG GLYCAN homepage. At the top, there is a navigation bar with tabs for KEGG2, PATHWAY, BRITE, MODULE, LIGAND, COMPOUND, GLYCAN, and REACTION. Below the navigation bar, there is a search input field labeled "Enter G numbers" with several buttons below it: Filter, Pathway mapping, Brite mapping, Get title, Get entry, and Clear. The main content area is titled "KEGG GLYCAN Structure Database". It contains a paragraph about the database being a collection of experimentally determined glycan structures from CarbBank and KEGG pathways. It also mentions the Composite Structure Map (CSM) which is computationally generated. There are links for DBGET search, LIGAND relational database search, and Monosaccharide codes. Below this, there is a section titled "KEGG Pathway Maps for Glycans" with a small map showing molecular pathways.

KEGG REACTION, RPAIR, RCLASS, ENZYME (生化学反応情報)

- REACTAION (生化学反応)
 - 生体内反応のデータベース
 - 代謝系の酵素反応がメイン
- RPAIR(基質-生成物変化)
- RCLASS(反応分類)
 - RPAIRのパターンによる反応分類
- ENZYME(酵素番号)
 - IUBMBの酵素番号

REACTION, RPAIR, RCLASS

- R00259 acetyl-CoA:L-glutamate N-acetyltransferase を例に -

Firefox ▾

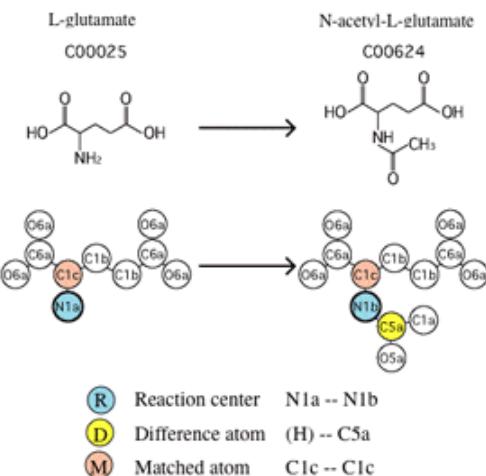
KEGG REACTION: R00259

www.kegg.jp/dbget-bin/www_bget?m:R00259

Google

REACTION: R00259

Entry	R00259	Reaction
Name	acetyl-CoA:L-glutamate N-acetyltransferase	
Definition	Acetyl-CoA + L-Glutamate \leftrightarrow CoA + N-Acetyl-L-glutamate	
Equation	$C00024 + C00025 \leftrightarrow C00010 + C00624$	
RPair	<ul style="list-style-type: none"> RP00007 C00010_C00024_main RP04458 C00025_C00624_main RP08475 C00024_C00624_trans 	
Enzyme	2.3.1.1	
Pathway	<ul style="list-style-type: none"> rn00330 Arginine and proline metabolism rn01100 Metabolic pathways rn01110 Biosynthesis of secondary metabolites 	
Orthology	<ul style="list-style-type: none"> K00618 amino-acid N-acetyltransferase [EC:2.3.1.1] K00619 amino-acid N-acetyltransferase [EC:2.3.1.1] K00620 glutamate N-acetyltransferase / amino-acid N-acetyltransferase [EC:2.3.1.35 2.3.1.1] K11067 N-acetylglutamate synthase [EC:2.3.1.1] K14681 argininosuccinate lyase / amino-acid N-acetyltransferase [EC:4.3.2.1 2.3.1.1] K14682 amino-acid N-acetyltransferase [EC:2.3.1.1] 	



- Reactionの基質と生成物の間で、原子の由来関係を持つ化合物のペアを Reactant Pair と定義
- RPAIRは、Reactant Pairを原子アラインメントして、反応前後の変化を RDMパターンとしてデータ化
- Reaction は RPAIRの組み合わせで表現できる
- Reactant Pairは、生化学的意味に基づきラベル付け可能
- RCLASSは、mainとラベル付けされた Reactant pairの変化の類似性に基づいた反応の分類

LIGANDをbfindでキーワード検索(1)

- 例: phenylalanine -

The figure consists of three screenshots of the KEGG LIGAND Database interface, illustrating the search process for the compound "Phenylalanine".

Screenshot 1: Main Search Interface

- The title bar says "KEGG LIGAND Database".
- The URL is "www.kegg.jp/kegg/ligand.html".
- The search bar at the top right contains "Search LIGAND" and "for Phenylalanine".
- The search results table shows the following rows:

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

- Below the table is a search bar: "Search LIGAND for Phenylalanine" with "Go" and "Clear" buttons.
- A red box highlights the "Search LIGAND" button and the "for Phenylalanine" input field.

Screenshot 2: DBGET Search Result for LIGAND

- The title bar says "DBGET Search Result: LIGAND Phe...".
- The URL is "www.kegg.jp/dbget-bin/www_bfind_sub?mode=bfind&max_h=100".
- The search bar at the top right contains "Search LIGAND" and "for Phenylalanine".
- The results table shows the following rows:

KEGG COMPOUND
C00079 KegDraw Jmol L-Phenylalanine; (S)-alpha-Amino-beta-phenylpropionic acid
C00355 KegDraw Jmol 3,4-Dihydro-L-phenylalanine; L-Dopa; 3-Hydroxy-L-tyrosine; L-beta-(3,4-Dihydrophenyl)alanine; Levodopa; Dihydro-L-phenylalanine
C02057 KegDraw Jmol Phenylalanine; DL-Phenylalanine; alpha-Amino-beta-phenylpropionic acid
C02265 KegDraw Jmol D-Phenylalanine; D-alpha-Amino-beta-phenylpropionic acid
C03519 KegDraw Jmol L-Phenylalanine; D-alpha-Amino-beta-phenylpropionic acid

- Below the table is a link: "... display all".

Screenshot 3: DBGET Search Result for COMPOUND

- The title bar says "DBGET Search Result: COMPOUND ...".
- The URL is "www.kegg.jp/dbget-bin/www_bfind_sub?mode=bfind&mode=1".
- The search bar at the top right contains "Search COMPOUND" and "for Phenylalanine".
- The results table shows the following rows:

KEGG REACTION
R00031 1,2-Benzenediol:oxygen oxidoreductase; Oxygen + 2 L-Tyrosine => 2 3,4-Dihydrox-L-phenylalanine
R00045 3,4-Dihydro-L-phenylalanine:oxygen oxidoreductase; Oxygen + 2 3,4-Dihydrox-L-phenylalanine => 2 Dopachrome + 2 H ₂ O
R00068 L-Phenylalanine racemase (ATP-hydrolysing); ATP + L-Phenylalanine + H ₂ O => AMP + Diphosphate + D-Phenylalanine
R00067 ATP:L-phenylalanine adenyltransferase; ATP + L-Phenylalanine => Diphosphate + N-Adenyl-L-phenylalanine
R00066 L-phenylalanine:NAD ⁺ oxidoreductase (deaminating); L-Phenylalanine + H ₂ O + NAD ⁺ => Phenylpyruvate + NH ₃ + NADH + H ⁺

- Below the table is a link: "... display all".
- A red box highlights the first result row: "C00079 [KegDraw](#) [Jmol](#) L-Phenylalanine; (S)-alpha-Amino-beta-phenylpropionic acid".

KEGG COMPOUND Entry

The screenshot shows the KEGG Compound entry for C00079. The main content includes:

- Entry:** C00079 Compound
- Name:** L-Phenylalanine; (S)-alpha-Amino-beta-phenylpropionic acid
- Formula:** C9H11NO2
- Exact mass:** 165.079
- Mol weight:** 165.1891
- Structure:** A chemical structure diagram of L-phenylalanine.
- Remark:** Same as: D00021
BRITE hierarchy
- Reaction:** R00686 R00687 R00688 R00689 R00690 R00691 R00692 R00693
R00694 R00695 R00697 R00698 R00699 R01375 R01376 R01795
R03680 R06744 R07211 R08435 R08463 R08652 R08690 R09535
R09578 R09579
- Pathway:** ko00360 Phenylalanine metabolism
ko00400 Phenylalanine, tyrosine and tryptophan biosynthesis
ko00940 Phenylpropanoid biosynthesis
ko00960 Tropane, piperidine and pyridine alkaloid biosynthesis
ko00966 Glucosinolate biosynthesis
ko00970 Aminocycl-(RNA) biosynthesis
map01060 Biosynthesis of plant secondary metabolites
map01061 Biosynthesis of phenylpropanoids
map01063 Biosynthesis of alkaloids derived from shikimate pathway
map01064 Biosynthesis of alkaloids derived from ornithine, lysine and nicotinic acid
map01070 Biosynthesis of plant hormones
ko01100 Metabolic pathways
ko01110 Biosynthesis of secondary metabolites
ko02010 ABC transporters
ko04974 Protein digestion and absorption
ko04978 Mineral absorption
- Enzyme:** 1.4.1.20 1.4.3.2 1.11.1.7 1.11.1.21
1.13.12.9 1.14.13.124 1.14.16.1 2.3.1.53
2.6.1.1 2.6.1.5 2.6.1.9 2.6.1.28
2.6.1.57 2.6.1.58 2.6.1.64 2.6.1.70
2.7.7.54 3.4.17.23 4.1.1.28 4.1.1.53
4.2.1.51 4.2.1.91 4.3.1.24 4.3.1.25
5.1.1.11 6.1.1.20
- Other DBs:** CAS: 63-91-2
PubChem: 3379
ChEBI: 17295
KNApSAcK: C00001386
PDB-CCD: PHE
3DMET: B01151
NIKKAJI: J9.175H
- KCF data:** Show

構造表示、
構造情報(mol, KCF)、
構造検索、構造表示(&編集)、

各種データベースへのリンク
REACTION, PATHWAY, ENZYME

外部データベースへのリンク
PubChem, ChEBI, etc.

LinkDB情報
GenomeNet内部でリンクされているDBや
対応関係のとれる外部DBを表示

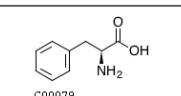
SIMCOMP search

Firefox ▾ SIMCOMP Search www.genome.jp/tools-bin/strsearch_view?pid=4442 Google

SIMCOMP Search

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

Query C00079

Structure 

C00079

Database COMPOUND DRUG KNAPSAcK REACTION

Options Global search Local search Customized search
► Option details

Feedback KEGG GenomeNet Kyoto University Bioinformatics Center

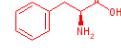
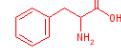
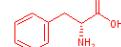
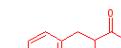
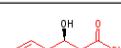
Firefox ▾ SIMCOMP Search www.genome.jp/tools-bin/search_list?DATABASE=compound&TARGET=compound Google

SIMCOMP Search Result

Database : KEGG COMPOUND Number of entries in a page: 20 Hide structure

Page : 1 Go of 21 Items : 1 - 20 of 413 Top Previous Next Bottom

Top 10 Clear Select operation Exec

No	Entry	Structure	Name
1	C00079		L-Phenylalanine (S)-alpha-Amino-beta-phenylpropionic acid
2	C02057		Phenylalanine DL-Phenylalanine alpha-Amino-beta-phenylpropionic acid
3	C02265		D-Phenylalanine D-alpha-Amino-beta-phenylpropionic acid
4	C00082		L-Tyrosine (S)-3-(p-Hydroxyphenyl)alanine (S)-2-Amino-3-(p-hydroxyphenyl)propionic acid Tyrosine
5	C01536		DL-Tyrosine 3-(p-Hydroxyphenyl)alanine 2-Amino-3-(p-hydroxyphenyl)propionic acid Tyrosine
6	C03290		L-threo-3-Phenylserine

LIGANDをbfindでキーワード検索 (2)

- 例: phenylalanine -

Firefox - KEGG LIGAND Database + www.kegg.jp/kegg/ligand.html

KEGG LIGAND Database
Molecular building blocks of life in the chemical space

KEGG2 PATHWAY BRITE MODULE LIGAND COMPOUND GLYCAN REACTI

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 number respectively. ENZYME is derived from the IUBMB/IUPAC Enzyme Nomenclature, but the others are internally developed and maintained.

Database	Identifier	Content	Specialized entry point
COMPOUND	C number	Chemical compound structures	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	

Search LIGAND for Phenylalanine Go Clear

bfind mode bget mode

Firefox - DBGET Search Result: LIGAND Phe... + www.kegg.jp/dbget-bin/www_bfind_sub?mode=bfind&max_h

KEGG LIGAND Database - Search term: Phenylalanine

Database: LIGAND - Search term: Phenylalanine

Go Clear

C00079 **KeptRaw Jml**
L-Phenylalanine, (S)-alpha-Amino-beta-phenylpropionic acid

C00355 **KeptRaw Jml**
3,4-Dihydro-L-phenylalanine, L-Ospra, 3-Hydroxy-L-tyrosine, L-beta-(3,4-Dihydrophenyl)alanine, Levodopa, Dihydro-L-phenylalanine

C02057 **KeptRaw Jml**
Phenylalanine, DL-Phenylalanine, alpha-Amino-beta-phenylpropionic acid

C02058 **KeptRaw Jml**
D-Phenylalanine, D-alpha-Amino-beta-phenylpropionic acid

C03519 **KeptRaw Jml**
L-phenylalanine, D-phenylalanine

... display all

KEGG REACTION

R00031 1,2-Benzenediol:oxygen oxidoreductase; Oxygen + 2 L-Tyrosine <=> 2,3,4-Dihydroxy-L-phenylalanine

R00045 3,4-dihydroxy-L-phenylalanine:oxygen oxidoreductase; Oxygen + 2 3,4-Dihydroxy-L-phenylalanine <=> 2 Dopaquinone + 2 H2O

R00686 L-Phenylalanine racemase (ATP-hydrolysing); ATP + L-Phenylalanine + H2O <=> AMP + Diphosphate + D-Phenylalanine

R00687 ATP:L-phenylalanine adenylyltransferase; ATP + L-Phenylalanine <=> Diphosphate + N-Adenyl-L-phenylalanine

R00688 L-phenylalanine:NAD+ oxido-reductase (deaminating); L-Phenylalanine + H2O + NAD+ <=> Phenylpyruvate + NH3 + NADH + H+

R00689 L-phenylalanine:oxygen oxido-reductase (deaminating); L-Phenylalanine + H2O + Oxygen <=> Phenylpyruvate + NH3 + Hydrogen peroxide

R00690 L-Phenylalanine:oxygen 2-oxidoreductase (decarboxylating); L-Phenylalanine + Oxygen <=> 2-Phenylacetamide + CO2 + H2O

R00691 L-Argenote hydro-lyase (decarboxylating; L-phenylalanine-forming); L-Arogenate <=> L-Phenylalanine + H2O + CO2

R00692 L-phenylalanine:pyruvate aminotransferase; L-Phenylalanine + Pyruvate <=> Phenylpyruvate + L-Alanine

R00693 Acetyl-CoA:L-phenylalanine N-acetyltransferase; Acetyl-CoA + L-Phenylalanine <=> CoA + N-Acetyl-L-phenylalanine

R00694 L-Phenylalanine:2-oxoglutarate aminotransferase; L-Phenylalanine + 2-Oxoglutarate <=> Phenylpyruvate + L-Glutamate

R00695 L-Aspartate:phenylpyruvate aminotransferase; L-Aspartate + Phenylpyruvate <=> Oxaloacetate + L-Phenylalanine

R00697 L-phenylalanine ammonia-lyase (trans-cinnamate-forming); L-Phenylalanine <=> trans-Cinnamate + NH3

R00698 L-phenylalanine:oxygen oxido-reductase (decarboxylating); L-Phenylalanine + Oxygen <=> 2-Phenylacetamide + CO2

R00699 L-phenylalanine carboxy-lyase (phenylethylamine-forming); L-Phenylalanine <=> Phenethylamine + CO2

R00731 L-Tyrosine:oxygen oxido-reductase; L-Tyrosine + Oxygen <=> 3,4-Dihydroxy-L-phenylalanine + H2O

R01374 D-phenylalanine:acceptor oxido-reductase (deaminating); D-Phenylalanine + H2O + Acceptor <=> Phenylpyruvate + NH3 + Reduced acceptor

KEGG REACTION Entry

The screenshot shows the KEGG REACTION entry for R00697. The main content includes:

- Entry:** R00697
- Name:** L-phenylalanine ammonia-lyase (trans-cinnamate-forming)
- Definition:** L-phenylalanine <=> trans-Cinnamate + NH₃
- Equation:** C00079 <=> C00423 + C00014
- Rpair:** RP01058 C00079_C00423 main
RP05821 C00014_C00079 leave
- Enzyme:** 4.3.1.24 4.3.1.25
- Pathway:** rn00360 Phenylalanine metabolism
rn00910 Nitrogen metabolism
rn00940 Phenylpropanoid biosynthesis
rn01100 Metabolic pathways
rn01110 Biosynthesis of secondary metabolites
- Orthology:** K10775 phenylalanine ammonia-lyase [EC:4.3.1.24]
K13064 phenylalanine/tyrosine ammonia-lyase [EC:4.3.1.25]

Chemical structures shown in the reaction equation:

Cc1ccccc1Cc2c(N)cccc2C(=O)O <=> O=Cc1ccccc1Cc2c(N)cccc2 + N

A red box highlights the reaction equation and its components. A red box also highlights the "All links" section on the right side of the page.

反応式(物質名、C番号、図)、

各種データベースへのリンク
RPAIR, PATHWAY, ENZYME, KO

LinkDB情報

GenomeNet内部でリンクされているDBや
対応関係のとれる外部DBを表示

KEGG RPAIR Entry

Firefox KEGG RPAIR: RP01058 www.kegg.jp/dbget-bin/www_bget?rp:RP01058 Google Help

RPAIR: RP01058

Entry	RP01058	RPair
Name	C00079_C00423	
Compound	C00079 L-Phenylalanine C00423 trans-Cinnamate	
Type	main	
RDM	2 1 C1b-C2b:-*:C1c+C8y-C2b+C8y 2 C1c-C2b:N1a-*:C1b+O6a-C2b+O6a	
RClass	RC00361	
Related pair	RP01074 RP01342	
Reaction	R00897	
Enzyme	4.3.1.24 4.3.1.25	
KCF data	Show	

アライメントの結果(図)

ペアのフラグ情報(生化学的意味)

RDMの文字列表記

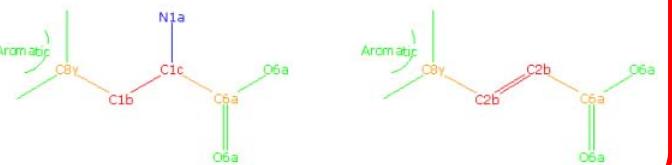
各種データベースへのリンク

(COMPOUND, RCLASS, Related RPAIR,
REACTION, ENZYME)

KEGG RCLASS Entry

Firefox KEGG RCLASS: RC00361 www.kegg.jp/dbget-bin/www_bget?rc:RC00361 Google Help All links

RCLASS: RC00361

Entry	RC00361	RClass
Definition	C1b-C2b:--*:C1c+C8y-C2b+C8y C1c-C2b:N1a-*:C1b+C8a-C2b+C8a	
RPAIR	RP01058 RP01074 RP01342	DB search
Related class	DB search	
Reaction	R00697 R00737 R01168	
Enzyme	4.3.1.3 4.3.1.23 4.3.1.24 4.3.1.25	
Pathway	rn00340 Histidine metabolism rn00360 Phenylalanine metabolism rn00910 Nitrogen metabolism rn00940 Phenylpropanoid biosynthesis rn01100 Metabolic pathways rn01110 Biosynthesis of secondary metabolites	
Orthology	K01745 histidine ammonia-lyase [EC:4.3.1.3] K10774 tyrosine ammonia-lyase [EC:4.3.1.23] K10775 phenylalanine ammonia-lyase [EC:4.3.1.24] K13064 phenylalanine/tyrosine ammonia-lyase [EC:4.3.1.25]	

RDM変換パターン(文字列、図)

RCLASSに含まれる RPAIR
各種データベースへのリンク
(RPAIR, Related RCLASS,
REACTION, ENZYME, PATHWAY, KO)

GenomeNetからの化合物データベース一括検索機能

GenomeNet

www.genome.jp

GenomeNet

KEGG KEGG2 PATHWAY BRITE MEDICUS DBGET

Search All databases for Phenylalanine Go Clear

Chemical substance

L-Phenylalanine; (S)-alpha-Amino-beta-phenylpropionic acid
C00355 KegDraw Jmol
3,4-Dihydroxy-L-phenylalanine; L-Dopa; 3-Hydroxy-L-tyrosine; L-beta-(3,4-Dihydroxyphenyl)alanine;

カテゴリー1～3のデータベース

統合データベースを選択しキーワードを入力するとメニューに表示されているデータベース全てに対する検索となる。

DBGET Search Result: All databases... +

www.genome.jp/dbget-bin/www_bfind_sub?mode=bfind&ma

Chemical substance

103024702 [PubChem]
D-Phenylalanine, N-[(phenylmethoxy)carbonyl]-, 4-chloro-2-[(4-chlorophenyl)amino]carbonyl]phenyl ester

103025974 [PubChem]
)isoquinolinyl)methyl]-3-phenylpropyl ester; L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, (1R,2S)-2-[(2S)-4-amino-1,4-dioxo-2-[(2-quinolinylcarbonyl)amino]butyl]amino]-1-[(3S,4aS,8aS)-3-[(1,1-dimethylethyl)amino]carbonyl]octahydro-2(1H,8aH,9aH,10aH)-3-phenyl-2-(trimethylammonio)propanoate; L-Phenylalanine betaine

103032560 [PubChem]
2-Methylpropyl N-[[((2R,5R)-5-(6-amino-9H-purin-9-yl)-4-fluoro-2,5-dihydrofuran-2-yl)oxy)methyl] (phenoxy)phosphoryl]L-phenylalaninate; Mono(isobutyl-phenylalanine) amide

103044993 [PubChem]
poly(lysine-co-phenylalanine)
... » display all

CHEBI

41654 [ChEBI]
N-[(2S)-2-[(4S)-2-amino-1,4,5,6-tetrahydropyrimidin-4-yl]-2-((1S)-1-carboxy-2-phenylethyl)carbamoyl]amino)acetyl]L-leucyl-L-phenylalanine

53490 [ChEBI] [KEGG-link]
N-formyl-L-methionyl-L-leucyl-L-phenylalanine; [CPD:C11596]

21371 [ChEBI]
L-phenylalanine amide

61957 [ChEBI]
L-phenylalanine amide group

29997 [ChEBI]
L-phenylalanine residue
... » display all

英 語: <http://www.genome.jp/>
日本語: <http://www.genome.jp/ja/>

Kyoto University

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KEGGのシステム情報、ツール (PATHWAY, BRITE, KEGG MAPPER)

KEGG: Kyoto Encyclopedia of Genes and Genomes

Firefox KEGG: Kyoto Encyclopedia of Genes... www.kegg.jp/kegg/ Search Help Japanese

KEGG Home
Release notes
Current statistics
Plea from KEGG

KEGG Database
KEGG overview
Searching KEGG
KEGG mapping
Color codes

KEGG Objects
Pathway maps
Brite hierarchies

KEGG Software
KegTools
KEGG API
KGML

KEGG FTP
Subscription

GenomeNet

DBGET/LinkDB

Feedback

Kanehisa Labs

KEGG: Kyoto Encyclopedia of Genes and Genomes

Announcement
The KEGG website at www.kegg.jp has become the primary site of the KEGG database developed by Kanehisa Laboratories (see the [article](#) in the NAR 2012 Database Issue). The GenomeNet website at www.genome.jp operated by Kyoto University Bioinformatics Center will continue to mirror the KEGG database and provide additional KEGG-based analysis services (see [Release notes](#)).

Main entry point to the KEGG web service
KEGG2 KEGG Table of Contents Update notes

Data-oriented entry points

- KEGG PATHWAY** KEGG pathway maps [Pathway list]
- KEGG BRITE** BRITE functional hierarchies [Brite list]
- KEGG MODULE** KEGG modules [Module list]
- KEGG DISEASE** Human diseases [Cancer | Infectious disease]
- KEGG DRUG** Drugs [ATC drug classification]
- KEGG ORTHOLOGY** Ortholog groups [KO system]
- KEGG GENOME** Genomes [KEGG organisms]
- KEGG GENES** Genes and proteins Release history
- KEGG LIGAND** Chemical information [Compound classification]

Entry point for wider society
KEGG MEDICUS Health-related information resource

Organism-specific entry points
KEGG Organisms Enter org code(s) Go hsa hsa eco

Analysis tools

- KEGG Mapper** KEGG PATHWAY/BRITE/MODULE mapping tools
- KEGG Atlas** Navigation tool to explore KEGG global maps
- KAAS** KEGG automatic annotation server
- BLAST/Fasta** Sequence similarity search
- SIMCOMP** Chemical structure similarity search
- PathPred** Biodegradation/biosynthesis pathway prediction

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Firefox KEGG - Table of Contents www.kegg.jp/kegg/kegg2.html Search Google

KEGG - Table of Contents

KEGG2 PATHWAY BRITE MODULE DISEASE DRUG KO GENOME GENES LIGAND DBGET

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 BLAST / FASTA search KAAS automatic annotation Map organisms to taxonomy Generate taxonomy tree KEGG organisms
KEGG LIGAND KEGG COMPOUND KEGG GLYCAN KEGG REACTION			SIMCOMP / SUBCOMP search KCaM search E-zyme reaction prediction PathPred pathway prediction PathComp path computation PathSearch reaction search	COMPOUND GLYCAN REACTION RPAIR RCLASS ENZYME
See Kanehisa et al. (2012) for the new features of KEGG.				
KEGG for specific organisms				
KEGG Organisms - the list of currently available organisms				
Select Organism <input type="text"/> Go Clear (examples) hsa mmu sce eco bsu syn				
KEGG Pangenomes - the list of pangenomes defined from KEGG organisms				
KEGG mapping for genome comparison and combination				

KEGG PATHWAY

生体内(外)の分子間ネットワーク図

The screenshot shows the KEGG PATHWAY Database homepage. At the top, there's a navigation bar with links for KEGG2, PATHWAY, BRITE, MODULE, DISEASE, DRUG, KO, GENOME, GENES, LIGAND, and DBGET. Below the navigation is a search bar with 'Select prefix' dropdowns for 'map' and 'Organism', and an 'Enter keywords' input field with a 'Go' button. A 'Help' link is also present. The main content area is titled 'Pathway Maps' and contains a brief introduction. It lists several categories: 1. Global Map, 2. Metabolism (with a red box around 'Carbohydrate'), 3. Genetic Information Processing, 4. Environmental Information Processing, 5. Cellular Processes, 6. Organismal Systems, and 6. Human Diseases. Below this, it mentions 'Drug Development'. Under 'Pathway Mapping', it describes the process and provides three tools: 'Search Pathway', 'Search&Color Pathway', and 'Color Pathway'. A large blue box highlights the 'Carbohydrate' section, which links to 'Glycolysis / Gluconeogenesis'.

<http://www.genome.jp/kegg/pathway.html>

Carbohydrate

→ Glycolysis / Gluconeogenesis

• 代謝系

- 12カテゴリ
- 中間代謝、二次代謝、薬の代謝、全体像

• 制御系

- 20カテゴリ
- 遺伝制御、環境シグナル、細胞プロセス、生体システム他

• 疾患

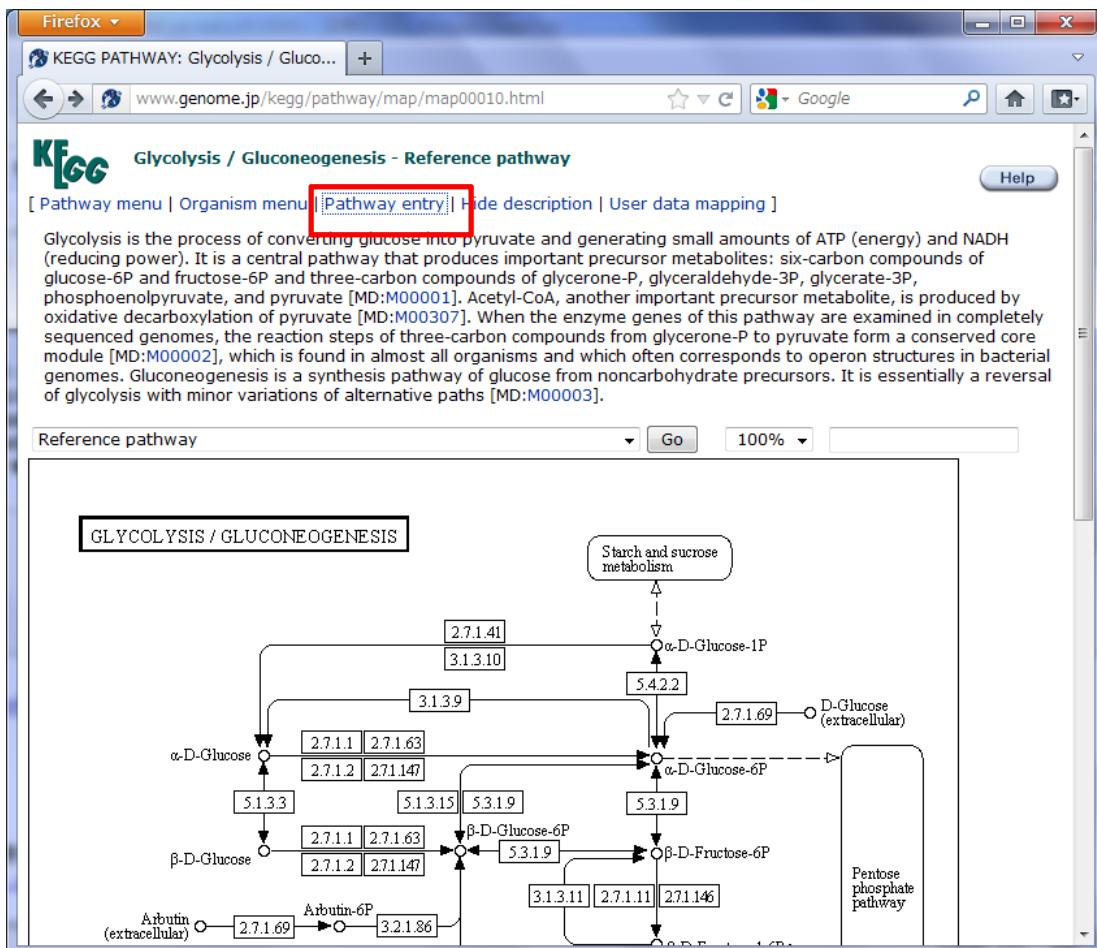
- がん、免疫・神経変性・循環器・代謝疾患、感染症

• 薬の開発

- 開発の歴史、標的ベース、構造ベース

KEGG PATHWAY

マップの例：解糖系



- 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
 - 生物種の階層分類
- Pathway entry
 - パスウェイデータベースのテキストバージョン
- Hide description
 - マップの説明を隠す
- User data mapping
 - マップ中のオブジェクトへの色付け
- – マップの拡大縮小

KEGG PATHWAY

テキストエントリー

Firefox

KEGG PATHWAY: map00010

www.genome.jp/dbget-bin/www_bget?pathway+map00010

PATHWAY: map00010

Help

Entry map00010 Pathway

Name Glycolysis / Gluconeogenesis

Description Glycolysis is the process of converting glucose into pyruvate and generating small amounts of ATP (energy) and NADH (reducing power). It is a central pathway that produces important precursor metabolites: six-carbon compounds of glucose-6P and fructose-6P and three-carbon compounds of glycerone-P, glyceraldehyde-3P, glycerate-3P, phosphoenolpyruvate, and pyruvate [MD:MO0001]. Acetyl-CoA, another important precursor metabolite, is produced via oxidative decarboxylation of pyruvate [MD:MO00307]. When the enzyme genes of this pathway are examined in completely sequenced genomes, the reaction steps of three-carbon compounds from glycerone-P to pyruvate form a conserved core module [MD:MO0002], which is found in almost all organisms and which often corresponds to operon structures in bacterial genomes. Gluconeogenesis is a synthesis pathway of glucose from noncarbohydrate precursors. It is essentially a reversal of glycolysis with minor variations of alternative paths [MD:MO0003].

Class Metabolism; Carbohydrate Metabolism
BRITE hierarchy

Pathway map map00010 Glycolysis / Gluconeogenesis

All links

- Ontology (4)
 - KEGG BRITE (2)
 - GO (2)
- Pathway (45)
 - KEGG PATHWAY (3)
 - KEGG MODULE (9)
- Disease (4)
 - KEGG DISEASE (4)
- Chemical substance
 - KEGG COMPOUND (1)
- Chemical reaction
 - KEGG ENZYME (45)
 - KEGG REACTION (1)
 - KEGG ORTHOLOGY (1)
- All databases (266)

Download RDF

- Pathway entry

- Entry

- マップ番号 (map|ko|ec|rn|生物種コード+番号)

- Name, Description

- パスウェイの説明とモジュールとの関係

- Class

- 階層分類情報

- Pathway map

- マップとオーソログテーブルへのリンク

- Disease

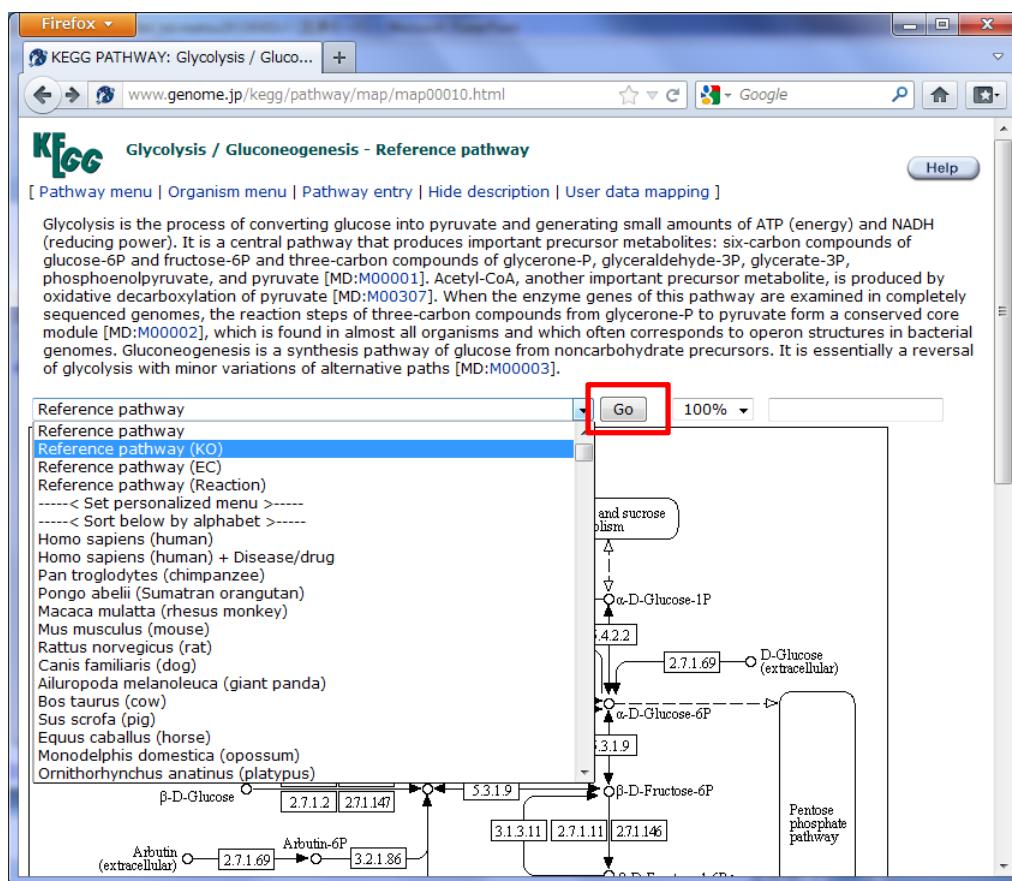
- Reference

- モジュール

- 生物種間での保存、複合体、オペロンを考慮した機能単位

KEGG PATHWAY

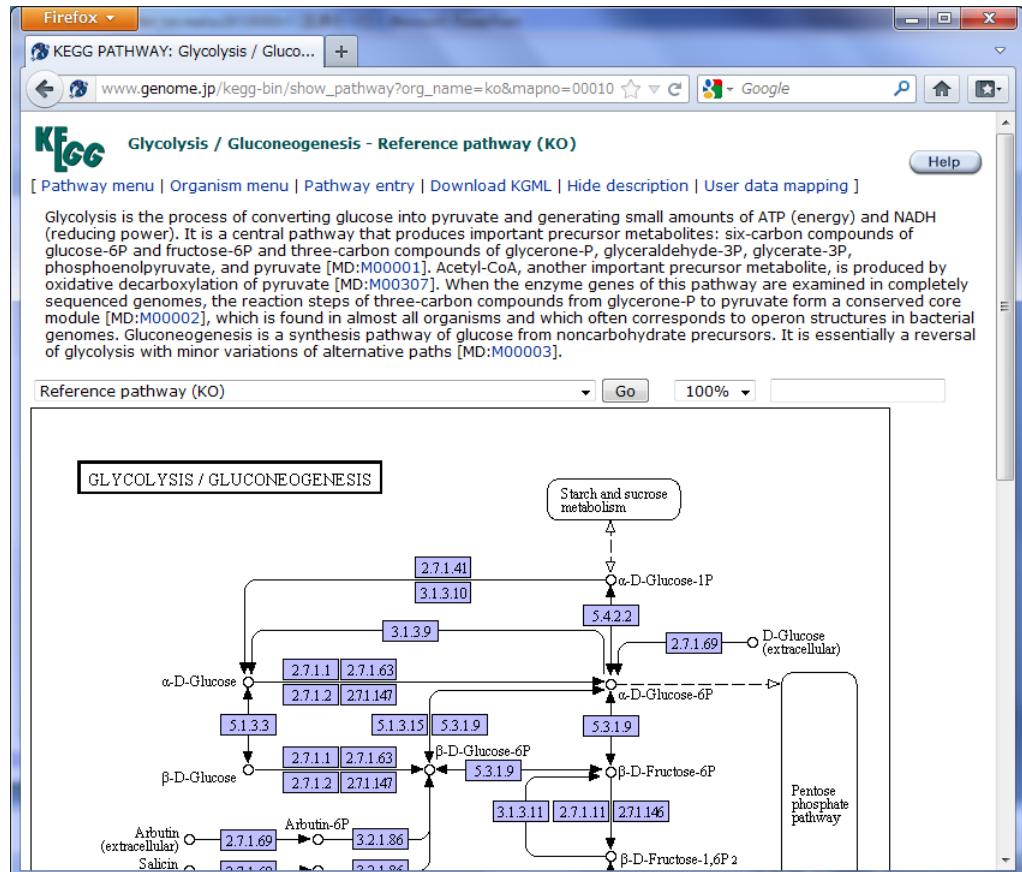
マップの例：解糖系



- [Reference pathway](#)
 - K0, EC, Reactionへのリンク
 - (K0) オーソログエントリーへのリンク
 - (EC) 酵素エントリーへのリンク
 - (Reaction) 反応エントリーへのリンク
- [生物種名](#)
 - 各生物種の遺伝子エントリーへのリンク
- [Set personalized menu](#)
 - 生物種の選択
- [Sort below by](#)
 - 生物種名のソート

KEGG PATHWAY

マップの例：解糖系 (EC)



- Reference pathway (EC)

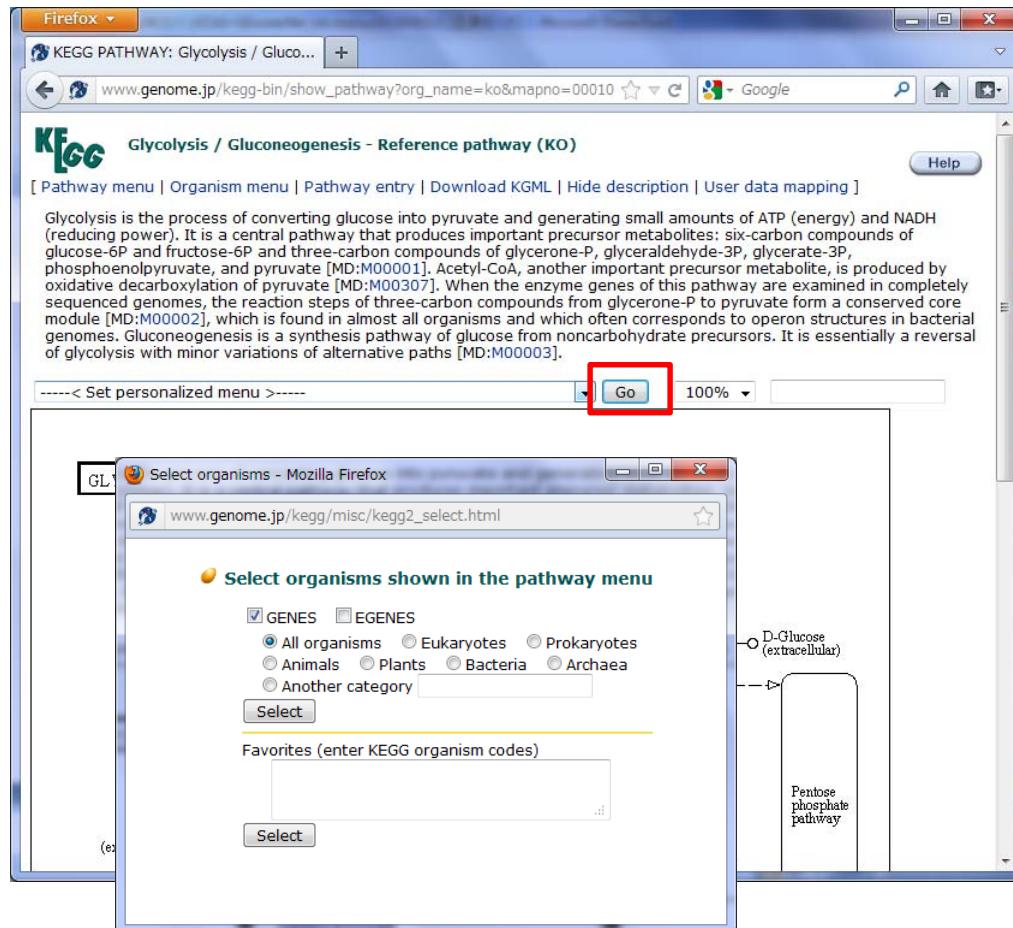
- 従来のリファレンスに対応
- 対応する酵素エントリーのある箱に色づけ

- Reference pathway (KO)

- 対応するオーソログエントリーのある箱に色づけ
- KEGG GENES に登録されている生物種が持つ遺伝子に関して配列の類似度を元に定義されているオーソログ情報
- 酵素によってはオーソログが定義できないものもある

KEGG PATHWAY

生物種の選択



- リストの生物種を限定する
 - カテゴリーは KEGG 生物種一覧のものが指定可能
 - Mammals, Protists, Actinobacteria など
 - 生物種コードも KEGG 生物種一覧のものが指定可能
 - hsa (ヒト), mmu (マウス), eco (大腸菌) など

PATHWAY の検索とマッピング

The screenshot shows the KEGG PATHWAY Database search interface in a Firefox browser window. The URL is www.genome.jp/kegg/pathway.html. The search bar contains 'hsa' in the 'Select prefix' field and 'cancer' in the 'Enter Keywords' field. A red box highlights this search input area. Below the search bar, there's a 'Pathway Maps' section with a brief introduction and a list of categories: 0. Global Map, 1. Metabolism, 2. Genetic Information Processing, 3. Environmental Information Processing, 4. Cellular Processes, 5. Organismal Systems, 6. Human Diseases. Another red box highlights the 'Search Pathway' link in the 'Pathway Mapping' section at the bottom, which also lists 'Search&Color Pathway' and 'Color Pathway'.

キーワード検索

- Entry, Name, Description フィールドとマップ中のオブジェクト（遺伝子、オーソログ、反応、化合物）や注釈を対象とした検索
- 複数キーワードは AND 検索

オブジェクトマッピング KEGG Mapper

- マップ中のオブジェクトを指定してパスウェイにマッピング
- 複数オブジェクトを指定するとマッチしたものすべてをマッピング
- Search Pathway
 - 指定したオブジェクトを赤く色づけ
- Search & Color Pathway
 - 指定したオブジェクトを自由に色づけ
- Color Pathway
 - 指定したパスウェイにオブジェクトの色データを与えて色づけ、数値を与えることも可能

PATHWAY のキーワード検索

Firefox KEGG PATHWAY Database www.genome.jp/kegg/pathway.html Google

KEGG PATHWAY Database
Wiring diagrams of molecular interactions, reactions, and relations

Select prefix Enter keywords
hsa Organism cancer 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 various organisms.

- 0. Global Map
- 1. Metabolism
- Carbohydrate Energy Lipid Nucleotide Amino acid Other amino acid Glycan Cofactor/vitamin Terpenoid/PK Other secondary metabolite Xenobiotics Overview
- 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 genomics, transcriptomics, proteomics, and metabolomics, to the KEGG pathway maps for interpretation of higher-level systemic functions.

- Search Pathway - basic pathway mapping tool
- Search&Color Pathway - advanced pathway mapping tool

Firefox Pathway Search Result www.kegg.jp/kegg-bin/search_pathway_text?map=hsa&keyword=cancer Google

Pathway Text Search

Number of entries in a page 20 Hide thumbnail

Items : 1 - 19 of 19

Entry	Thumbnail Image	Name	Description	Object
hsa05215		Prostate cancer - Homo sapiens (human)	Prostate cancer constitutes a major health problem in Western countries. It is the most frequently diagnosed cancer in men worldwide. The prostate cancer pathway map shows the molecular mechanisms underlying prostate cancer development, including signaling pathways involving MAPK, PI3K/Akt, and Wnt signaling, as well as genetic alterations such as PTEN loss and AR mutations.	...010; MAPK signaling pathway hsa05215: Prostate cancer hsa04110: Cell cycle
hsa05223		Non-small cell lung cancer - Homo sapiens (human)	Lung cancer is a leading cause of cancer death among men and women in industrialized countries. The non-small cell lung cancer pathway map shows the molecular mechanisms underlying lung cancer development, including signaling pathways involving RAS, PI3K/Akt, and NF-κB, as well as genetic alterations such as EGFR mutations and TP53 loss.	...RAF) 3845 (KRAS hsa05223: Non-small cell lung cancer hsa04110: Cell cycle hsa04115: p53 signaling pathway
hsa05213		Endometrial cancer (EC) - Homo sapiens (human)	Endometrial cancer (EC) is the most common gynaecological malignancy and the fourth leading cause of cancer death in women worldwide. The endometrial cancer pathway map shows the molecular mechanisms underlying EC development, including signaling pathways involving MAPK, PI3K/Akt, and Wnt signaling, as well as genetic alterations such as PTEN loss and BRAF mutations.	...: MAPK signaling pathway hsa05213: Endometrial cancer hsa04310: Wnt signaling pathway



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<http://www.genome.jp/kegg/pathway.html>

PATHWAY のオブジェクトに好きな色を付ける

The screenshot shows two browser windows. The left window is the 'KEGG PATHWAY Database' with a search bar for 'cancer'. The right window is 'KEGG Mapper: Color Objects in KEGG Pathways' with a search input field containing 'K01803 red,blue' and 'C00118 pink', and a red box highlighting this input. A red box also highlights the 'Exec' button at the bottom of the search form.

KEGG PATHWAY Database

Wiring diagrams of molecular interactions, reactions, and relations

KEGG2 PATHWAY BRITE MODULE DISEASE DRUG KO GENOME GENES LIGAND DBGET

Select prefix Enter keywords
hsa Organism cancer 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:

0. Global Map
1. Metabolism
- Carbohydrate Energy Lipid Nucleotide Amino acid Other amino acid Glycan Cofactor/vitamin Terpenoid/PK Other secondary metabolite Xenobiotics Overview
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

KEGG Mapper: Color Objects in KEGG Pathways

KEGG Mapper Search Pathway Color Pathway Search Brite Color Brite Join Brite

Search against: Reference pathway (KO)

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) ファイルが選択されていません

If necessary, change default bgcolor: pink

Include aliases
 Use uncolored diagrams
 Display objects not found in the search

Exec Clear

- オブジェクトの色を指定する
(html で使える色指定ならOK)
- Example をコピペ

<http://www.genome.jp/kegg/pathway.html>

PATHWAY のオブジェクトに好きな色を付ける

Search PATHWAY

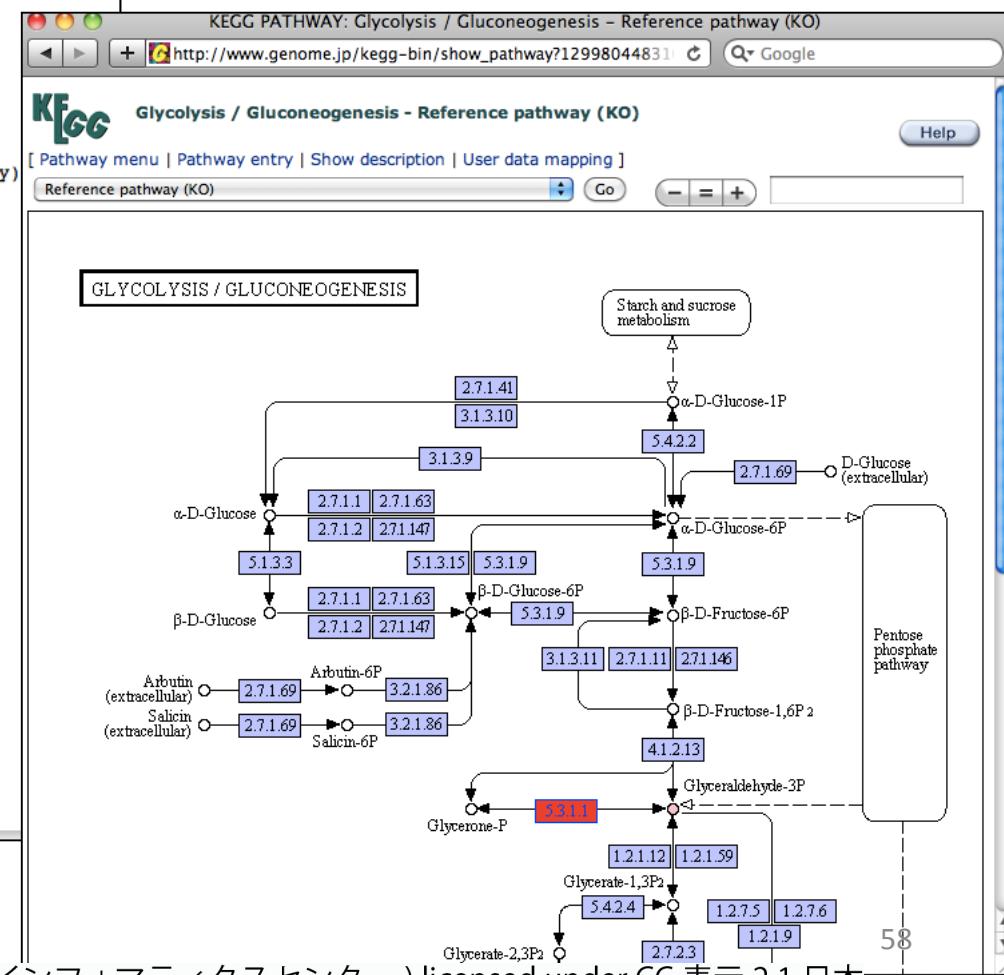
http://www.genome.jp/kegg-bin/color_pathway

Pathway Search Result

Sort by the pathway list

Show all objects

- ko00562 Inositol phosphate metabolism (2)
- ko00010 Glycolysis / Gluconeogenesis (2)
 - cpd:C00118 D-Glyceraldehyde 3-phosphate; (2R)-2-Hydroxy-3-(phosphonoxy) ko:K01803 TPI, tpiA; triosephosphate isomerase (TIM) [EC:5.3.1.1]
- ko00051 Fructose and mannose metabolism (2)
- ko01100 Metabolic pathways (2)
- ko00710 Carbon fixation in photosynthetic organisms (2)
- ko01110 Biosynthesis of secondary metabolites (2)
- ko01120 Microbial metabolism in diverse environments (2)
- ko00900 Terpenoid backbone biosynthesis (1)
- ko00730 Thiamine metabolism (1)
- ko00052 Galactose metabolism (1)
- ko00030 Pentose phosphate pathway (1)
- ko00040 Pentose and glucuronate interconversions (1)
- ko00750 Vitamin B6 metabolism (1)
- ko00331 Clavulanic acid biosynthesis (1)
- ko00680 Methane metabolism (1)



KEGG GENOME

<http://www.genome.jp/kegg/genome.html>

KEGG GENOME Database

Organisms and ecosystems with genome sequence information

KEGG2 PATHWAY BRITE KO GENES SSDB GENOME Organisms

Enter KEGG organism code or use Organism button to select

Organism Go Clear (Examples) hsa mmu dme cel ath sce eco bsu syn mja

KEGG Organisms and Ecosystems

KEGG GENOME has been a collection of KEGG organisms (see [release history](#)), which are the organisms with known complete genome sequences supplemented by those with massive EST datasets (see also KEGG GENES). KEGG GENOME is being extended in three ways. First, it now contains metagenomes representing environmental samples (ecosystems) of genome sequences for multiple species. Second, KEGG organisms with high-quality KOALA annotation can now be combined computationally to examine, for example, reconstructed pathways for pangenomes and organism groups. Third, virus genomes will be integrated and virus genes will be annotated.

Category	Genome	Identifiers	Gene catalog	Annotation
Organisms	GENOME	T0 numbers or three-letter organism codes	GENES	KOALA
		T1 numbers or four-letter organism codes starting with "d"	DGENES	KAAS
		T2 numbers or four-letter organism codes starting with "e"	EGENES	KAAS
Metagenomes		T3 numbers	MGENES	KAAS
Pangenomes		Generic species names	GENES	KOALA
Viruses	VGENOME	RefSeq identifiers	VGENES	None

- KEGG 生物種ごとの入り口
 - GENES/DGENES : ゲノムが決定された生物種
 - EGENES : ESTで作成された遺伝子セット
 - MGENES : メタゲノムデータ
 - Pangenomes : 近縁生物種をまとめたもの
 - Viruses
- 生物種の組み合わせ

KEGG Organism Groups

An organism group is defined as a combination of KEGG organisms, enabling the analysis of combined pathway maps for the group, for example, in symbiosis or pathogenesis.

Define organism group (enter three-letter organism codes): Go

(Metagenome example)
hsa+T30003 Homo sapiens (human) + gut microbiome *New!*

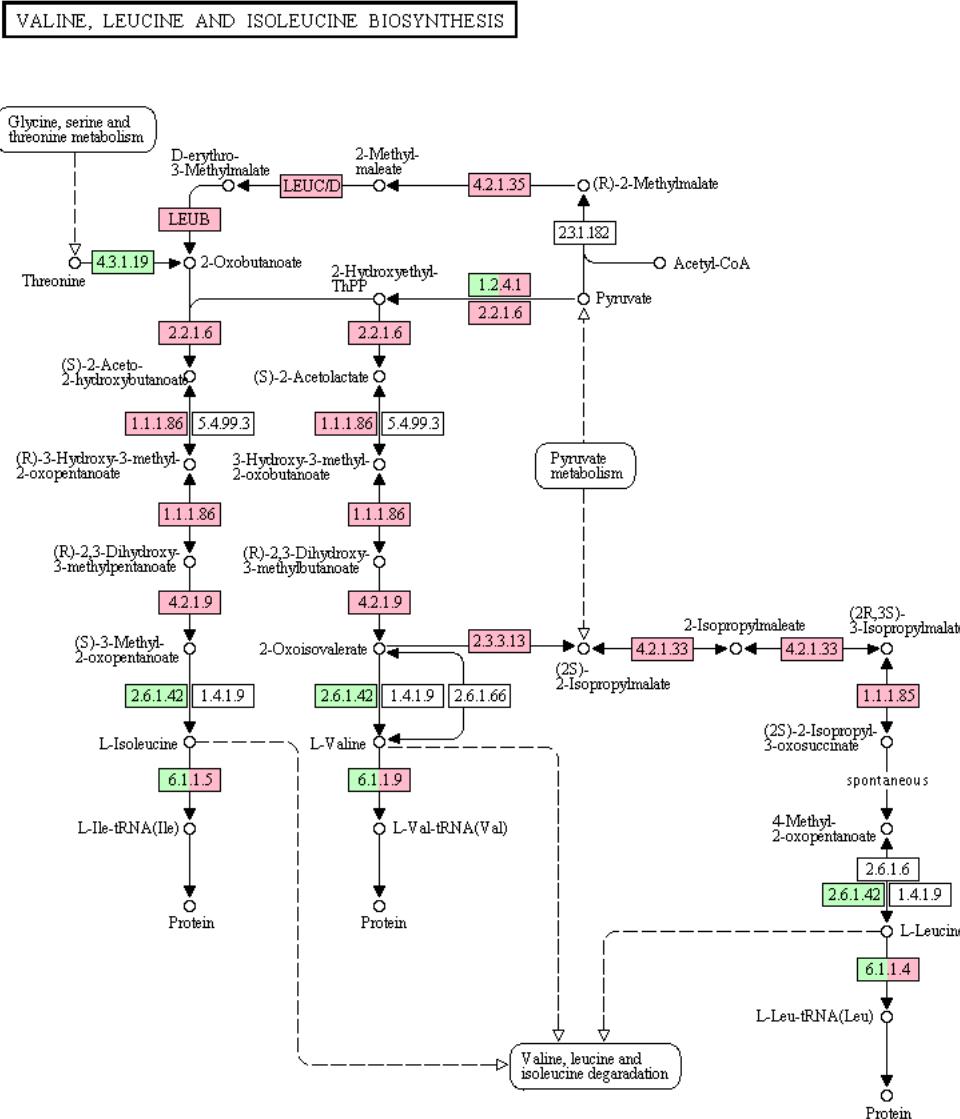
(Symbiosis examples)

dja+mlo Lotus japonicus (lotus) + Mesorhizobium loti
api+buc Acyrthosiphon pisum (pea aphid) + Buchnera aphidicola
bmy+wbm Brugia malayi (filaria) + Wolbachia

(Pathogenesis examples)

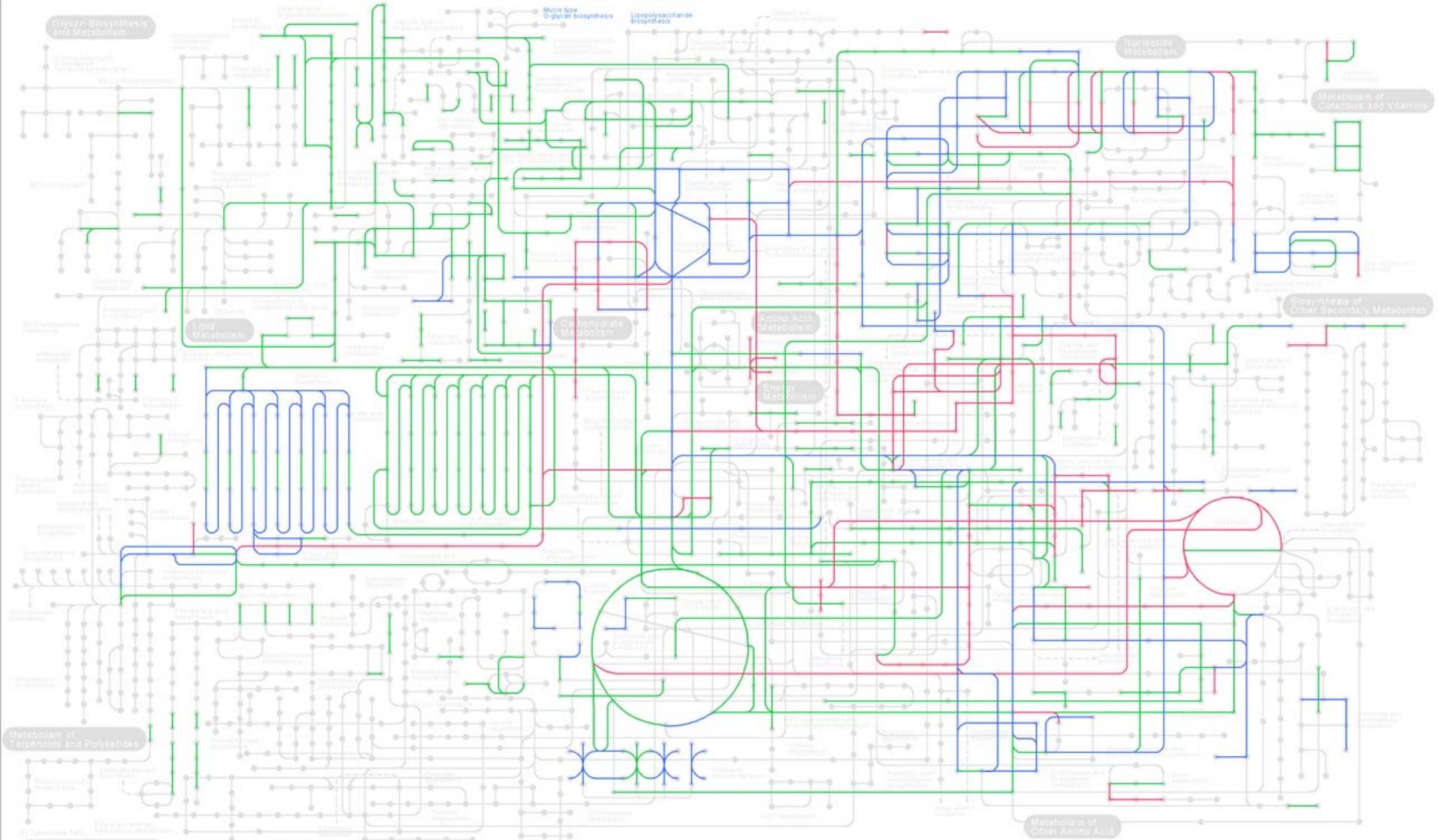
hsa+pfa Homo sapiens (human) + Plasmodium falciparum
aga+pfa Anopheles gambiae (mosquito) + Plasmodium falciparum

複数生物種の情報を PATHWAY にマッピング



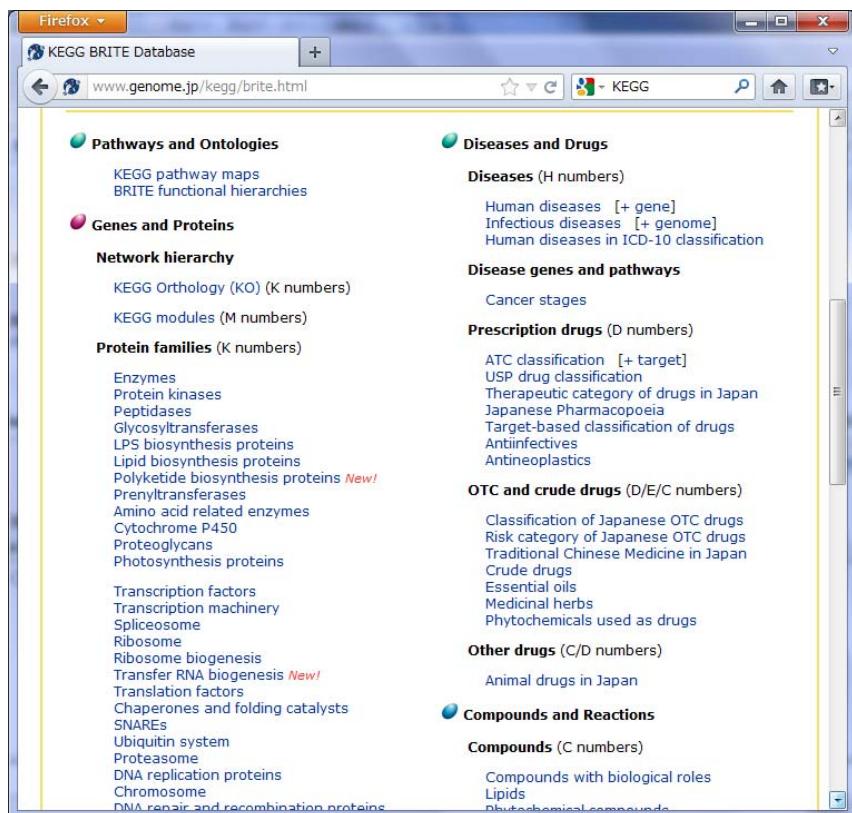
- 共生関係
 - 寄生関係
 - ヒトと腸内細菌叢など
 - アブラムシ
 - 昆虫
 - ブフネラ
 - アブラムシの共生細菌

複数生物種の情報を PATHWAY にマッピング



KEGG BRITE

- 機能の階層分類情報 -



- Pathway and ontology
 - KEGG PATHWAY, KEGG BRITE のエントリ一を階層で表現
- Genes and Proteins
 - 遺伝子や蛋白質の機能やネットワークの分類。分類対象はKO
- Compound and Reactions
 - 化合物の構造や機能による分類、酵素反応の種類による分類
- Drug and Diseases
 - 薬物や疾患のような医薬系の情報の分類
- Cell and Organisms
 - KEGGの登録生物の系統分類

KEGG BRITE

- 機能の階層分類情報 -

The screenshot shows the KEGG BRITE Database interface. At the top, there's a navigation bar with links for KEGG2, PATHWAY, BRITE, MODULE, DISEASE, DRUG, KO, GENOME, GENES, LIGAND, and DBGET. Below the navigation bar, there's a section titled "Functional Hierarchies" with a brief description of what KEGG BRITE is. A search bar is present with the placeholder "Search BRITE hierarchies for". Under the "Brite Mapping" section, there's a list of tools: "Search Brite - basic brite mapping tool", "Search&Color Brite - advanced brite mapping tool", and "Join Brite - selected brite hierarchy manipulation tool". The bottom of the page has links for "Pathways and Ontologies" and "Diseases and Drugs".

- キーワード検索

- BRITE階層情報のテキスト検索

- オブジェクトマッピング KEGG Mapper

- マップ中のオブジェクトを指定してBRITEにマッピング
 - 複数オブジェクトを指定するとマッチしたもののすべてをマッピング
 - Search BRITE
 - 指定したオブジェクトを赤く色づけ
 - Search & Color BRITE
 - 指定したオブジェクトを自由に色づけ
 - Join BRITE
 - BRITEに別の関係情報をマッピング
(例: GPCRのBRITE(ko04030)に、GPCRとリガンドの関係情報をマッピング)

そのほかのKEGGのツール群

ゲノムネットケミカル情報解析ツール

Firefox ▾

GenomeNet

www.genome.jp

Google

GenomeNet Database Resources

- Release notes
- Acknowledgments
- DBGET**
 - Overview
 - DB release info
- KEGG**
- varDB**
- Community DBs**
- Bioinformatics tools**
 - Other tools
- Feedback**

DBGET: Integrated Database Retrieval System

- DBGET search
- LinkDB search

KEGG: Kyoto Encyclopedia of Genes and Genomes

- KEGG2 - Table of contents
- KEGG PATHWAY - Systems information: pathways
- KEGG BRITE - Systems information: ontologies
- KEGG Organisms - Organism-specific entry points
- KEGG GENES - Genomic information
- KEGG LIGAND - Chemical information

KEGG MEDICUS: Health-related info resource

- MEDICUS search

varDB: Antigenic variation database

Community Databases

- CYORF - Cyanobacteria annotation database
- BSORF - Bacillus subtilis genome database
- EXPRESSION - Gene expression profile database

DB growth curve

GenomeNet Bioinformatics Tools

Sequence Analysis

- BLAST / FASTA - Sequence similarity search
- MOTIF - Sequence motif search
- CLUSTALW / MAFFT / PRRN - Multiple alignment

Genome Analysis

- KAAS - KEGG automatic annotation server
- EGassembler - EST consensus contigs
- GENIES - Gene network prediction

Chemical Analysis

- SIMCOMP / SUBCOMP - Chemical structure search
- KC2M - Chemical structure search
- PathComp** - Possible reaction path computation
- PathSearch - Similar reaction path search
- PathPred - Reaction pathway prediction
- E-zyme - Enzymatic reaction prediction

Kyoto University Bioinformatics Center

KEGG API

KEGG API はプログラムなどから KEGG を利用するためのウェブサービスです。前半では、KEGG データベースから情報を取得したり検索したりするために KEGG API を使う方法を説明します。後半のリファレンスで KEGG API の全機能を解説します。例として主に Ruby 言語を使って解説しますが、SOAP と WSDL を扱うことのできる言語 (Perl, Python, Java など) であれば簡単に KEGG API を利用することができます。

目次

- イントロダクション
- KEGG API の使い方
 - Ruby の場合
 - Perl の場合
 - Perl の注意点
 - Python の場合
 - Java の場合
- KEGG API リファレンス
 - WSDL ファイル
 - 用語の凡例

KEGG API を使うと、もっと柔軟に KEGG のデータを扱うことができます。

<http://www.kegg.jp/kegg/soap/>

KGML: KEGG Markup Language

XML フォーマットでパスウェイ中のオブジェクトのつながりを表現

KEGG: Kyoto Encyclopedia of Genes and Genomes
http://www.genome.jp/kegg/

KEGG Home
Introduction
Overview
Release notes
Current statistics

KEGG Identifiers
Pathway maps
Brite hierarchies

KEGG XML

KEGG API
KEGG FTP
KegTools

GenomeNet
DBGET/LinkDB
Feedback

New features
Module maps
Disease/drug maps
3rd global map
Combined maps

KEGG: Kyoto Encyclopedia of Genes and Genomes

A grand challenge in the post-genomic era is a complete computer representation of the cell, the organism, the ecosystem, and the biosphere, which will enable computational prediction of higher-level complexity of cellular processes and organism behaviors from genomic and molecular information. Towards this end we have been developing a bioinformatics resource named KEGG as part of the research projects of the Kanehisa Laboratories in the Bioinformatics Center of Kyoto University and the Human Genome Center of the University of Tokyo.

Main entry point to the KEGG web service
[KEGG2](#) [KEGG Table of Contents](#) [Update notes](#) [Help](#)

Data-oriented entry points

- [KEGG PATHWAY](#) Pathway maps for systemic functions
- [KEGG BRITE](#) Functional hierarchies and ontologies
- [KEGG MODULE](#) Module maps for functional units
- [KEGG DISEASE](#) Human diseases
- [KEGG DRUG](#) Drugs
- [KEGG ORTHOLOGY](#) KO system and ortholog annotation
- [KEGG GENES](#) Genes and proteins
- [KEGG GENOME](#) Genomes
- [KEGG COMPOUND](#) Chemical compounds
- [KEGG GLYCAN](#) Glycans
- [KEGG REACTION](#) Reactions

Organism-specific entry points
[KEGG Organisms](#) Select [Organism](#) (example) hsa

KGML (KEGG Markup Language)
http://www.genome.jp/kegg/xml/

KEGG KEGG2 PATHWAY BRITE DISEASE DRUG

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KEGG Identifiers
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Brite hierarchies

KEGG XML

KEGG API
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KGML (KEGG Markup Language)

XML representation of KEGG pathway maps

The KEGG Markup Language (KGML) is an exchange format of the KEGG graph objects, especially the KEGG pathway maps that are manually drawn and updated. KGML enables automatic drawing of KEGG pathways and provides facilities for computational analysis and modeling of protein networks and chemical networks. The KGML files for metabolic pathway maps contain two types of graph object patterns, how boxes (enzymes) are linked by "relations" and how circles (compounds) are linked by "reactions". The KGML files for non-metabolic pathway maps contain only the aspect of how boxes (proteins) are linked by "relations". The prefix for the pathway map identifiers indicates the following.

- ko - reference pathway map linked to K numbers (KO identifiers)
- ec - reference pathway map linked to EC numbers
- org (three- or four-letter organism code) - organism-specific pathway map linked to genes

Documents

- [KEGG Markup Language manual](#)
- [KGML v0.7.1 DTD \[dtd | html \]](#)

Access methods

The entire set of KGML files may be downloaded from the FTP site (academic users only).

- <http://www.genome.jp/kegg/download/>

Note: academic users are requested to obtain a licensing agreement. Please refer to the page below.

KegTools

Firefox ▾

KEGG - KegTools

www.kegg.jp/kegg/download/kegtools.html

KEGG Home
Release notes
Current statistics
Plea from KEGG

KEGG Database
KEGG overview
Searching KEGG
KEGG mapping
Color codes

KEGG Objects
Pathway maps
Brite hierarchies

KEGG Software
KegTools
KEGG API
KGML

KEGG FTP
Subscription

GenomeNet

DBGET/LinkDB

Feedback

Kanehisa Labs

KegTools

KegTools are desktop applications that run on the Mac OS X, Windows, and Linux platforms. Currently, the following three applications are freely available.

KegHier

Java application for browsing BRITE hierarchy files

- KegHier 1.1.0 (December 22, 2011) for:
Mac OSX [dmg] Windows (exe) [zip] Windows (jar/bat) [zip] Linux [tar.gz]
- ReadMe file

KegArray

Java application for microarray data analysis

- KegArray 1.2.3 (October 16, 2009) for:
Mac OSX [dmg] Windows (exe) [zip] Windows (jar/bat) [zip] Linux [tar.gz]
- ReadMe file

KegDraw

Java application for drawing compound and glycan structures

- KegDraw 0.1.12beta (December 22, 2011) for:
Mac OSX [dmg] Windows (exe) [zip] Windows (jar/bat) [zip] Linux [tar.gz]
- ReadMe file