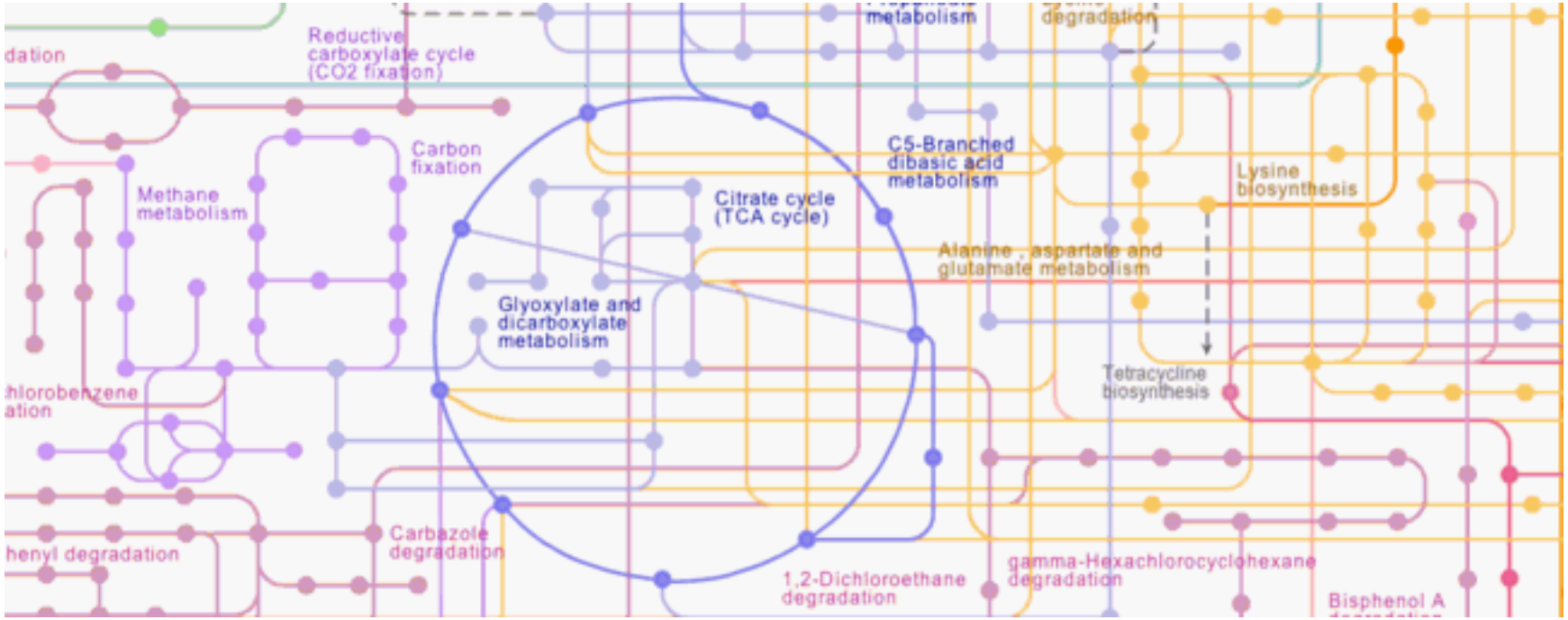


Metabolic Network and Cheminformatics

Masaaki Kotera,

Laboratory of Chemical Life Science,

Bioinformatics Centre, Institute for Chemical Research,
Kyoto University.

Metabolome Analysis

1. 試料
2. 成分分析(GC-MS, LC-MS, etc)
3. 代謝物同定

   MassBank, etc. (http://www.massbank.jp/)

4. データ解析
   - まずはデータの傾向を粗くつかむ

     KEGG, etc. (http://www.genome.jp/kegg/)
   - もっと詳しく調べる

     Metabolic network analyses

MS and NMR databases

- MassBank
  - http://www.massbank.jp/ -MS
- Human Metabolome Database
  - http://www.hmdb.ca/ - both MS and NMR
- Biological Magnetic Resonance Data Bank
  - http://www.bmrb.wisc.edu/structgen/ - NMR
- CHENOMX
  - http://www.chenomx.com/ - MS, 有料
- METLIN
  - http://metlin.scripps.edu/ - MS
- Fiehn Lib
  - http://fiehnlab.ucdavis.edu/Metabolite-Library-2007/ - MS

MassBank

http://www.massbank.jp/ja/database.html より抜粋

- MSn の類似スペクトル検索
- キーワードによるスペクトルの簡易検索
- イオン、中性脱離分子、分子式による検索
- 部分化学構造式での検索
- 中性脱離分子を利用したMSnのスペクトル検索
- スペクトル閲覧・比較ツール
- MSn の類似スペクトル一括検索サービス
- スペクトルのブラウズ
- スペクトルのカテゴリ別表示
- WEB-API による MassBank へのアクセス

メタボロームデータベース：多様な研究への対応とデータの共有化

- 使えるデータベース・ウェブツール
  - 実験医学増刊 Vol.29 No.15, 2011.
  - 日本発のデータベース戦略から，ゲノム・疾患情報の有効活用まで
- KNApSAcK
  - http://kanaya.naist.jp/KNApSAcK/
- MassBank
  - http://www.massbank.jp/

KEGG Mapper

http://www.genome.jp/kegg/mapper.html

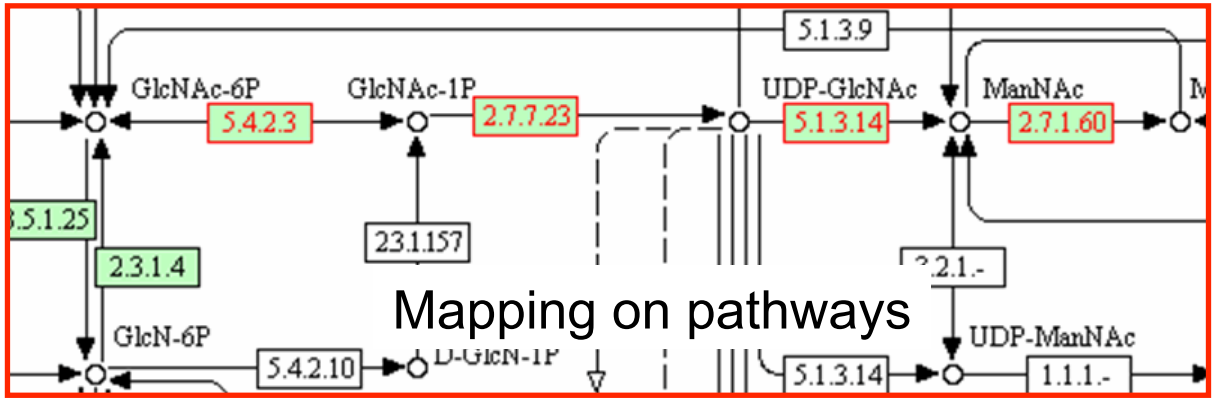
List of genes or compounds

11251
64579
27242
9331
51744
7436
8396
11001
8542
8611
26290
53340
7804
4585
55512
6361
6364
3579
914
5175
5553

KEGG Mapper

hsa04060 Cytokine-cytokine receptor interaction - Homo sapiens (human) (56)
hsa04510 Focal adhesion - Homo sapiens (human) (48)
hsa04062 Chemokine signaling pathway - Homo sapiens (human) (38)
hsa04650 Natural killer cell mediated cytotoxicity - Homo sapiens (human) (34)
(34)
hsa04810 Regulation of actin cytoskeleton - Homo sapiens (human) (33)
hsa04142 Lysosome - Homo sapiens (human) (31)
hsa00564 Glycerophospholipid metabolism - Homo sapiens (human) (31)
hsa04512 ECM-receptor interaction - Homo sapiens (human) (30)
hsa04010 MAPK signaling pathway - Homo sapiens (human) (30)
hsa04310 Wnt signaling pathway - Homo sapiens (human) (28)
hsa00510 N-Glycan biosynthesis - Homo sapiens (human) (28)
hsa04070 Phosphatidylinositol signaling system
hsa04145 Phagosome - Homo sapiens (human) (27)
hsa04666 Fc gamma R-mediated phagocytosis - Homo sapiens (human) (26)
hsa00520 Amino sugar and nucleotide sugar metabolism - Homo sapiens (human) (25)
hsa04910 Insulin signaling pathway - Homo sapiens (human) (25)
hsa04664 Fc epsilon RI signaling pathway - Homo sapiens (human) (24)

List of pathways

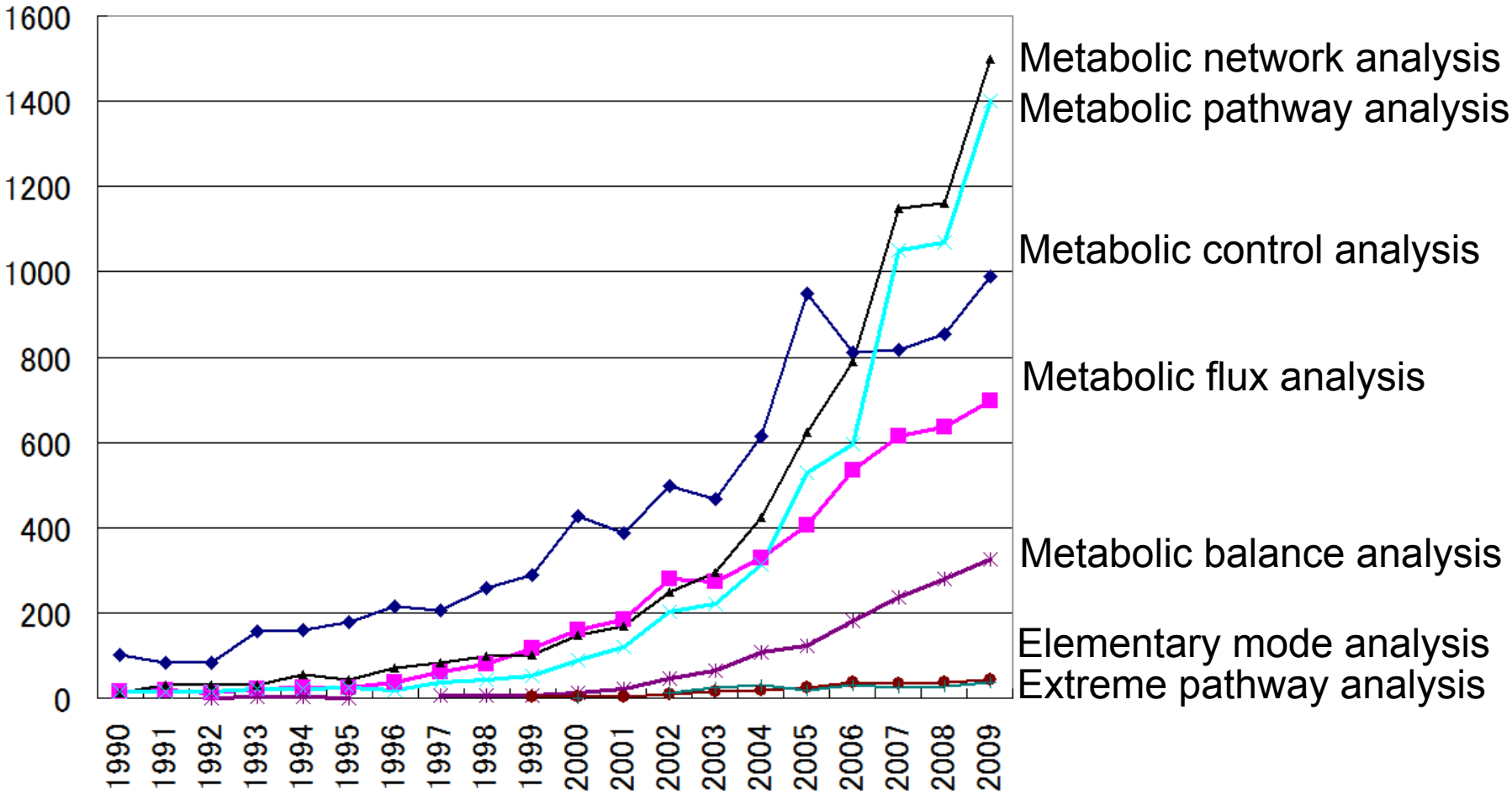


Mapping on pathways

What can we do with “Network Analysis”?

Taken from http://www.bloomsburyhotels.com/images/city/tubemap.gif

Words in fashion



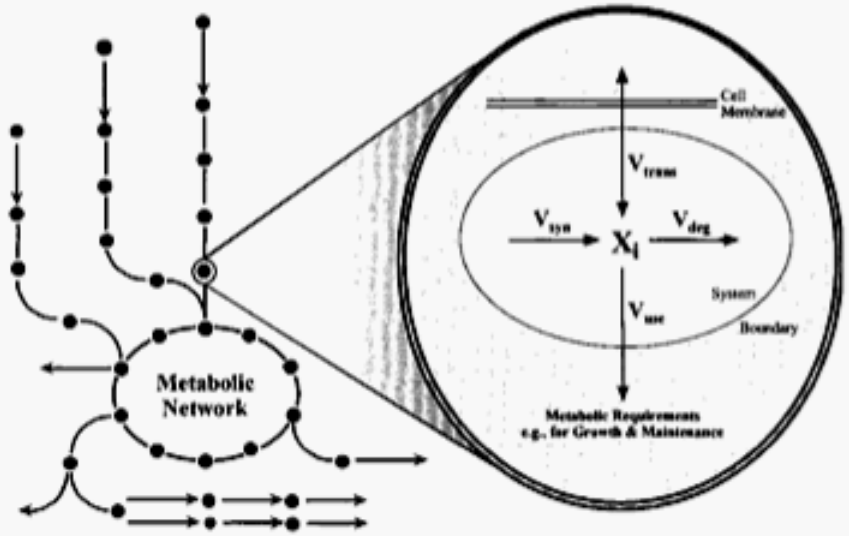
- Elementary modes
  - "minimal set of enzymes that could operate at steady state with all irreversible reactions proceeding in the appropriate direction" (Schuster et al., TIBTECH, 1999)

- Extreme pathways
  - "the edges of the flux cone, that is they are the basis from which all other fluxes can be obtained by linear combination" (Schilling et al., Journal of Theoretical Biology, 2000)

[Toward metabolic phenomics: analysis of genomic data using flux balances]
CH Schilling, JS Edwards, BO ... - Biotechnology progress, 1999 - Wiley Online Library

Fundamentals of Flux Balance Analysis

The fundamental principle underlying FBA is the conservation of mass. A flux balance can be written for each metabolite(X_i) within a metabolic system to yield the dynamic mass balance equations that interconnect the various metabolites.



Dynamic Flux Balances

$$\frac{dX}{dt} = S \bullet v - b$$

$$v = fn(X,...)$$

X = Metabolite Concentrations
S = Stoichiometric Matrix
v = Metabolic Reaction Fluxes (V_{syn}, V_{deg})
b = Net Transport out of Network (V_{use}- V_{trans})

Steady State Analysis

$$S \bullet v = b$$

Solve for Unknown Metabolic Fluxes **v**

A steady state assumption is made which produces the system of linear equations in the lower box, which simply states that the formation fluxes are balanced by degradation fluxes. This situation is analogous to Kirchhoff's current law used in electrical circuit analysis, where the sum of the currents coming in and out of a node must sum to zero.

Typically there are more fluxes in the system than metabolites. Thus, the system of equations is underdetermined and can therefore be formulated as a linear programming (LP) problem, in which one finds the optimal flux distribution that minimizes or maximizes a particular objective. Various objective function can be used such as those listed below:

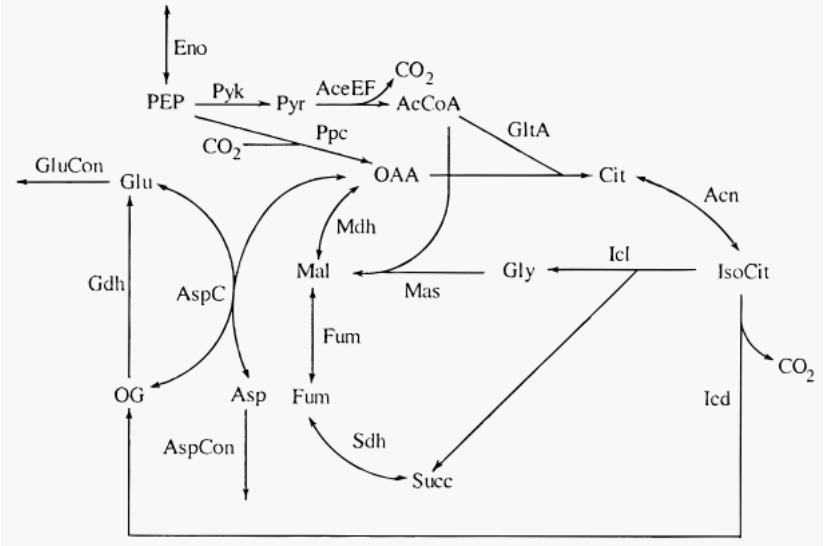
- *Minimize ATP production*
- *Minimize nutrient uptake*
- *Minimize redox production*
- *Maximize metabolite production*
- *Maximize biomass production (i.e growth)*
- *Minimize the Euclidean norm of the flux vector*

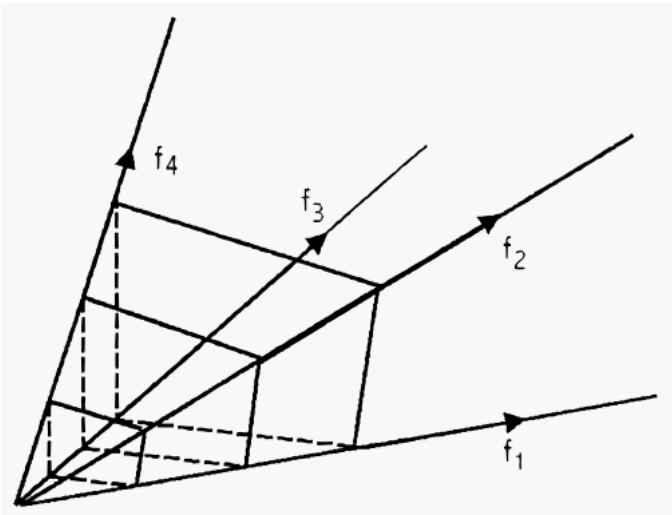
Metabolic pathway analysis: basic concepts and scientific applications in the post-genomic era

CH Schilling, S Schuster, BO Palsson, ... - Biotechnology ..., 1999 - interscience.wiley.com

This article reviews the relatively short history of **metabolic pathway analysis**. Computer-aided algorithms for the synthesis of metabolic pathways are discussed. Important algebraic concepts used in pathway analysis, such as null space and convex cone, are explained. It is **...**

引用元 220 - 関連記事 - 全 17 バージョン



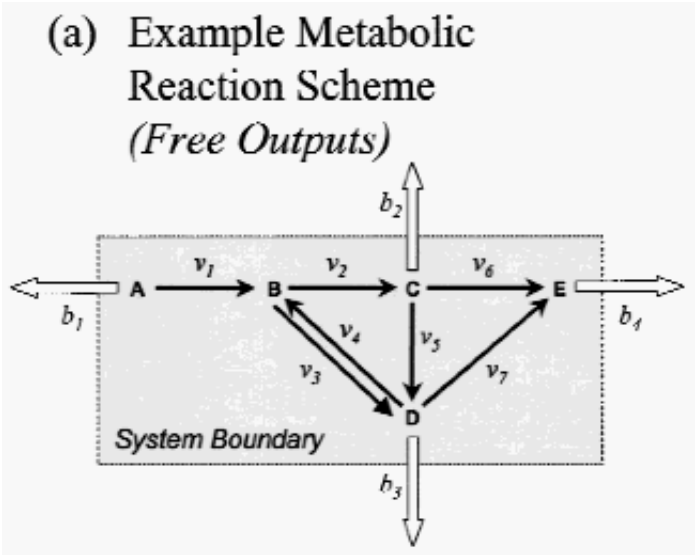


Combining pathway analysis with flux balance analysis for the comprehensive study of metabolic systems

… JS Edwards, D Letscher, BØ Palsson - Biotechnology and …, 2000 - interscience.wiley.com

Abstract: The elucidation of organism-scale metabolic networks necessitates the development of integrative methods to analyze and interpret the systemic properties of cellular metabolism. A shift in emphasis from single metabolic reactions to systemically defined ...

引用元 136 - 関連記事 - 全 8 バージョン



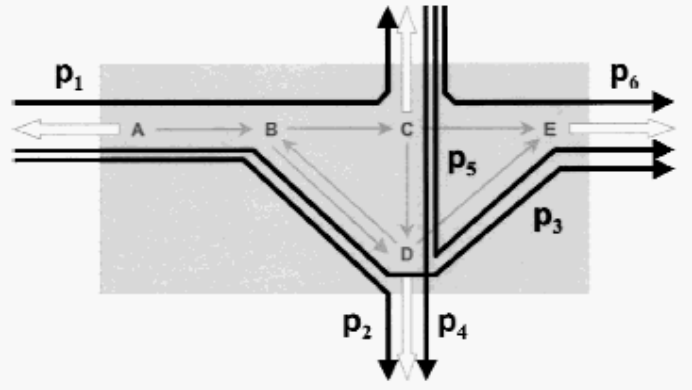
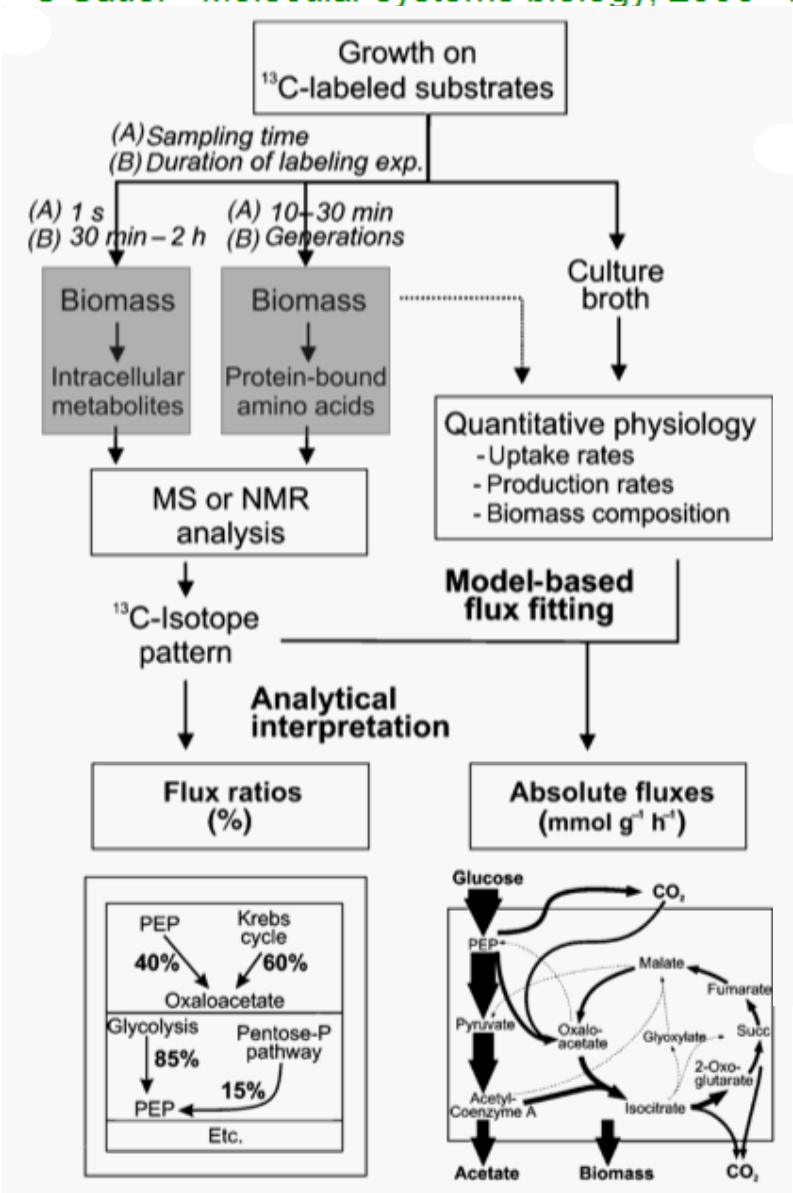


Table I. The eight extreme pathway vectors for the example network with free outputs.[a]

Pathway number	Internal fluxes							Exchange fluxes			
	v_1	v_2	v_3	v_4	v_5	v_6	v_7	b_1	b_2	b_3	b_4
$\mathbf{p}_1$	1	1	0	0	0	0	0	−1	1	0	0
$\mathbf{p}_2$	1	0	1	0	0	0	0	−1	0	1	0
$\mathbf{p}_3$	2	0	2	0	0	0	1	−2	0	0	1
$\mathbf{p}_4$	0	0	0	0	1	0	0	0	−1	1	0
$\mathbf{p}_5$	0	0	0	0	2	0	1	0	−2	0	1
$\mathbf{p}_6$	0	0	0	0	0	1	0	0	−1	0	1
$\mathbf{p}_7$	0	0	1	1	0	0	0	0	0	0	0
$\mathbf{p}_8$	0	1	0	1	1	0	0	0	0	0	0

Metabolic networks in motion: 13C-based flux analysis

U Sauer - Molecular systems biology, 2006 - nature.com



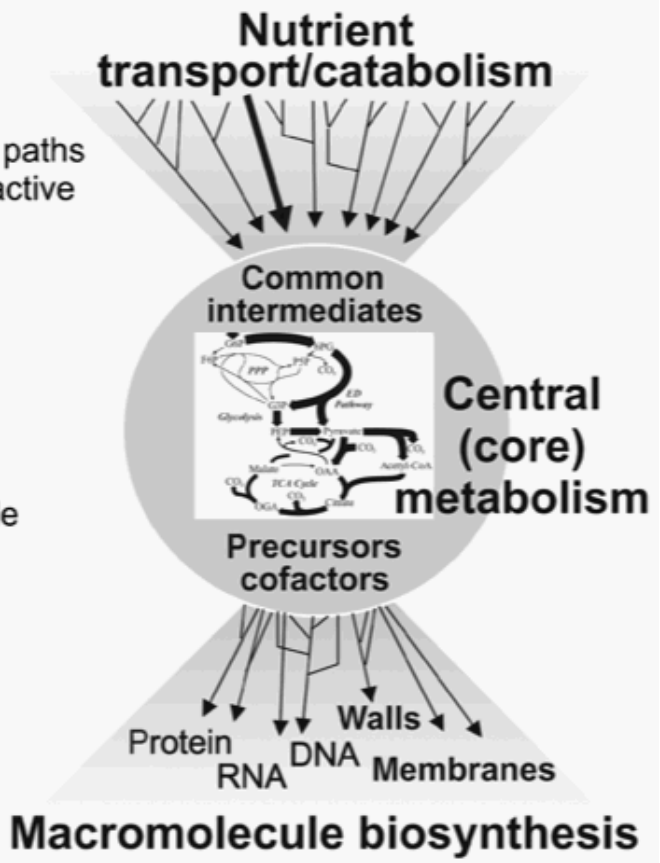
Schöller

rarius,

- Linear
- Convergent
- Few connections
- Typically one or few paths are simultaneously active
- One-way flux
- Organism specific

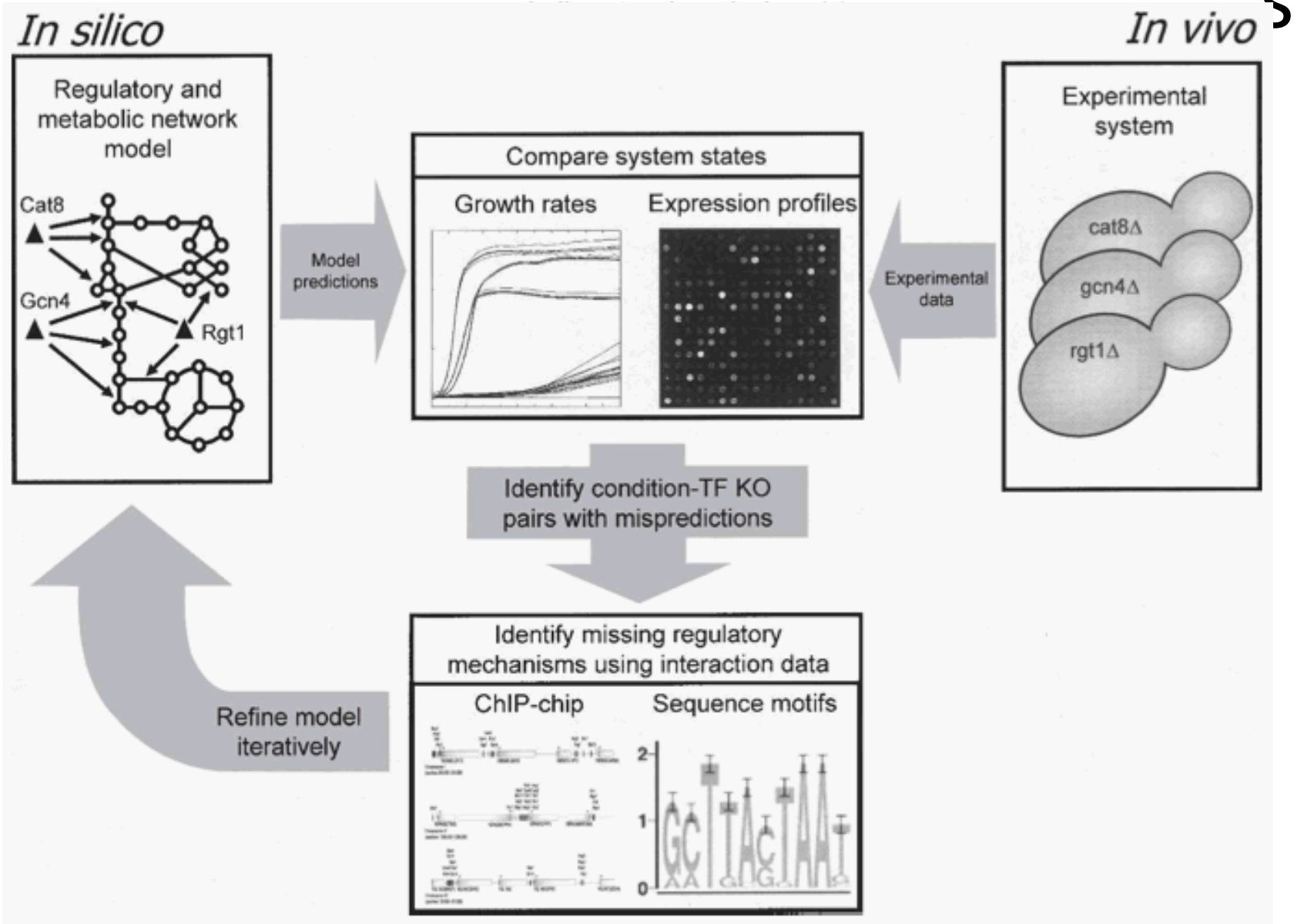
- Many cycles
- Many connections
- Redundant
- Flux direction variable
- Ubiquitous

- Linear
- Divergent
- Few connections



[Integrated analysis of regulatory and metabolic networks reveals novel regulatory mechanisms in Saccharomyces cerevisiae]

MJ Herrgård, BS Lee, V Portnoy, BØ ... - Genome research, 2006 - genome.cshlp.org

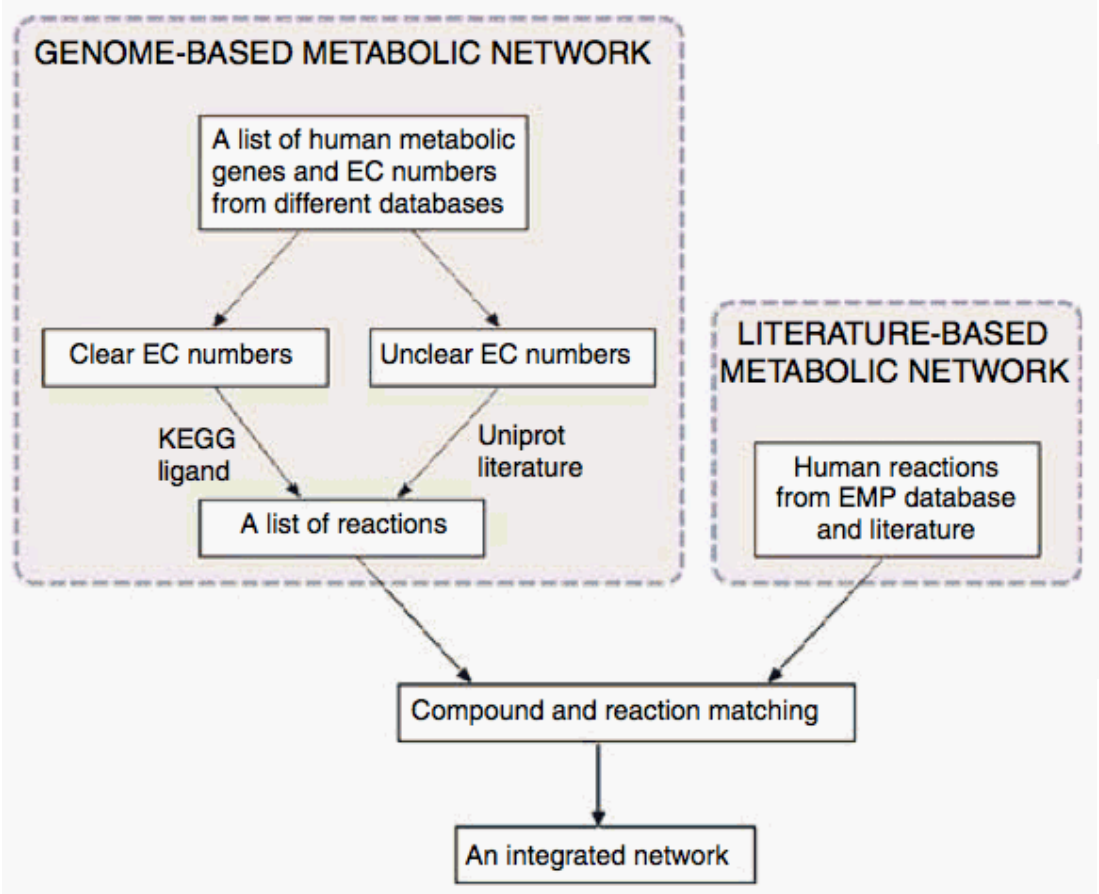


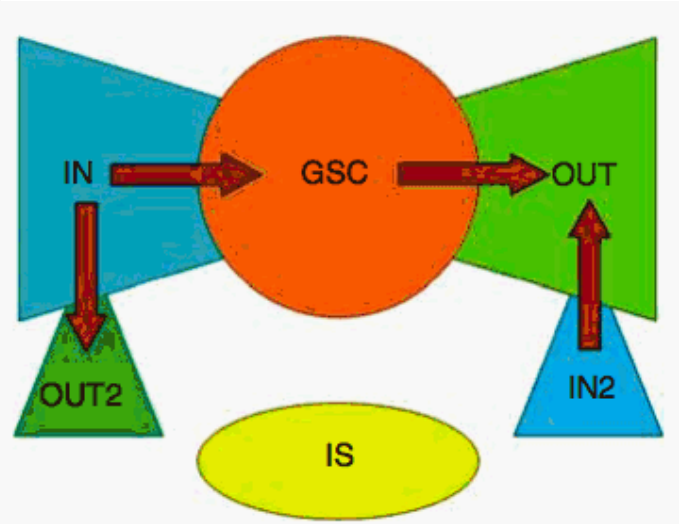
The Edinburgh human metabolic network reconstruction and its functional analysis

H Ma, A Sorokin, A Mazein, A Selkov, E ... - Molecular systems ..., 2007 - nature.com

... A main objective of human **metabolic network analysis** is to see how it is related with human disease. More than 10 000 human genes (half of the whole genome) have been reported to be related with one or more human diseases in the OMIM database (Hamosh et al, 2005). **...**

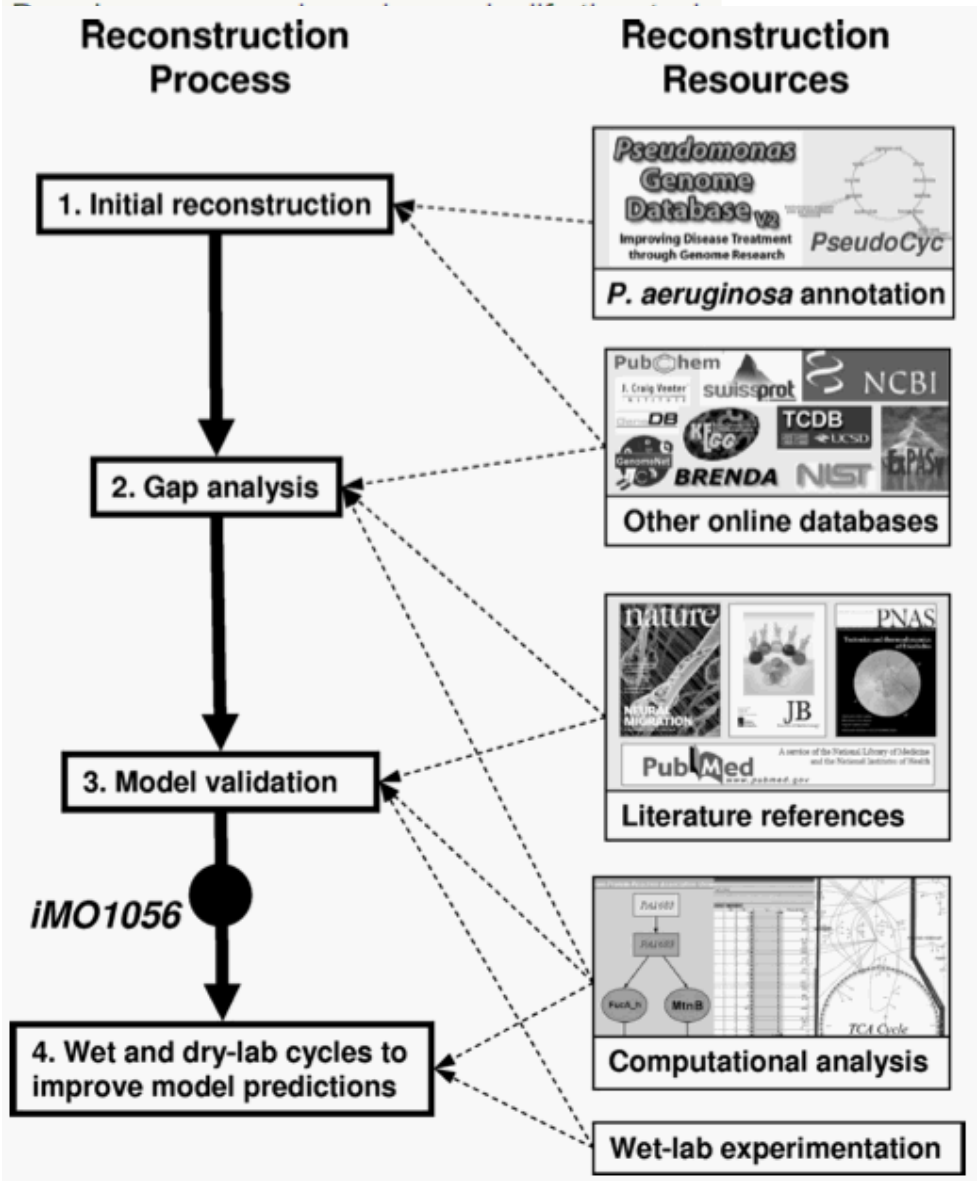
引用元 67 - 関連記事 - 全 13 バージョン

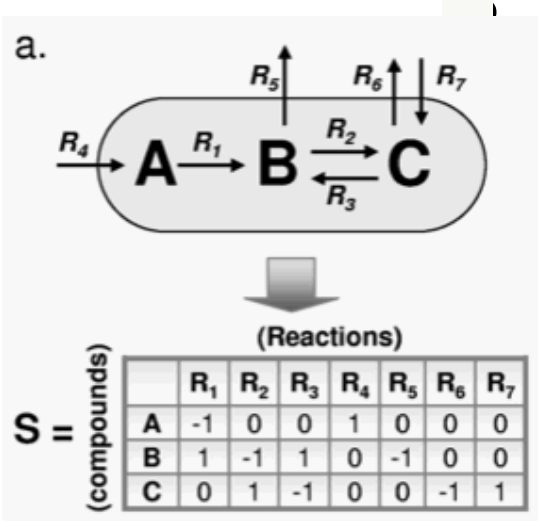




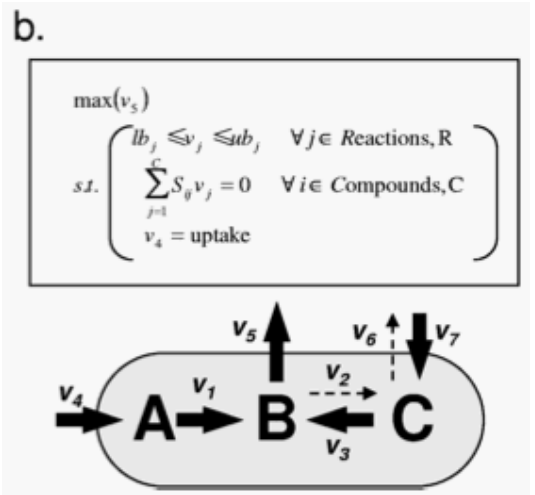
Genome-scale metabolic network analysis of the opportunistic pathogen Pseudomonas aeruginosa PAO1

MA Oberhardt, J Puchalka, KE Fryer, VAP … - Journal of …, 2008 - Am Soc Microbiol

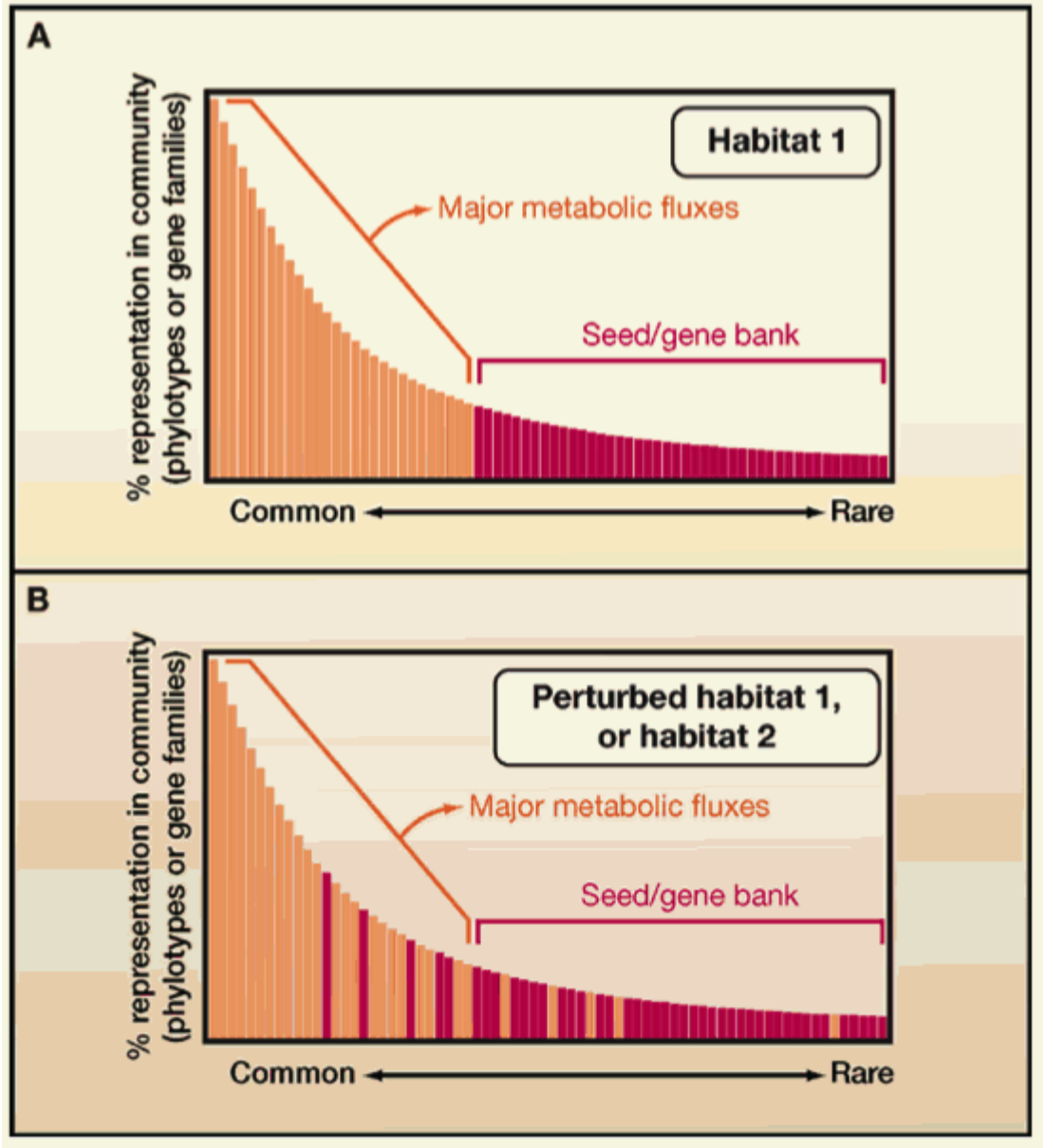




	R1	R2	R3	R4	R5	R6	R7
A	-1	0	0	1	0	0	0
B	1	-1	1	0	-1	0	0
C	0	1	-1	0	0	-1	1



[An invitation to the marriage of metagenomics and metabolomics]
PJ Turnbaugh, JI Gordon - Cell, 2008 - Elsevier



Underground metabolism

R D'Ari… - Bioessays, 1998 - Wiley Online Library

All enzymes are able to use alternative substrates. When these are naturally occurring metabolites, an 'underground reaction' takes place. Examples are presented in which **underground metabolism** of this sort produces an observable phenotype. Although biological **...**

Cited by 26 - Related articles - BL Direct - All 3 versions

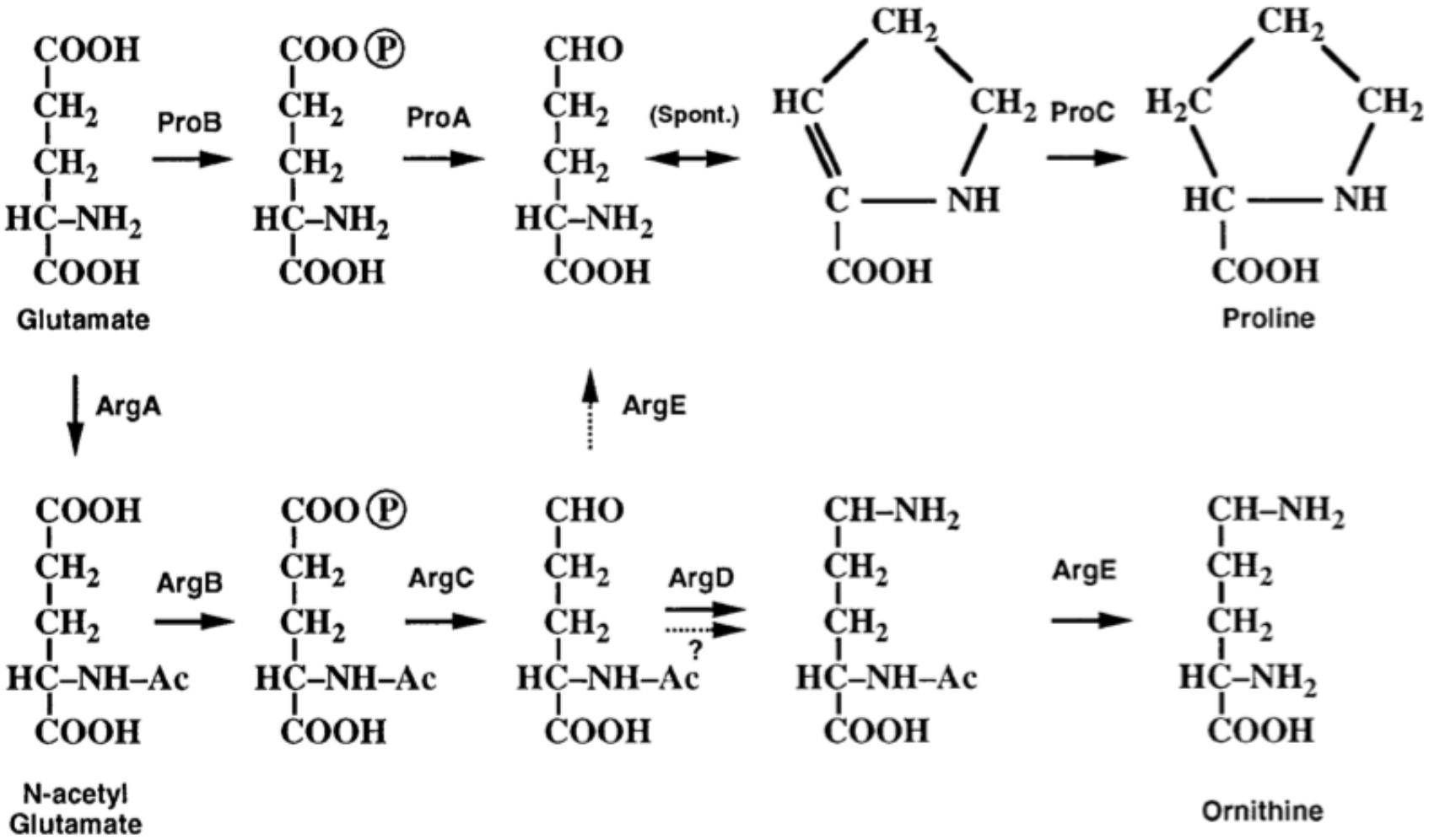


Figure 1. The ProBA bypass that functions in *argD* mutants. Dotted arrows indicate underground reactions. Enzymes are named by the corresponding *E. coli* gene names placed near the arrows. Ac: acetate.

パスウェイDBの選び方と使い方

- 使えるデータベース・ウェブツール
  - 実験医学増刊 Vol.29 No.15, 2011.
  - 日本発のデータベース戦略から，ゲノム・疾患情報の有効活用まで
- KEGG
  - http:www.genome.jp/kegg/
- Reactome
  - http://www.reactome.org/
- MetaCyc
  - http://metacyc.org/

KEGG PATHWAY

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

KEGG PATHWAY Database

Wiring diagrams of molecular interactions, reactions, and relations

KEGG2 PATHWAY BRITE DISEASE DRUG KO GENES GENOME LIGAND DBGET

Select prefix: map | Organism

Enter keywords: | Go | Help

Pathway Maps

KEGG PATHWAY is a collection of manually drawn pathway maps (see new maps, change history, and last updates) representing our knowledge on the molecular interaction and reaction networks for:

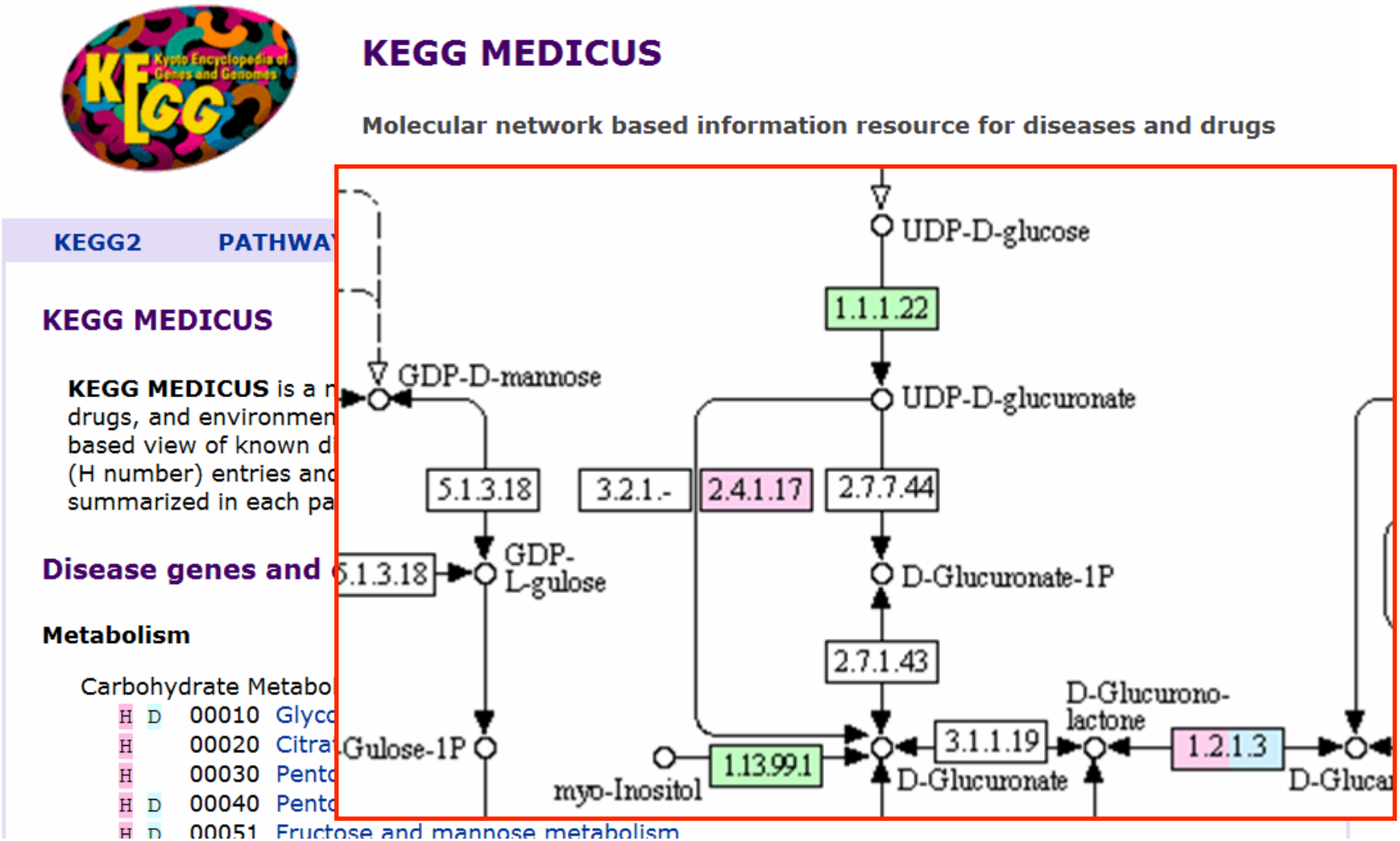
0. Global Map
1. Metabolism
Carbohydrate Energy Lipid Nucleotide Amino acid Other amino acid Glycan
Cofactor/vitamin Terpenoid/PK Other secondary metabolite Xenobiotics Overview
2. Genetic Information Processing
3. Environmental Information Processing
4. Cellular Processes
5. Organismal Systems
6. Human Diseases

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

7. Drug Development

KEGG MEDICUS

http://www.genome.jp/kegg/medicus.html



KEGG MEDICUS

http://www.genome.jp/kegg/medicus.html

KEGG MEDICUS

Molecular network based information resource for diseases and drugs

KEGG2 P

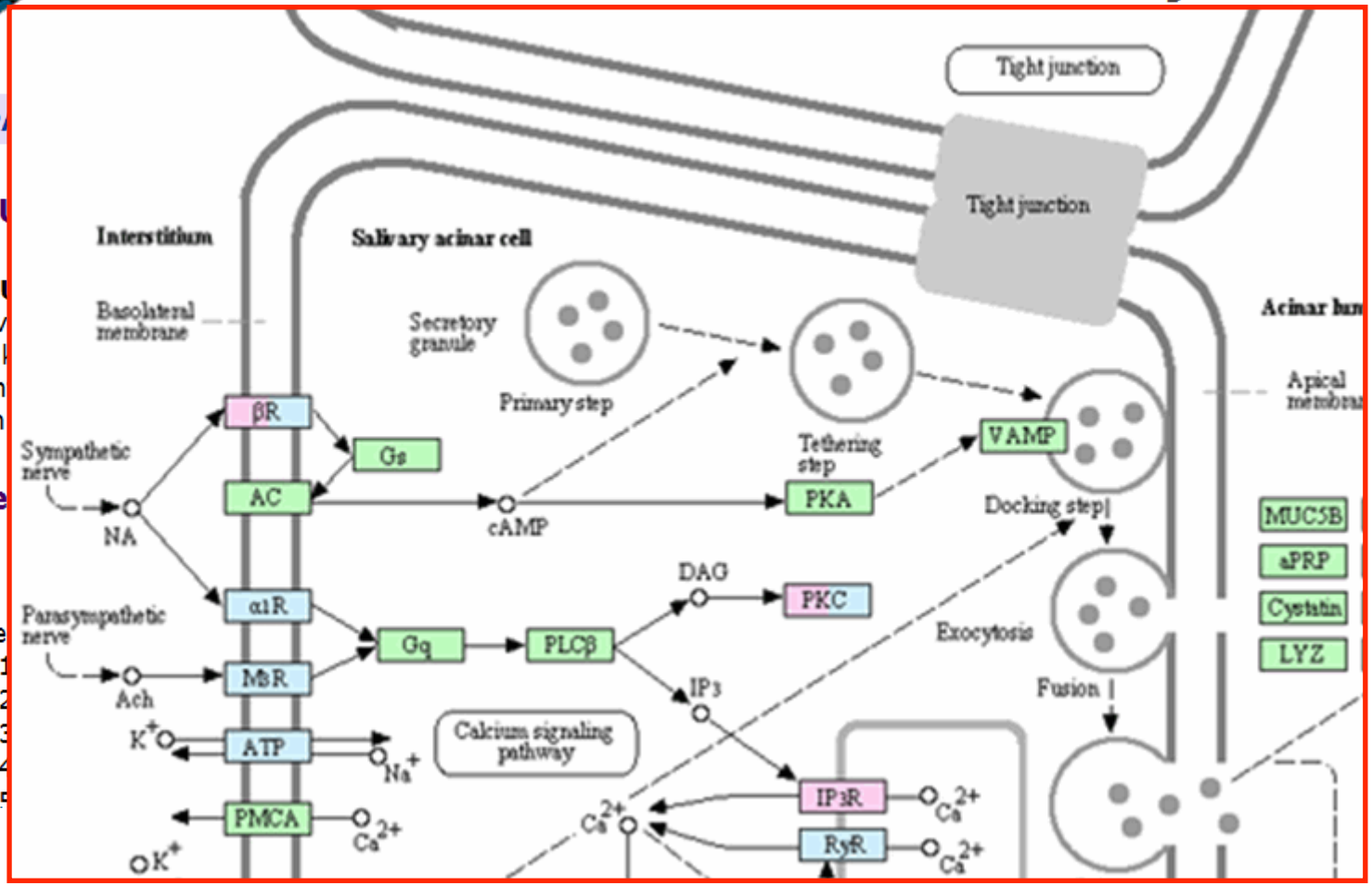
KEGG MEDICU

KEGG MEDICU
drugs, and env
based view of
(H number) en
summarized in

Disease gene

Metabolism

Carbohydrate
H D 0001
H 0002
H 0003
H D 0004
H D 0005



Why bother with chemical structures?

http://chemgarden.littlestar.jp/

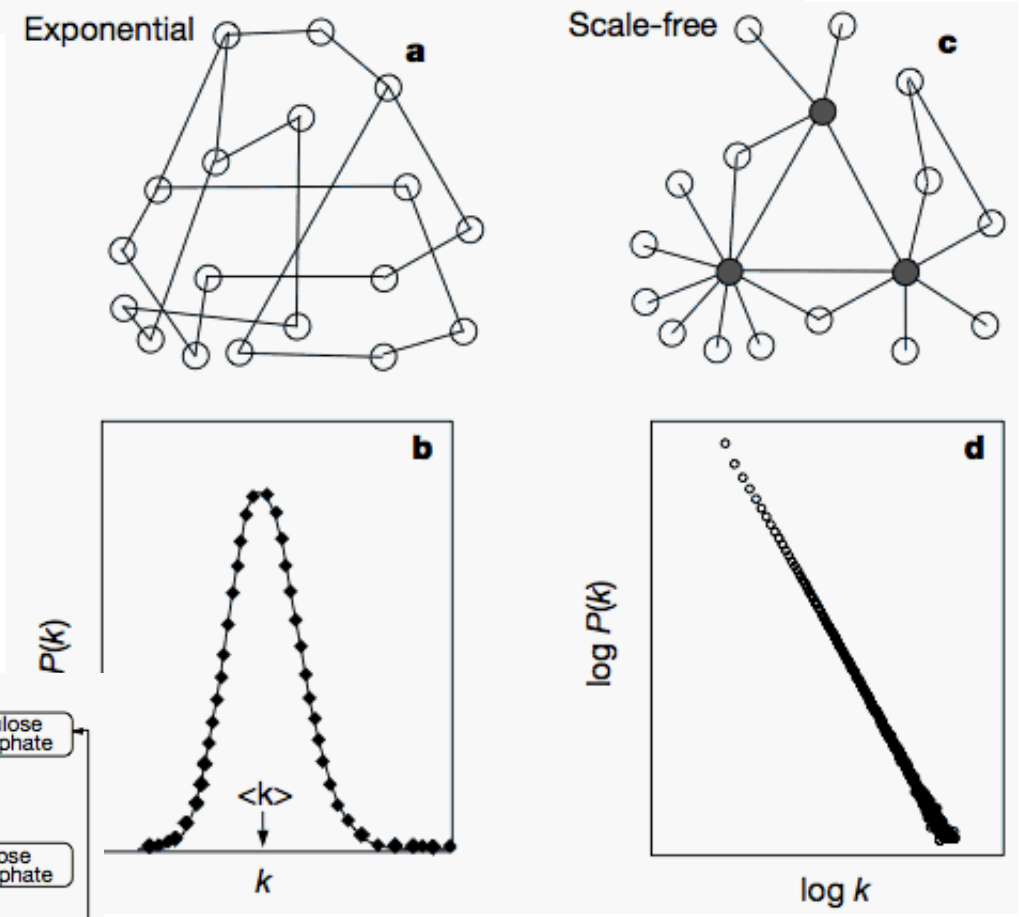
- Metabolic network is “small world”.
  - Jeong et al., *Nature*, 2000.
  - Fell and Wagner, *Nature Metabolic Engineering*, 2000.

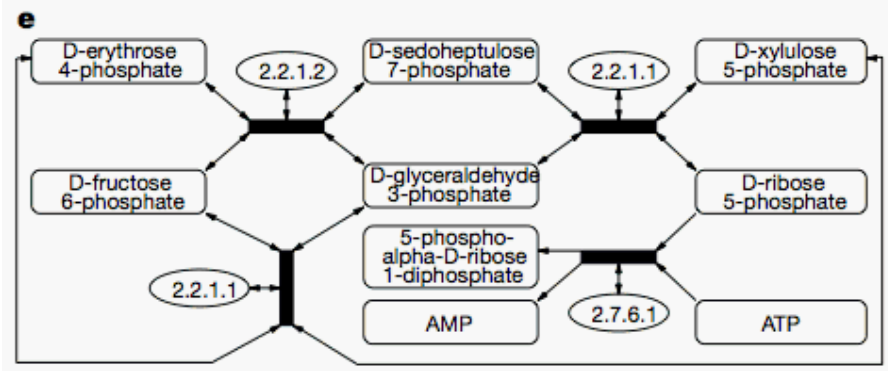
- No, it is not.
  - Ma and Zeng, *Bioinformatics*, 2003.
  - Arita, *PNAS*, 2004.

The large-scale organization of metabolic networks

H Jeong, B Tombor, R Albert, ZN Oltvai, AL Barabási - Nature, 2000 - nature.com

In a cell or microorganism, the processes that generate mass, energy, information transfer and cell-fate specification are seamlessly integrated through a complex network of cellular constituents and reactions 1 . However, despite the key role of these networks in sustaining cellular ...



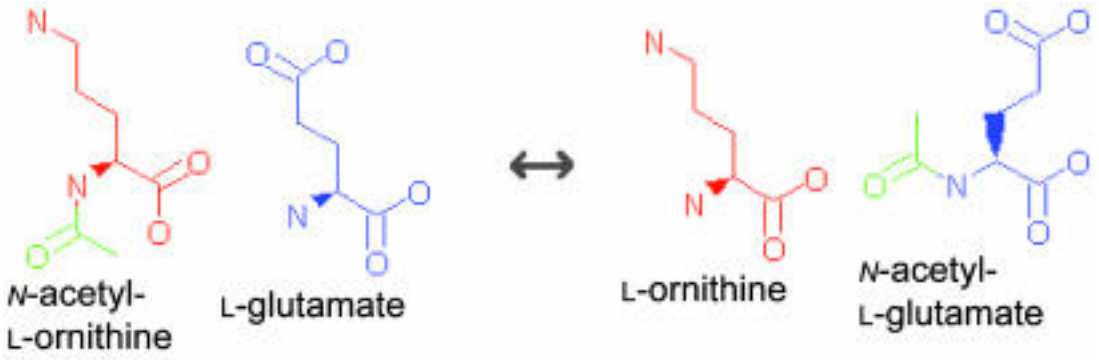


The metabolic world of Escherichia coli is not small

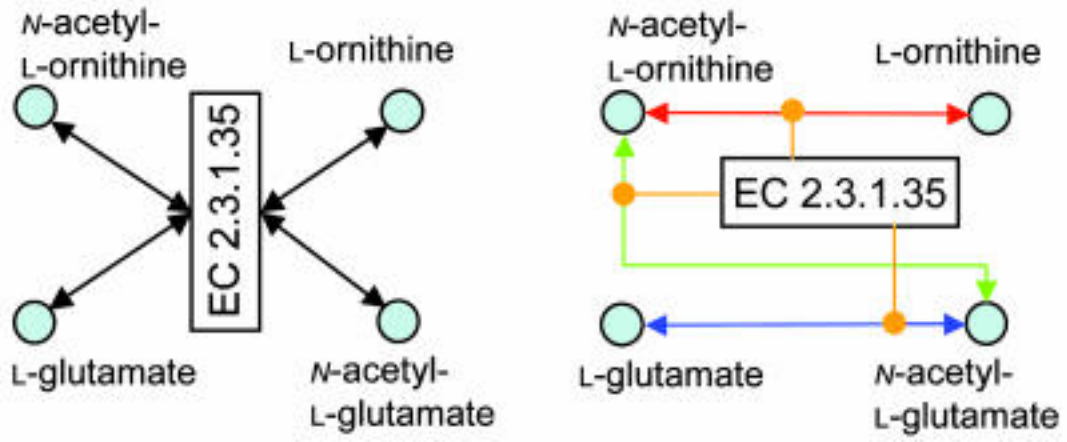
M Arita - Proceedings of the National Academy of ..., 2004 - National Acad Sciences

To elucidate the organizational and evolutionary principles of the metabolism of living organisms, recent studies have addressed the graph-theoretic analysis of large biochemical networks responsible for the synthesis and degradation of cellular building blocks [Jeong, ...

引用元 188 - 関連記事 - 全 20 バージョン



EC 2.3.1.35 *N*-acetyl- L-ornithine:L-glutamate *N*-acetyltransferase



The metabolic world of Escherichia coli is not small

M Arita - Proceedings of the National Academy of …, 2004 - National Acad Sciences

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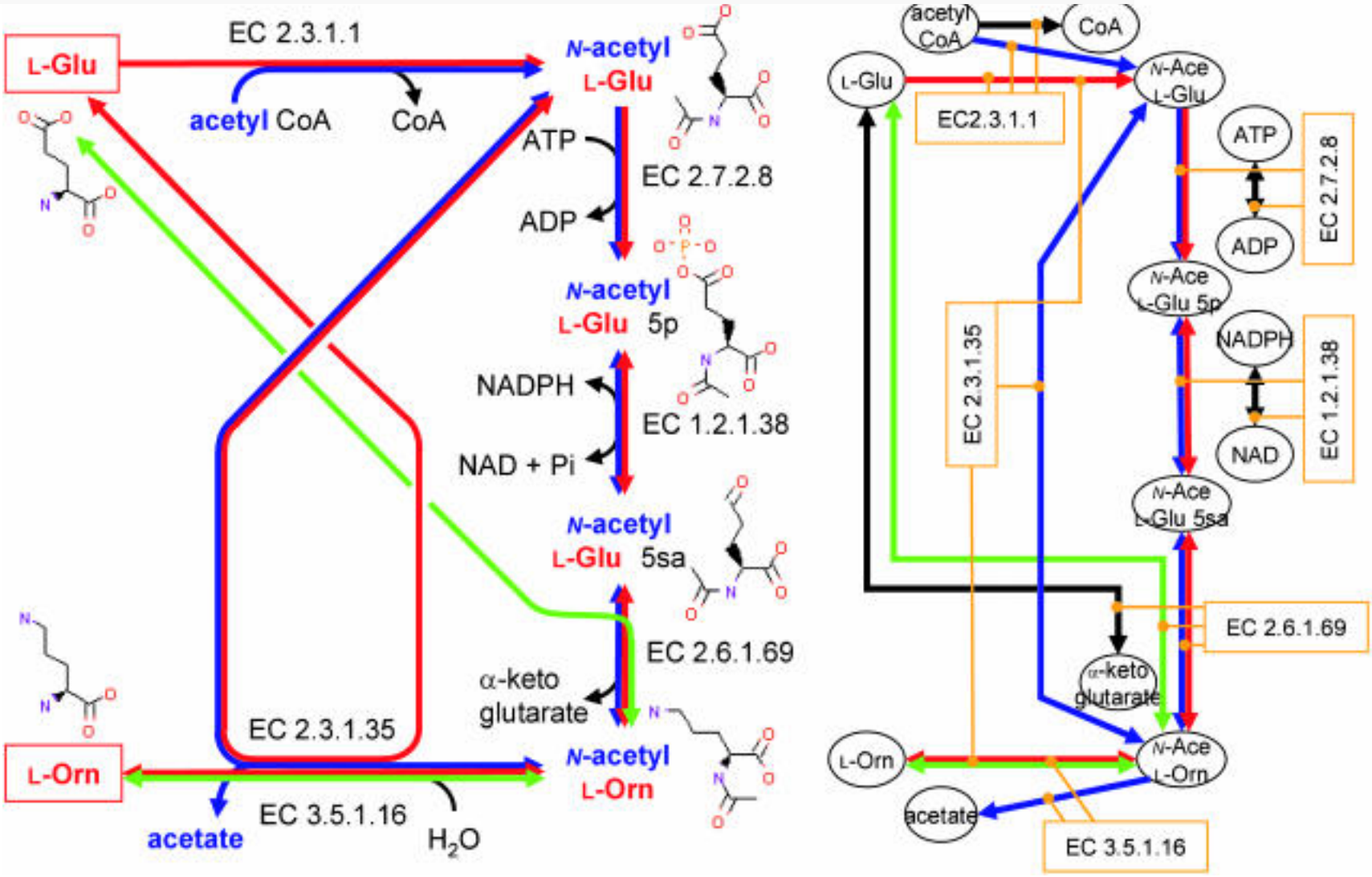
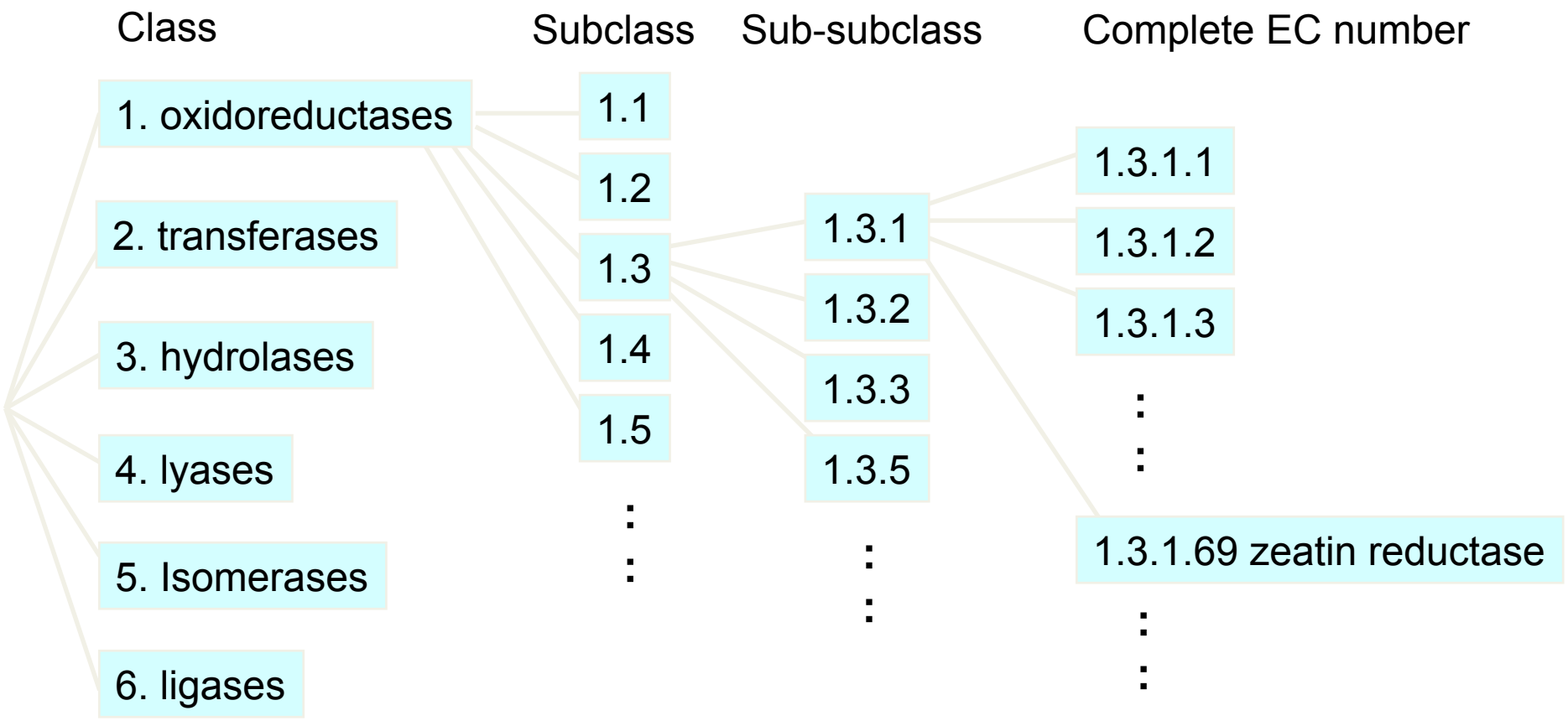
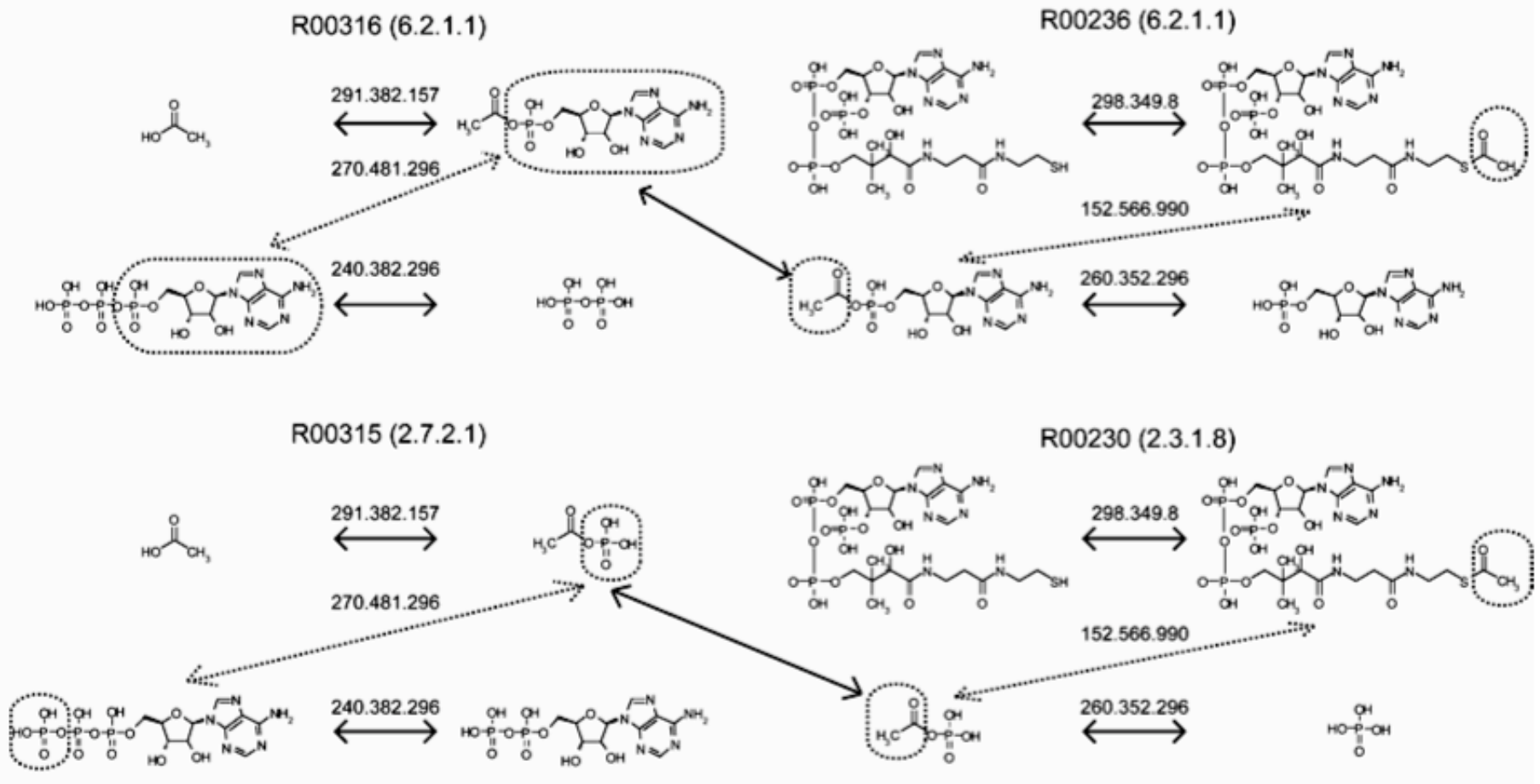


EC numbers as a classification of enzymes



[Computational assignment of the EC numbers for genomic-scale analysis of enzymatic reactions]
M **Kotera**, Y Okuno, M Hattori, S Goto… - Journal of the …, 2004 - ACS Publications
The EC (Enzyme Commission) numbers represent a hierarchical classification of enzymatic reactions, but they are also commonly utilized as identifiers of enzymes or enzyme genes in the analysis of complete genomes. This duality of the EC numbers makes it possible to ...
Cited by 78 - Related articles - All 8 versions



[PDF] RPAIR: a reactant-pair database representing chemical changes in enzymatic reactions
M **Kotera**, M Hattori, MA Oh, R Yamamoto… - Genome Inform, 2004 - jsbi.org
Masaaki Kotera kot@kuicr.kyoto-u.ac.jp Masahiro Hattori hattori@kuicr.kyoto-u.ac.jp Min-A Oh mina@kuicr.kyoto-u.ac.jp **...** Rumiko Yamamoto rumiko@scl.kyoto-u.ac.jp Tomoko Komeno ktomoko@scl.kyoto-u.ac.jp Junko Yabuzaki yzjunko@scl.kyoto-u.ac.jp
Cited by 20 - Related articles - View as HTML - All 2 versions

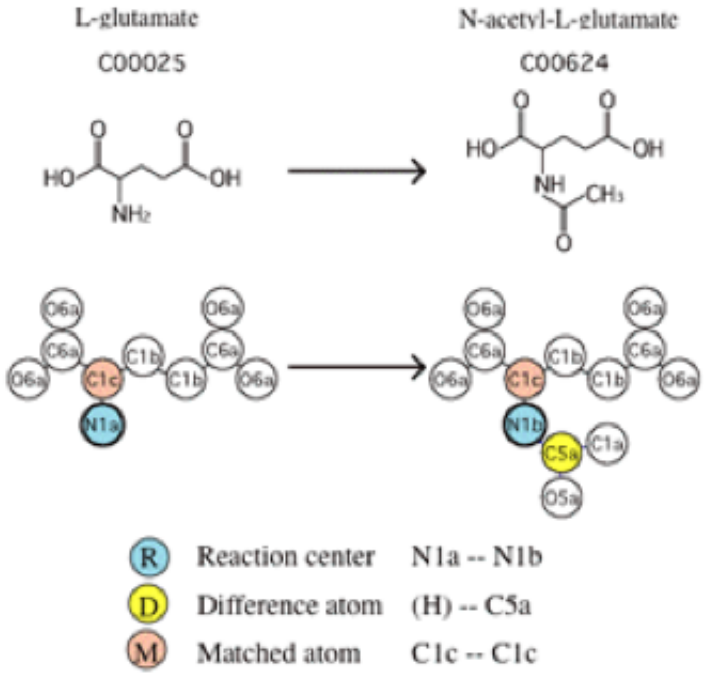
KEGG RPAIR Database

KEGG RPAIR is a collection of substrate-product pairs (reactant pairs) defined for each reaction in KEGG REACTION, together with the chemical structure transformation patterns characterized by the RDM patterns (see below). In general, a reaction consists of multiple reactant pairs, and the one that appears on the KEGG metabolic pathway map is called the main pair, such as RP04458 for the above acetylation reaction.

In order to distinguish functional groups and microenvironments of atoms, atomic species of C, N, O, S, and P are classified into 68 types, called KEGG atom types. They were first introduced for detecting biochemical similarities by graph-based chemical structure comparison [1].

- KEGG atom types

The RDM pattern is defined as KEGG atom type changes at the reaction center (R), the difference region (D), and the matched region (M) for each reactant pair. It characterizes chemical structure transformation patterns associated with enzymatic reactions [2].



(Example) RDM pattern for RP04458

What's "Chemoinformatics"?

- Chemical data storage and retrieval
  - Chemical file formats (SMILES, Molfiles, etc)
  - Chemical databases
- Virtual screening
- Quantitative structure-activity relationship (QSAR)

Google SSL beta search results

Term	Google search results
Bioinformatics	52,000,000
Chemoinformatics	1,070,000
Cheminformatics	940,000
Chem-bio informatics	38,900
Chemo–bio informatics	4,400
Biocheminformatics	2,760
Biochemoinformatics	2,160
Bio chemoinformatics	1,930
Bio cheminformatics	1,920
Chemical bioinformatics	909

CBI / JSBi 2011 合同大会

Chem-Bio Informatics Society(CBI)Annual Meeting 2011
The 2011 Annual Conference of the Japanese Socirty for Bioinformatics

計算科学の拓く新しい生命像

会期：2011 年 11 月 8 日（火）～ 10 日（木）
会場：神戸国際会議場　神戸コンベンションセンター
（ 神戸市中央区港島中町 6-9-1 ）

Chemical file formats

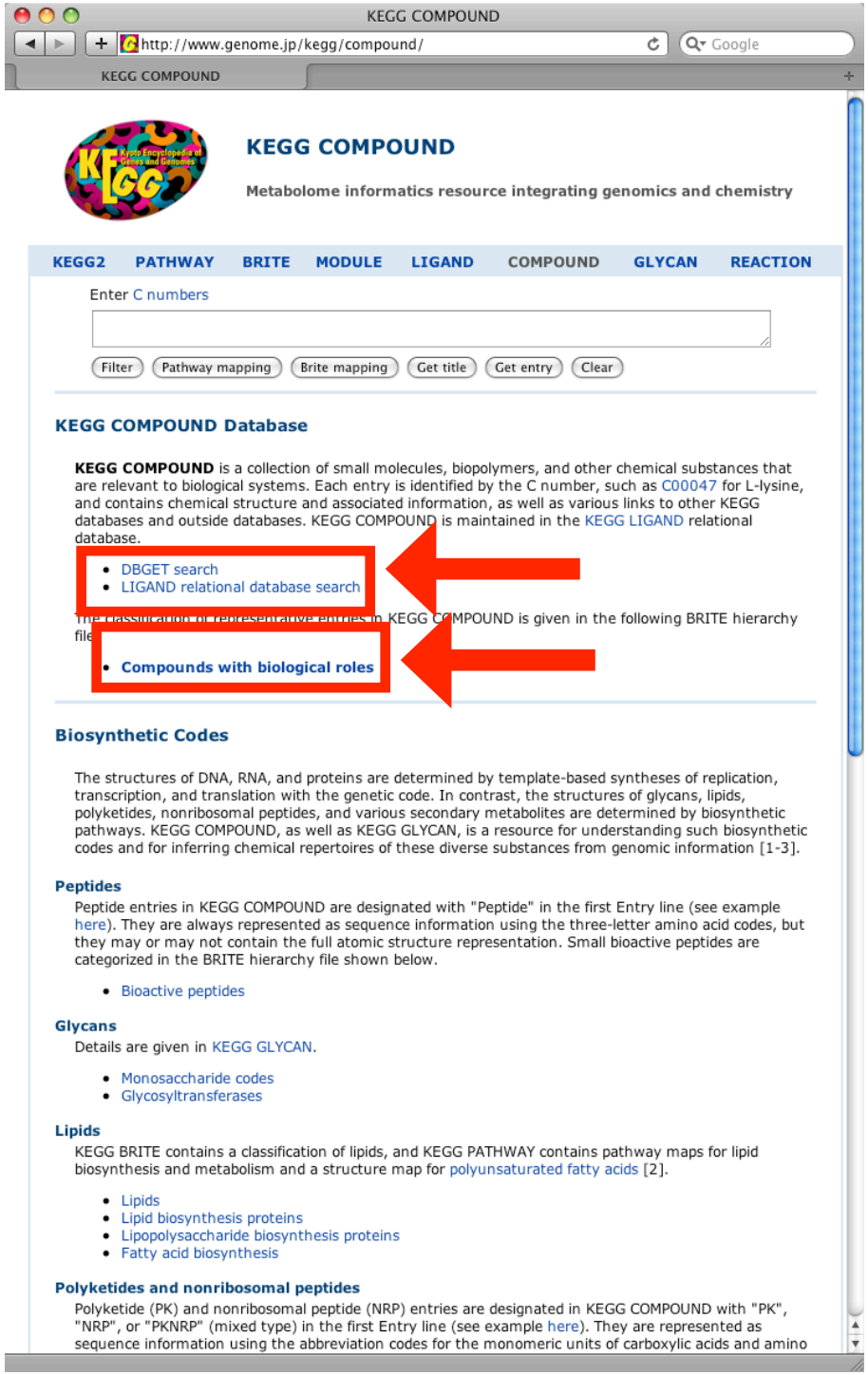
- Chemical line notations
  - SMILES … Simplified molecular input line entry specification
  - SLN … SYBYL Line Notation
  - InChI … The IUPAC International Chemical Identifier
- Chemical table files
  - Molfiles, SDF
  - KCF … KEGG Chemical Function
  - Protein Data Bank Format
- Chemical XML
  - CML … Chemical Markup Language

OpenBabel

- Free software mainly used for converting chemical file formats.
- Available for Windows, Unix, and Mac OS.
- Distributed under the GNU GPL.
- http://openbabel.org/

Chemical databases

- KEGG COMPOUND
  - http://www.genome.jp/kegg/compound/
- ChEBI
  - http://www.ebi.ac.uk/chebi/
- PubChem
  - http://pubchem.ncbi.nlm.nih.gov/
- ChemSpider
  - http://www.chemspider.com/
- ZINC
  - http://zinc.docking.org/
- Chemical Substances Database
  - http://www.saglasie.com/tr/chemical/

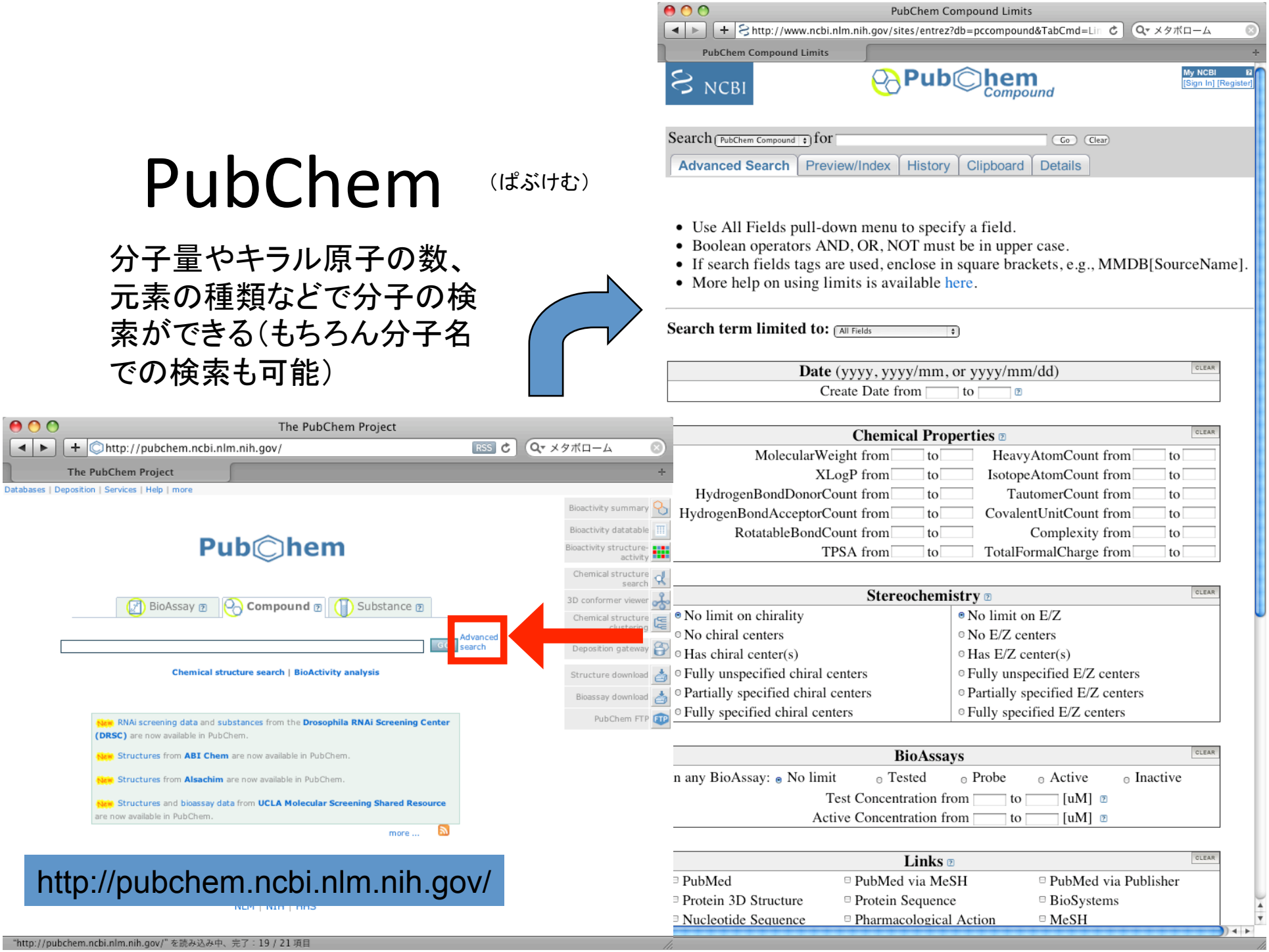


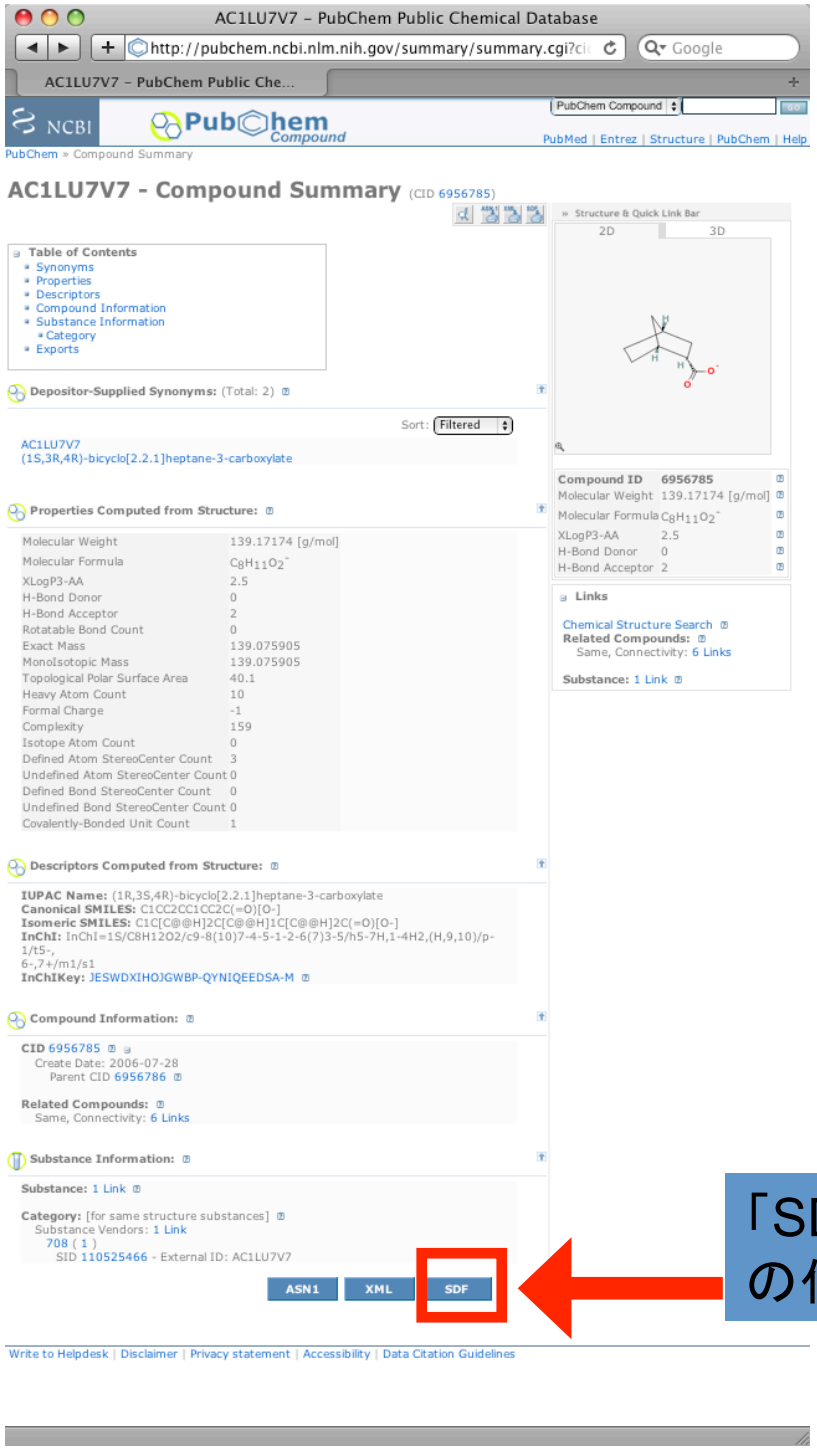
KEGG COMPOUND（けぐこんぱうんど）

生体分子の機能分類に基づいて検索ができる
（もちろん分子名での検索も可能）。

PubChem （ぱぶけむ）

分子量やキラル原子の数、元素の種類などで分子の検索ができる（もちろん分子名での検索も可能）





PubChem （ぱぶけむ）

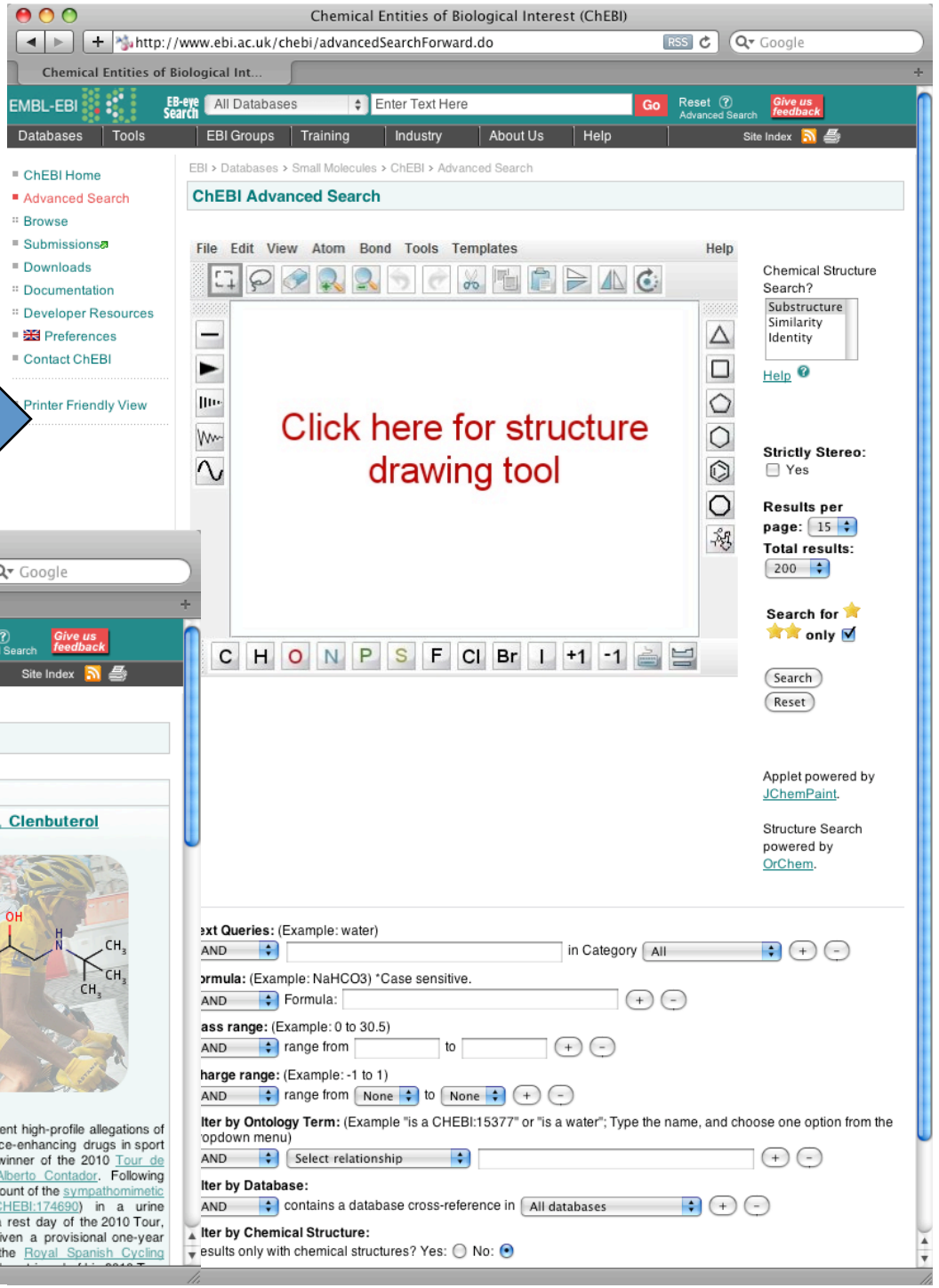
分子量やキラル原子の数、元素の種類などで分子の検索ができる（もちろん分子名での検索も可能）

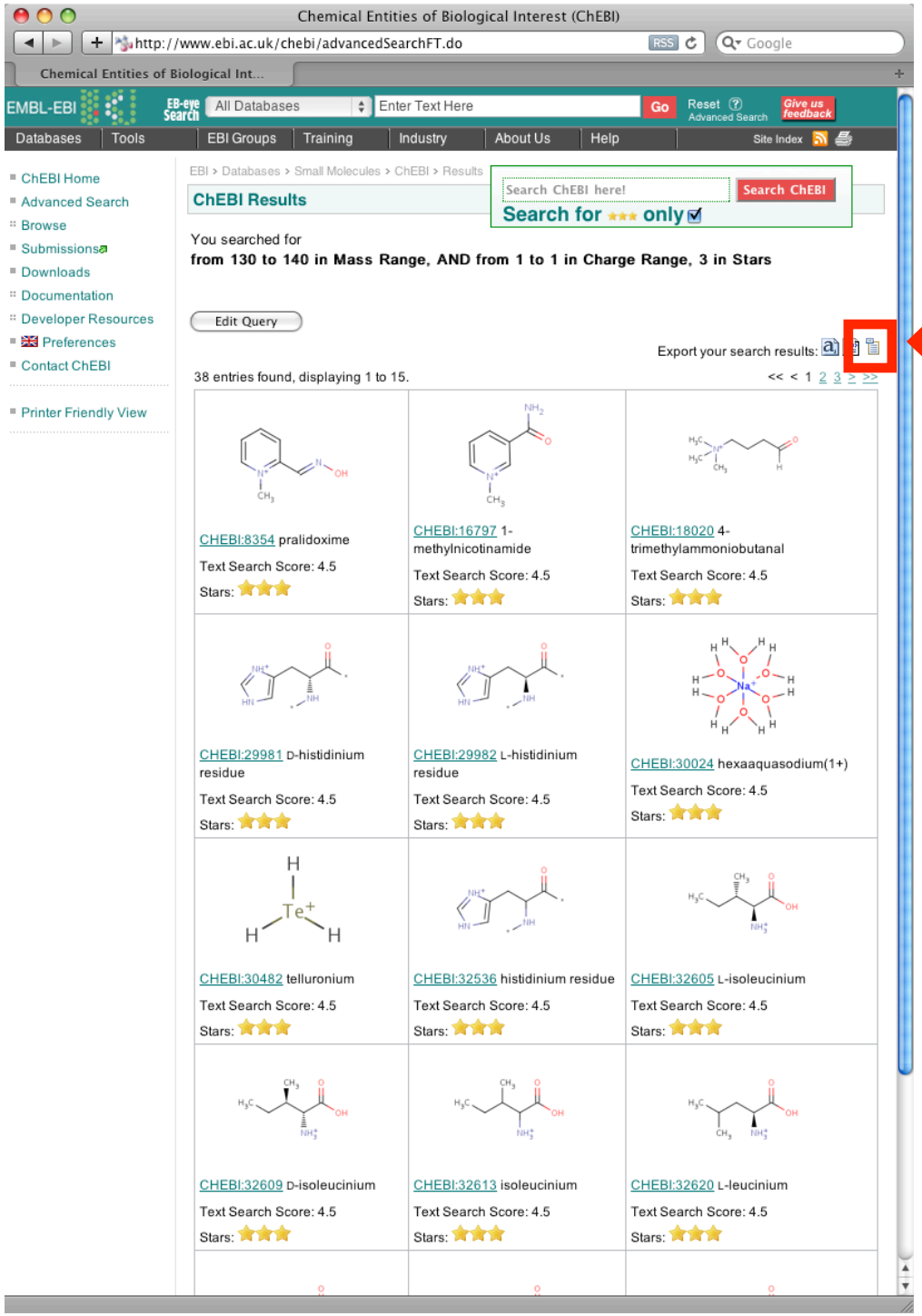
「SDF」をクリックするとSDF形式の化合物構造データが手に入る

（SDF = mol ファイルの拡張形式）

ChEBI （けびい、ちぇびい）

分子量や電荷数などの他、分子描画ツールで分子の検索ができる（もちろん分子名での検索も可能）。





ChEBI （けびい、ちぇびい）

ココをクリックするとSDF形式の化合物構造データが複数まとめてダウンロードできる。

（SDF = mol ファイルの拡張形式）

分子量や電荷数などの他、分子描画ツールで分子の検索ができる(もちろん分子名での検索も可能)。

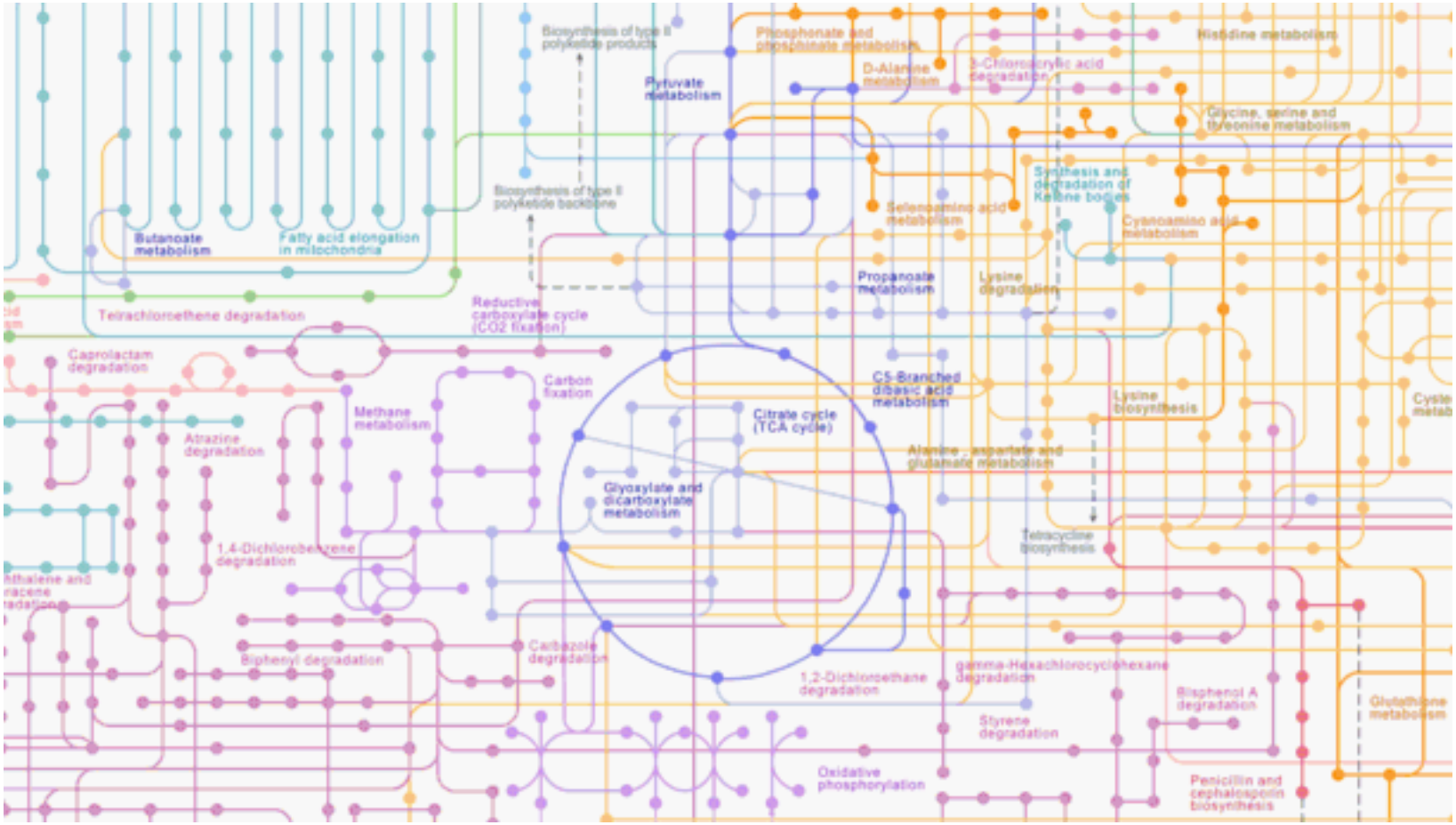
Reconstruction of metabolic networks

In the case a reference pathway…

- Exists,
  - **Which gene is mapped onto where?**
  - Are there any possible paths that are not found yet?
- Does not exist,
  - Which compound is converted into which compound?
  - Which gene is mapped onto that path?

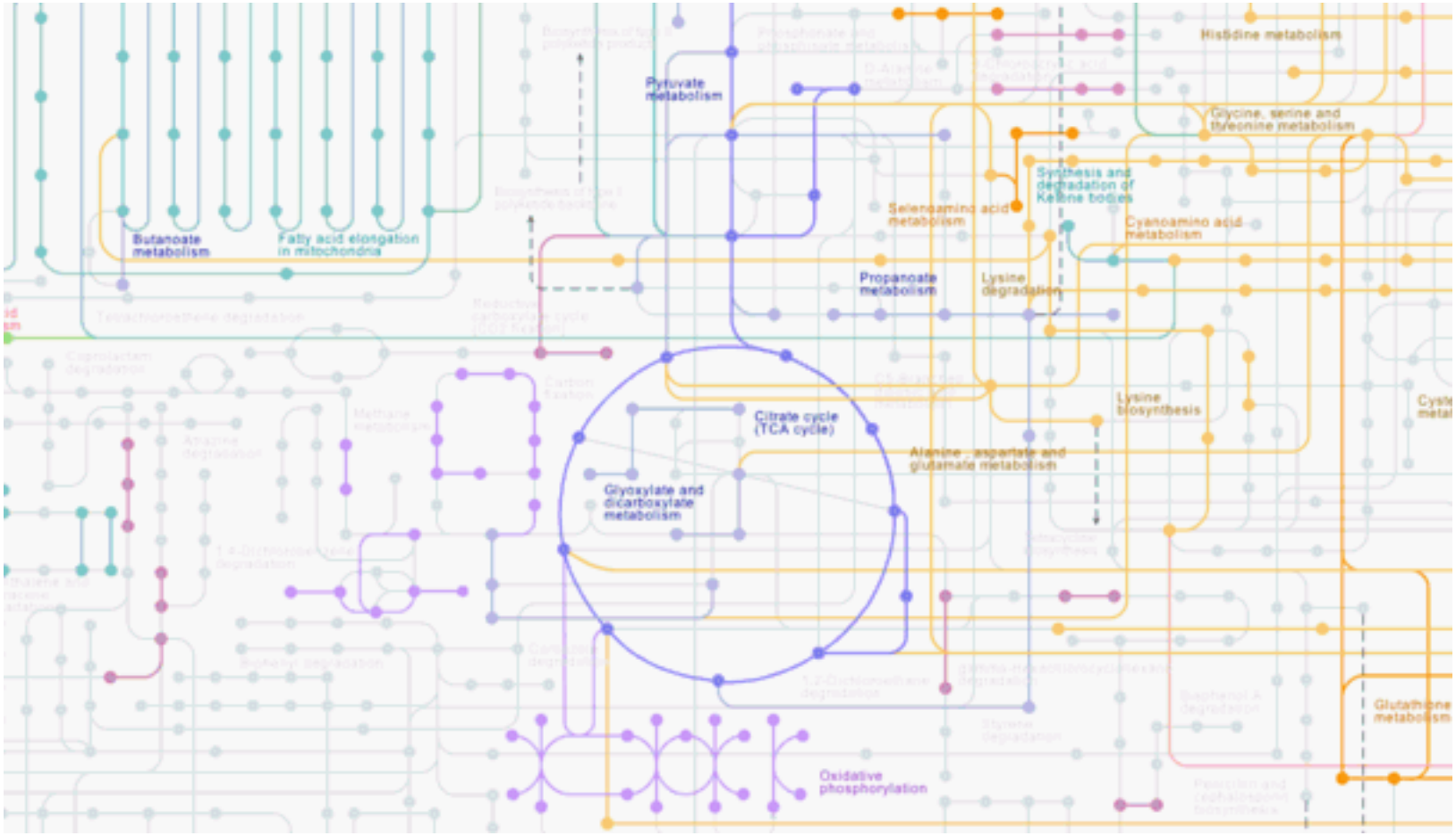
KEGG global map

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



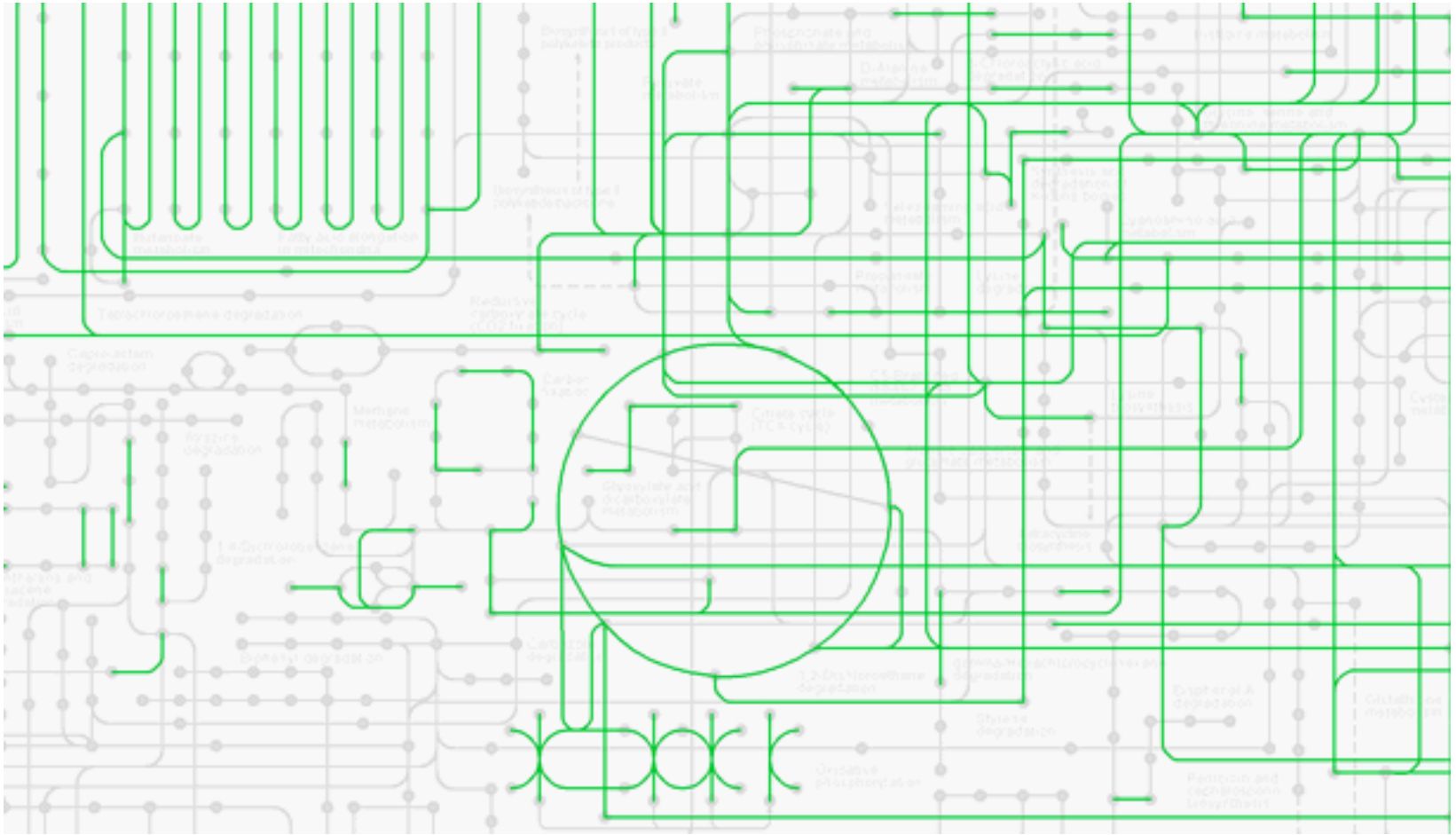
KEGG global map of human

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



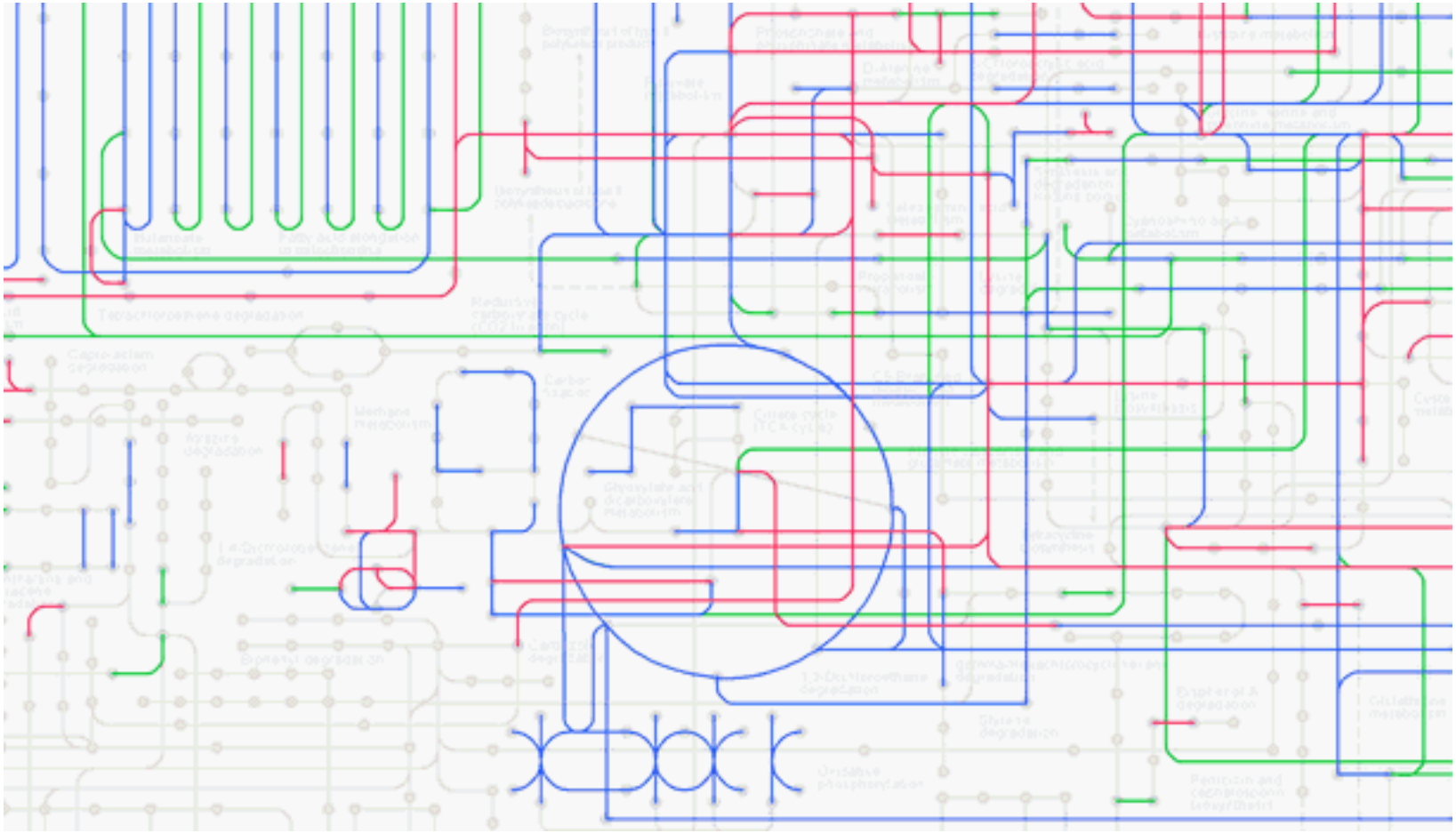
Human metabolome

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



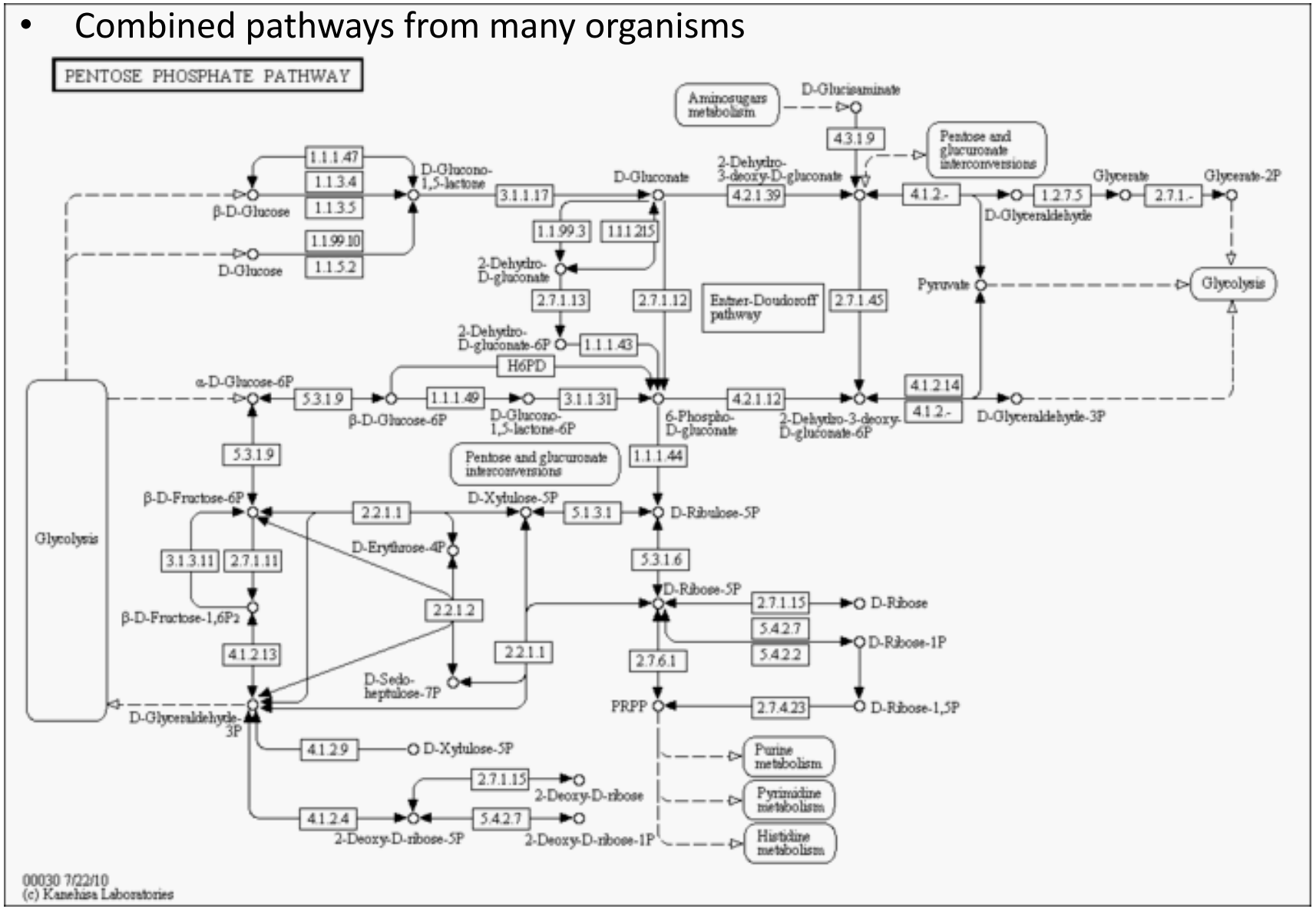
Human gut meta-metabolome

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



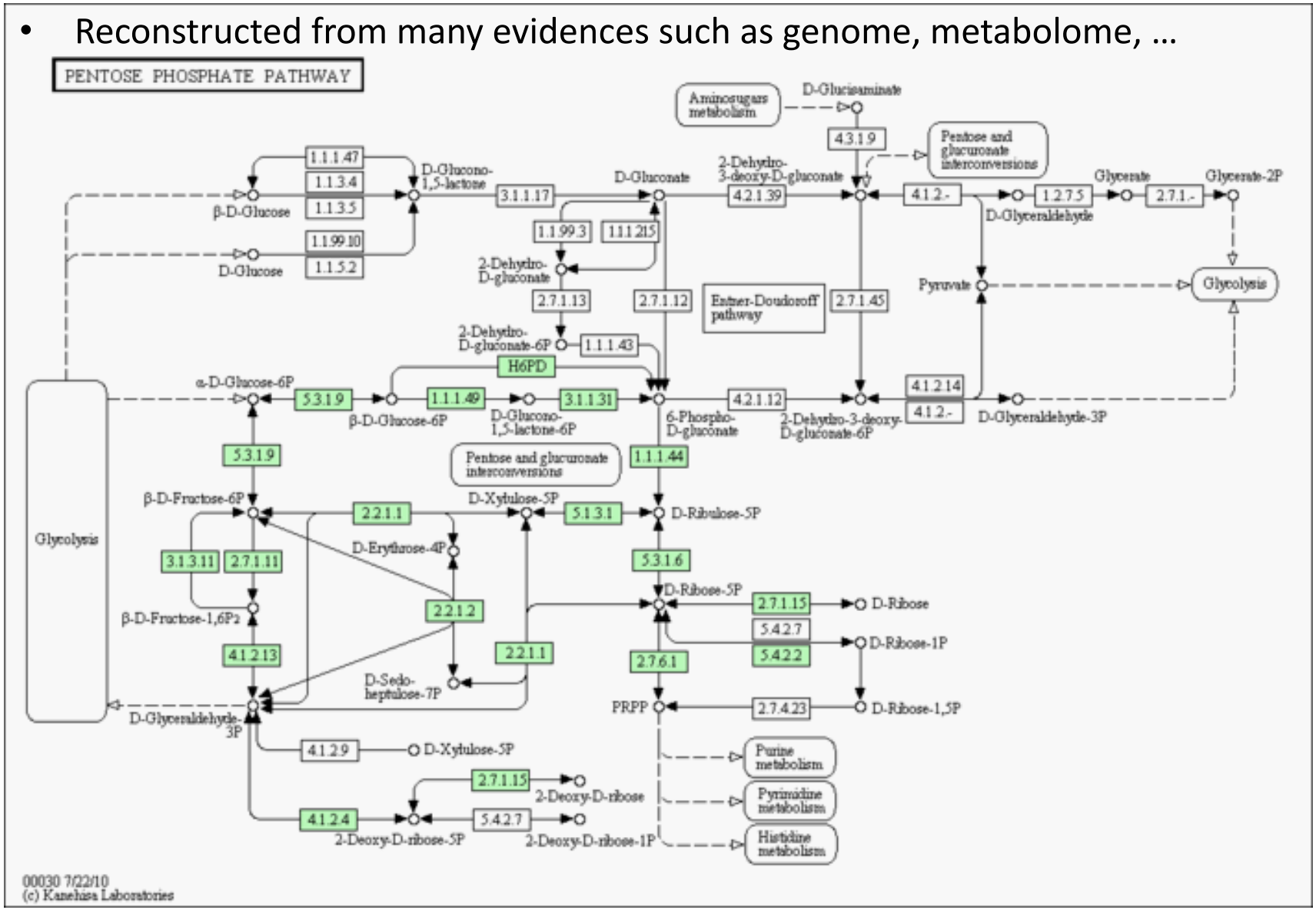
Reference pathways

- Combined pathways from many organisms



Organic-specific pathways

- Reconstructed from many evidences such as genome, metabolome, …



[HTML] Reconstruction of amino acid biosynthesis pathways from the complete genome sequence

H **Bono**, H **Ogata**, S **Goto**... - Genome research, 1998 - gb.cw.com.tw

The complete genome sequence of an organism contains information that has not been fully utilized in the current prediction methods of gene functions, which are based on piece-by-piece similarity searches of individual genes. We present here a method that utilizes a higher ...

Cited by 122 - Related articles - BL Direct - All 19 versions

Table 2. Results of Reconstructing Amino Acid Biosynthesis Pathways from Seven Complete Genomes

KEGG map ID	Amino acid	*Eco*	*Hin*	*Hpy*	*Bsu*	*Mja*	*Sy*	
00251	Gln	++	++	++	++	++	++	++
	Gln	++	++	++	++	++	++	++
00252	Asn	++	++	?	++	++	++	++
	Asp	++	++	?	++	++	++	++
	Ala	2.6.1	2.6.1	++	++	++	++	++
00260	Ser	++	++	++	++	++	++	++
	Gly	++	++	++	++	++		
	Thr	++	++	++	++	++		
00271	Met	++	++	–	++	–	+	++
00272	Cys	++	++	++				
00290	Val	++	++	–				
	Leu	++	++	–	++	+	++	++
	Ile	++	++	–	++	++	++	++
00300	Lys	2.6.1	2.6.1	2.6.1	2.6.1	?	?	?
00330	Arg	++	+	–	++	++	+	++
	Pro	++	++	++	+	–	++	++
00340	His	++	++	–	++	++	+	+
00400	Phe	++	++	?	++	?	++	++
	Tyr	++	++	?	++	?	++	++
	Trp	++	++	+	++	?	++	++

(++) Reconstruction is complete in the current version of KEGG; (+) reconstruction becomes complete by assigning a homologous gene; (2.6.1) reconstruction becomes complete by assuming wider specificity for an enzyme; (?) the pathway apparently exists but all missing enzymes are not yet resolved; (–) the pathway does not appear to exit.

Reference pathways

Bidirectional Best Hit

Orthologous Gene Table

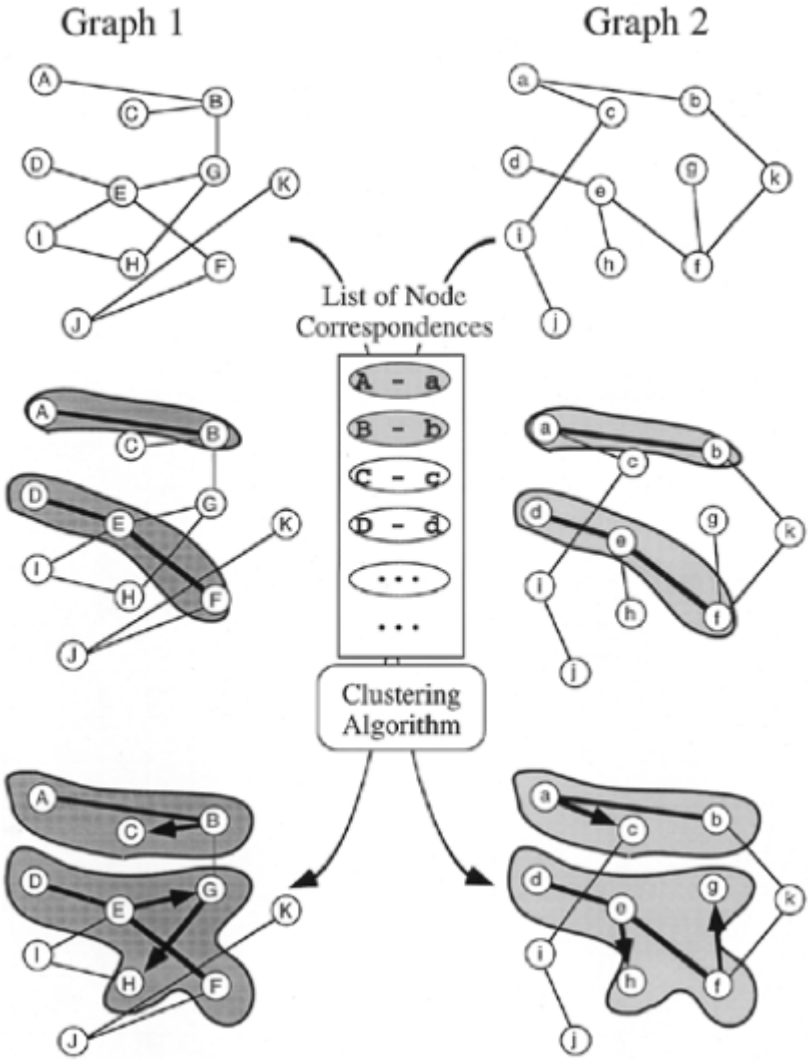
GFIT (Gene Function Identification Tool)

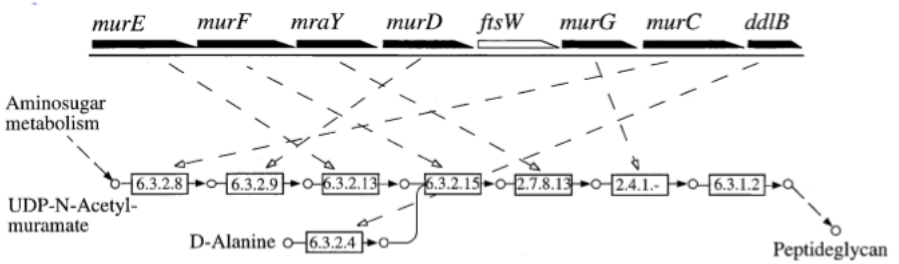
A heuristic graph comparison algorithm and its application to detect functionally related enzyme clusters

H **Ogata**, W **Fujibuchi**, S **Goto**... - Nucleic acids ..., 2000 - Oxford Univ Press

The availability of computerized knowledge on biochemical pathways in the KEGG database opens new opportunities for developing computational methods to characterize and understand higher level functions of complete genomes. Our approach is based on the concept of ...

Cited by 156 - Related articles - BL Direct - All 29 ve





Spe-cies	6.3.2.13	6.3.2.15	2.7.8.13	6.3.2.9	-	2.4.1.-	6.3.2.8	6.3.2.4
	3	4	5	2		6	1	3'
Eco	b0085 (murE)	b0086 (murF)	b0087 (mraY)	b0088 (murD)	b0089 (ftsW)	b0090 (murG)	b0091 (murC)	b0092 (ddlB)
Hin	HI1133	HI1134	HI1135	HI1136	HI1137	HI1138	HI1139	HI1140
Hpy	HP1494	HP0740	HP0493	HP0494	HP0743	HP1155	HP0623	HP0738
Rpr	RP597	RP596	RP595	RP410	RP280	RP412	RP247	RP249
Bsu	murE	murF	mraY	murD	spoVE	murG	murC	ddlA
Mtu	Rv2158c	Rv2157c	Rv2156c	Rv2155c	Rv2154c	Rv2153	Rv2152c	Rv2981c
Ctr	CT269	CT756	CT757	CT758	CT760	CT761	CT762	
Cpn	CPn0418	CPn0899	CPn0900	CPn0901	CPn0903	CPn0904	CPn0905	
Bbu	BB0201	BB0304	BB0303	BB0585	BB0302	BB0767	BB0817	BB0200
Tpa	TP0933	TP0386	TP0345	TP0903	TP0387	TP0523	TP0341	TP0670
Syn	slr0528	slr1351	sll0657	sll2010	slr1267	slr1656	slr1423	slr1874
Dra	DR0297	DR0768	DR1835	DR2496	DR2497	DR0626	DR0627	DR0362
Aae	aq_1747	aq_821	aq_053	aq_2075	aq_025	aq_1177	aq_1360	aq_521
Tma	TM0237	TM0236	TM0235	TM0234	TM0233	TM0232	TM0231	TM0259

The KEGG resource for deciphering the genome

M Kanehisa, S Goto, S Kawashima... - Nucleic acids ..., 2004 - Oxford Univ Press

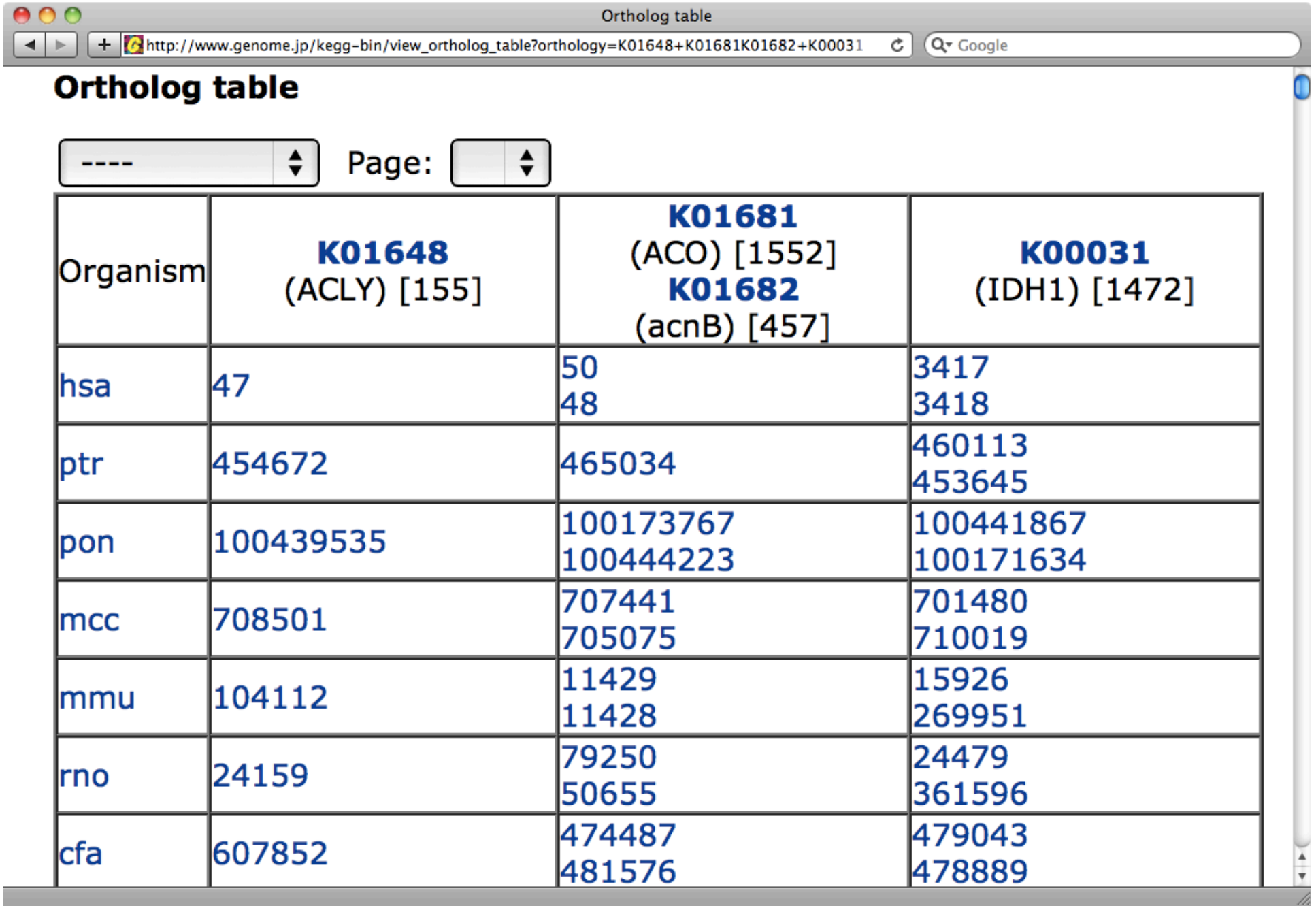
... New efforts are being made to abstract knowledge, both computationally and manually, about ortholog clusters in the KO (**KEGG Orthology**) database, and to collect and analyze carbohydrate structures in the GLYCAN database. ...

Cited by 1168 - Related articles - BL Direct - All 33 versions

Table 2. The hierarchy of KEGG orthology (KO)

01100 Metabolism
  01110 Carbohydrate metabolism
  01120 Energy metabolism
  01130 Lipid metabolism
  01140 Nucleotide metabolism
  01150 Amino acid metabolism
    00251 Glutamate metabolism
    .....
    00300 Lysine biosynthesis
      K00003 E1.1.1.3, thrA; homoserine dehydrogenase
      K00928 E2.7.2.4, lysC; aspartate kinase
      K00133 E1.2.1.11, asd; aspartate-semialdehyde dehydrogenase
      K01714 E4.2.1.52, dapA; dihydrodipicolinate synthase
      K00215 E1.3.1.26, dapB; dihydrodipicolinate reductase
      K00674 E2.3.1.117, dapD; 2,3,4,5-tetrahydropyridine-2-carboxylate *N*-succinyltransferase
      K00821 E2.6.1.17; *N*-succinyldiaminopimelate aminotransferase
      K01439 E3.5.1.18, dapE; succinyl-diaminopimelate desuccinylase
      K01778 E5.1.1.7, dapF; diaminopimelate epimerase
      K01586 E4.1.1.20, lysA; diaminopimelate decarboxylase
      .....
    00310 Lysine degradation
    .....
  01160 Metabolism of other amino acids
  .....
01200 Genetic information processing
01300 Environmental information processing
01400 Cellular processes
01500 Human disease


KEGG ORTHOLOGY (KO) Database
http://www.genome.jp/kegg/ko.html
Google
アップル
Yahoo! Japan
YouTube
Wikipedia
ニュース (289)
お役立ち
PBTweet+
KEGG ORTHOLOGY (KO) Database
Linking genomes to pathways by ortholog annotation
KEGG2
PATHWAY
BRITE
MODULE
KO
GENOME
GENES
SSDB
Organisms
Enter K numbers
(Example) K00161 K00162 K00163 K00627 K00382
Filter
Ortholog table
Pathway mapping
Brite mapping
Get title
Get entry
Clear
KEGG Orthology (KO) System
The KEGG reference pathways maps, BRITE functional hierarchies, and KEGG modules are represented in a general way to be applicable to all organisms. The KEGG Orthology (KO) system is the basis for this representation, consisting of manually defined ortholog groups that correspond to KEGG pathway nodes, BRITE hierarchy nodes, and KEGG module nodes.
KEGG Orthology (KO)
Once genes are assigned the KO identifiers, or the K numbers, by the genome annotation procedure described below, the organism-specific pathway maps, BRITE functional hierarchies, and KEGG modules are automatically generated (see KEGG mapping for details).
Search
ORTHOLOGY
for
Go
Clear
bfind mode
bget mode



Ortholog table

---- Page:

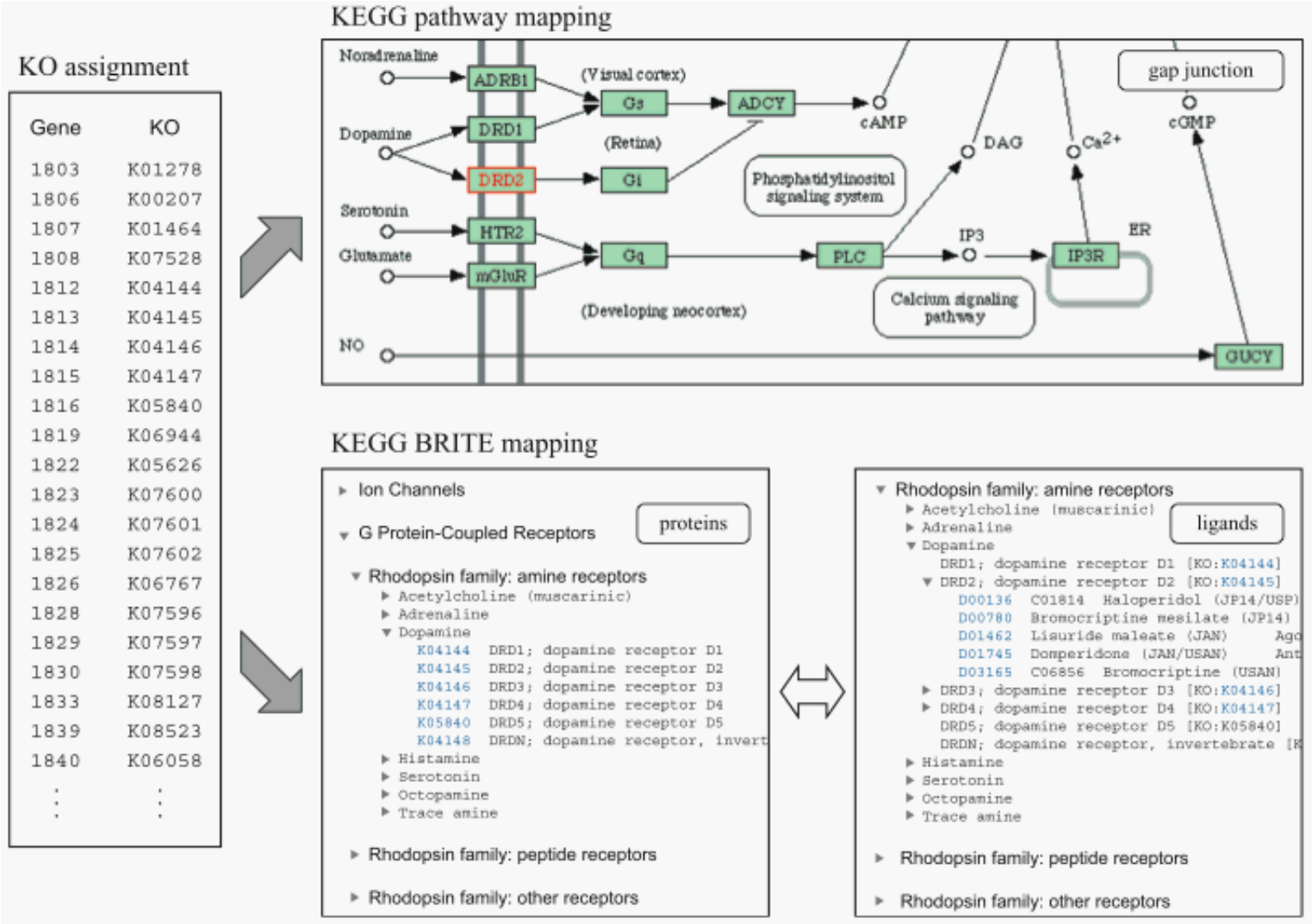
Organism	**K01648** (ACLY) [155]	**K01681** (ACO) [1552] **K01682** (acnB) [457]	**K00031** (IDH1) [1472]
hsa	47	50 48	3417 3418
ptr	454672	465034	460113 453645
pon	100439535	100173767 100444223	100441867 100171634
mcc	708501	707441 705075	701480 710019
mmu	104112	11429 11428	15926 269951
rno	24159	79250 50655	24479 361596
cfa	607852	474487 481576	479043 478889

KAAS: an automatic genome annotation and pathway reconstruction server

Y **Moriya**, M Itoh, S Okuda… - Nucleic Acids …, 2007 - Oxford Univ Press

The number of complete and draft genomes is rapidly growing in recent years, and it has become increasingly important to automate the identification of functional properties and biological roles of genes in these genomes. In the KEGG database, genes in complete genomes are ...

Cited by 121 - Related articles - All 11 versions

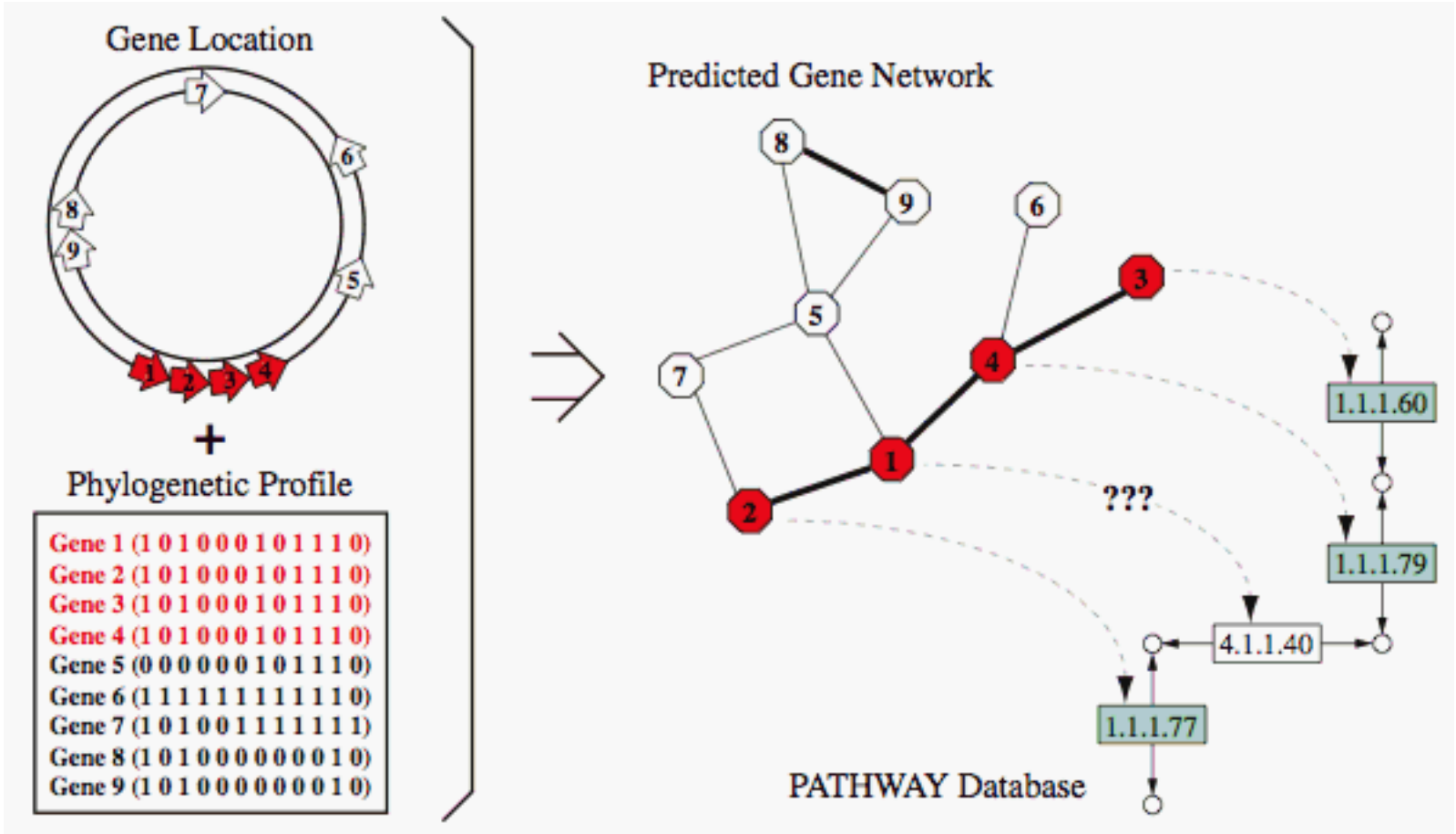


Prediction of missing enzyme genes in a bacterial metabolic network

Y **Yamanishi**, H **Mihara**, M Osaki… - FEBS …, 2007 - Wiley Online Library

The metabolic network is an important biological network which consists of enzymes and chemical compounds. However, a large number of metabolic pathways remains unknown, and most organism-specific metabolic pathways contain many missing enzymes. We present a ...

Cited by 21 - Related articles - BL Direct - All 5 versions



Reconstruction of metabolic networks

In the case a reference pathway…

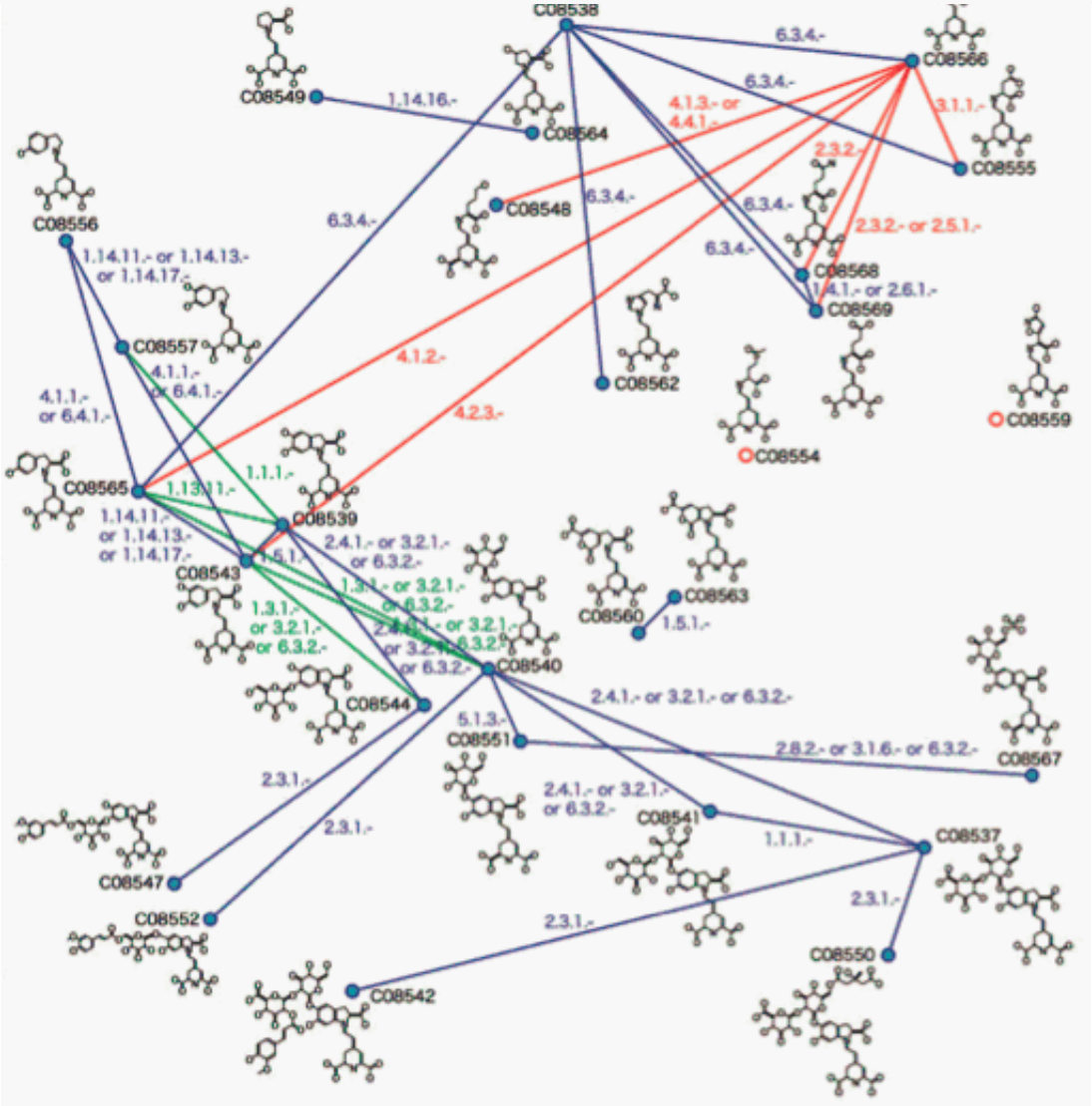
- Exists,
  - Which gene is mapped onto where?
  - Are there any possible paths that are not found yet?
- Does not exist,
  - **Which compound is converted into which compound?**
  - Which gene is mapped onto that path?

Eliciting possible reaction equations and metabolic pathways involving orphan metabolites

M Kotera, AG McDonald, S Boyce, KF … - Journal of Chemical …, 2008 - ACS Publications

The development of metabolomics has resulted in the discovery of an increasing number of orphan metabolites, which are defined as compounds that are known to be present in living organisms but whose synthetic/degradation pathways are unknown. In this paper, we describe a ...

引用元 6 - 関連記事 - 全 2 バージョン

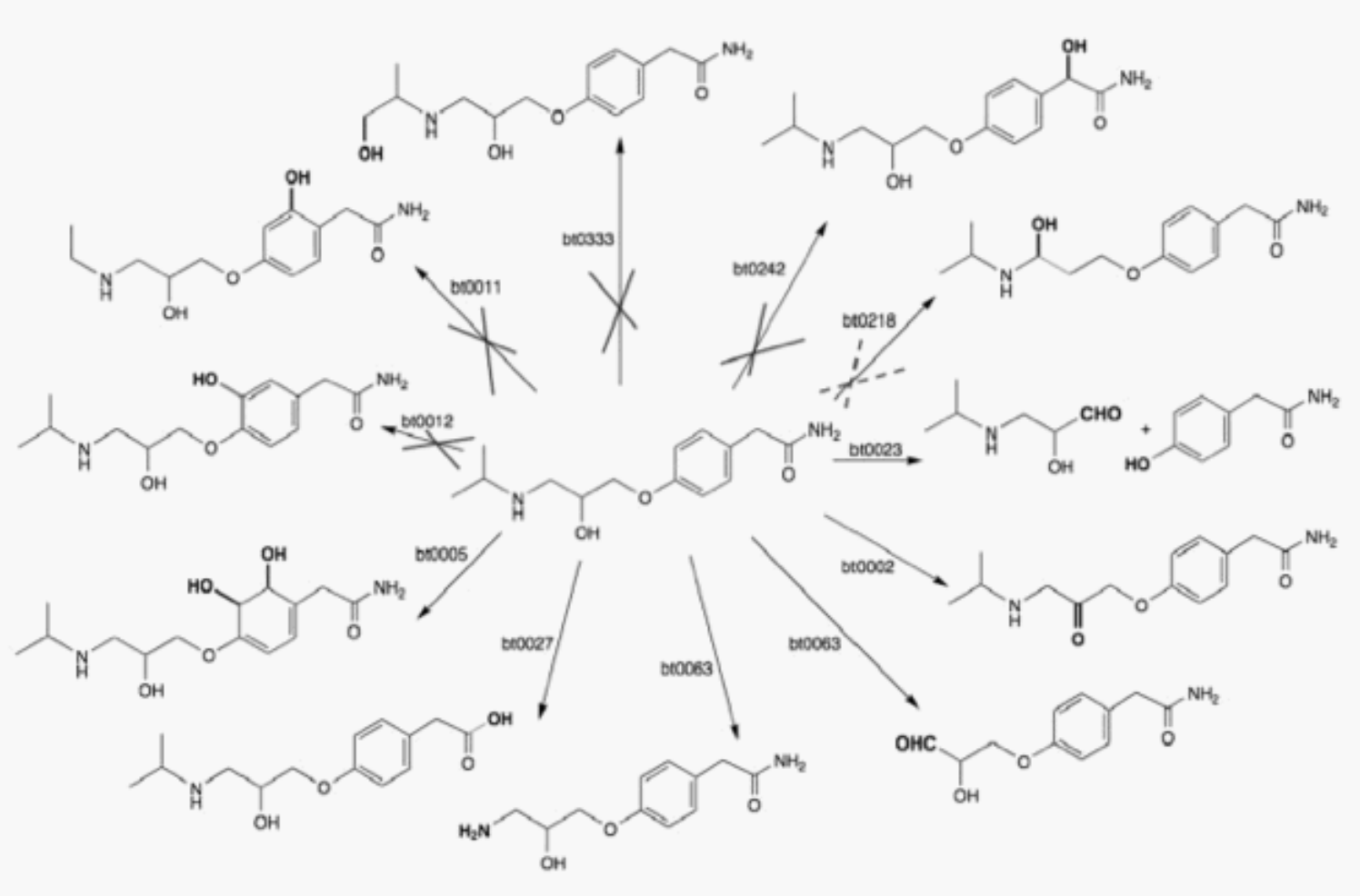


Data-driven extraction of relative reasoning rules to limit combinatorial explosion in biodegradation pathway prediction

K Fenner, J Gao, S Kramer, L Ellis, L Wackett - Bioinformatics, 2008 - Oxford Univ Press

Results: A total of 112 relative reasoning rules were identified and implemented. In one prediction step, ie as per one generation predicted, the use of relative reasoning decreases the predicted biotransformations by over 25% for 50 compounds used to generate the rules and by ...

引用元 8 - 関連記事 - 全 10 バージョン



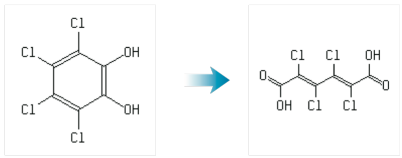
PathPred: an enzyme-catalyzed metabolic pathway prediction server

Y Moriya, D Shigemizu, M Hattori… - Nucleic Acids …, 2010 - Oxford Univ Press

The KEGG RPAIR database is a collection of biochemical structure transformation patterns, called RDM patterns, and chemical structure alignments of substrate-product pairs (reactant pairs) in all known enzyme-catalyzed reactions taken from the Enzyme Nomenclature and the ...

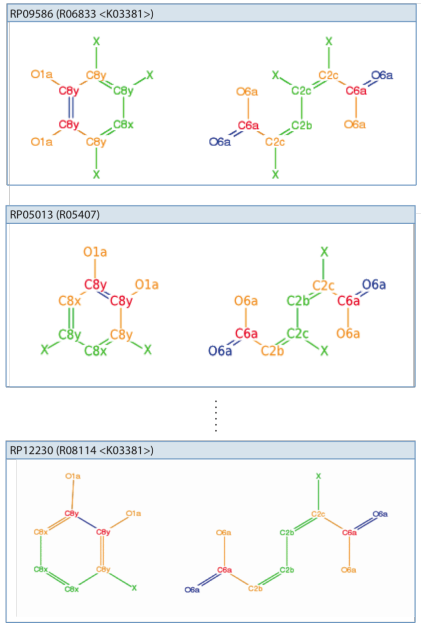
Cited by 5 - Related articles - All 6 versions

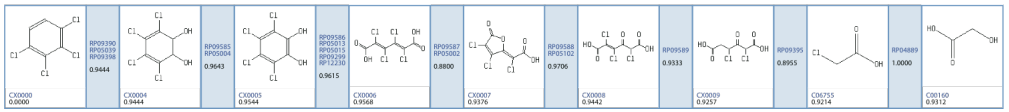
predicted reaction

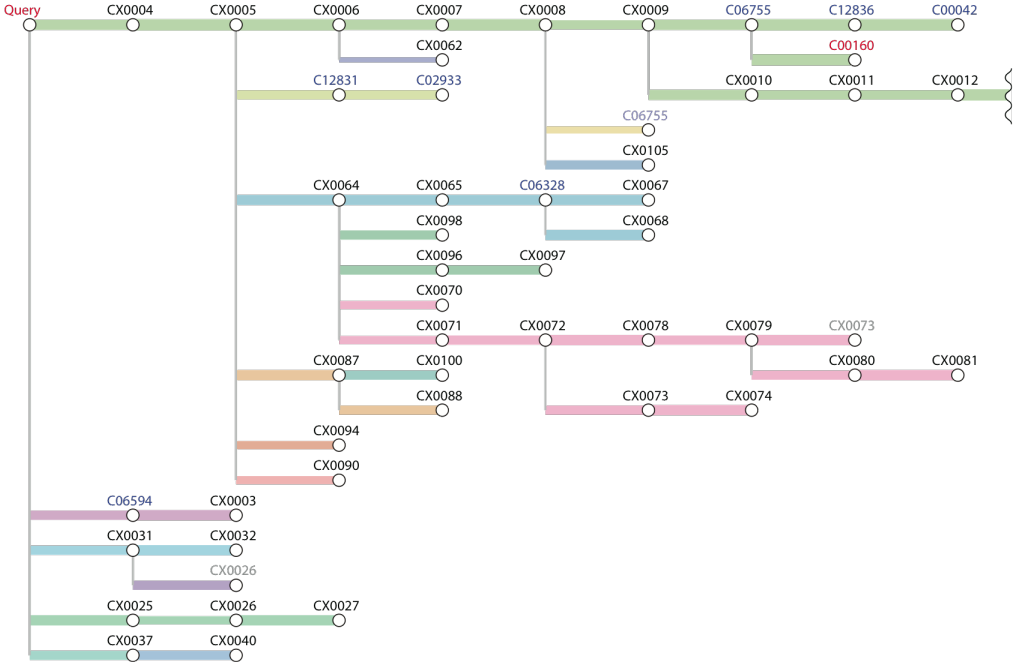


reaction score: 0.9615

reference rpairs







Reconstruction of metabolic networks

In the case a reference pathway…

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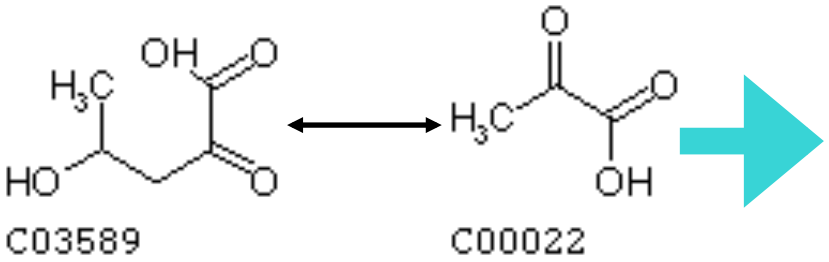
  - Are there any possible paths that are not found yet?
- Does not exist,
  - Which compound is converted into which compound?
  - **Which gene is mapped onto that path?**

Development of a chemical structure comparison method for integrated analysis of chemical and genomic information in the metabolic pathways

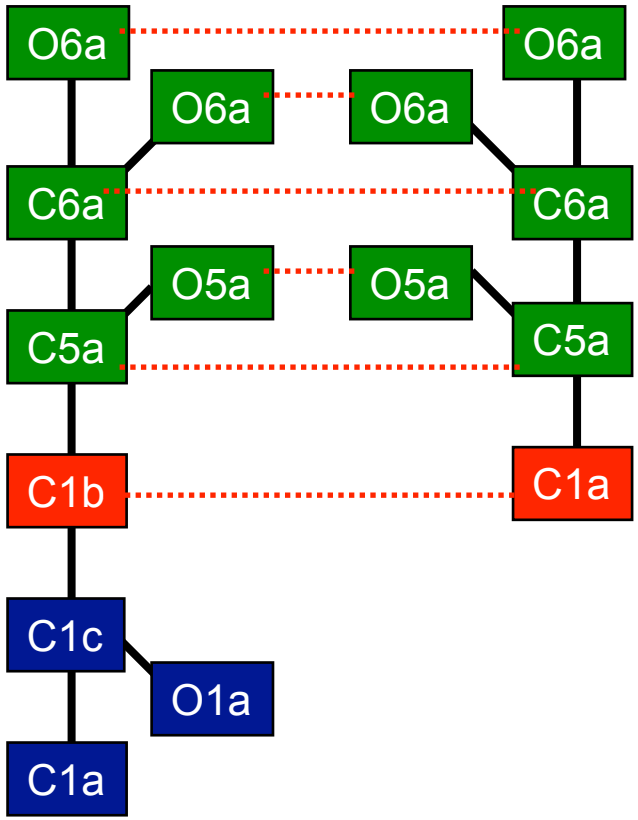
M Hattori, Y Okuno, S Goto, M Kanehisa - J. Am. Chem. Soc, 2003 - ACS Publications

Cellular functions result from intricate networks of molecular interactions, which involve not only proteins and nucleic acids but also small chemical compounds. Here we present an efficient algorithm for comparing two chemical structures of compounds, where the chemical ...

引用元 112 - 関連記事 - 全 4 バージョン



Atom alignment of the molecular graphs

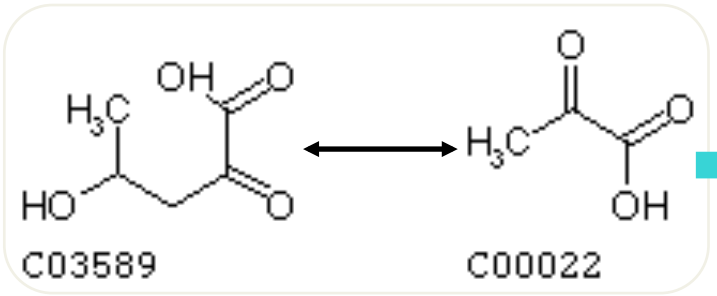


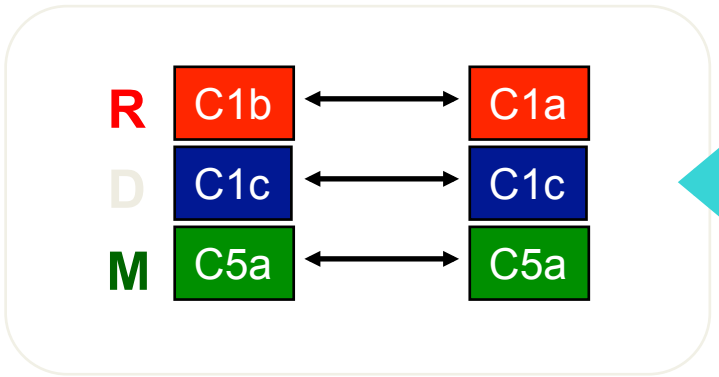
Computational assignment of the EC numbers for genomic-scale analysis of enzymatic reactions

M **Kotera**, Y Okuno, M Hattori, S Goto… - Journal of the …, 2004 - ACS Publications

The EC (Enzyme Commission) numbers represent a hierarchical classification of enzymatic reactions, but they are also commonly utilized as identifiers of enzymes or enzyme genes in the analysis of complete genomes. This duality of the EC numbers makes it possible to ...

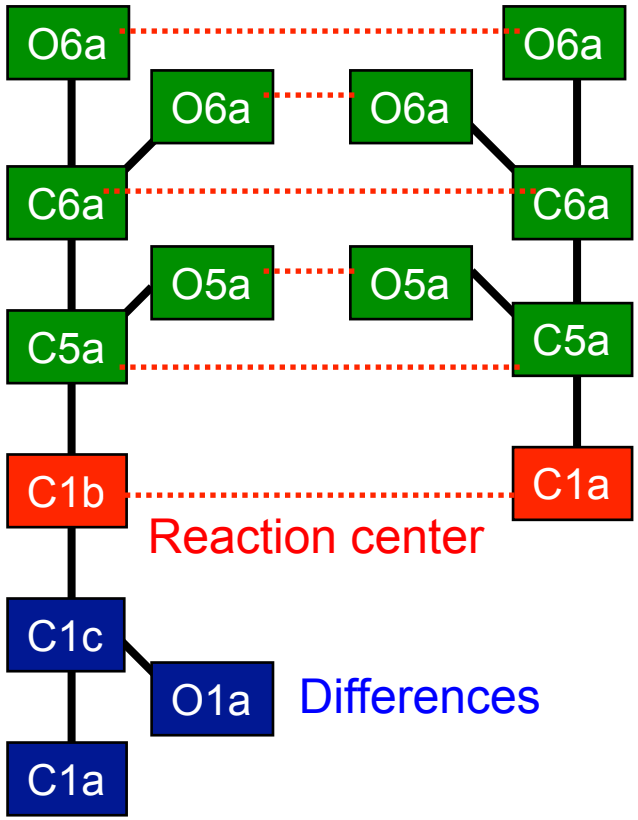
Cited by 78 - Related articles - All 8 versions





RDM chemical transformation pattern

Atom alignment of the molecular graphs

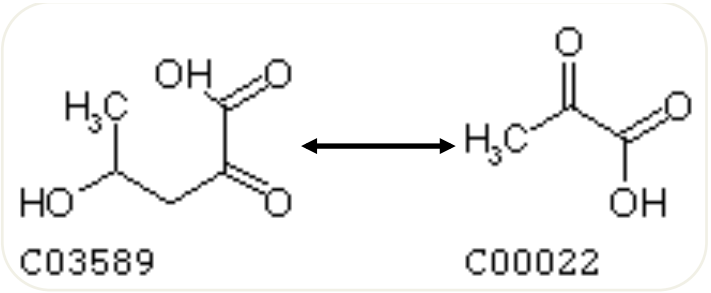


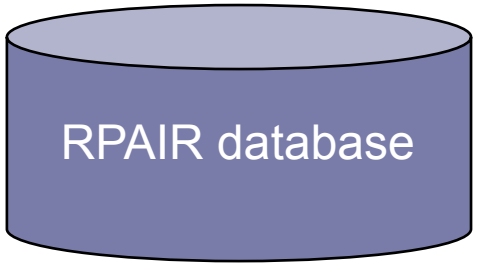
E-zyme: predicting potential EC numbers from the chemical transformation pattern of substrate-product pairs

Y Yamanishi, M Hattori, M Kotera, S Goto… - …, 2009 - Oxford Univ Press

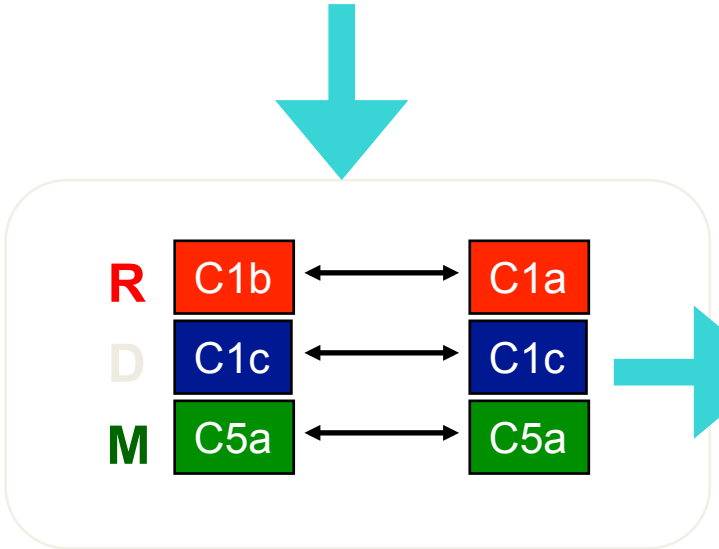
Results: In this article we propose a new method to predict the potential EC numbers to given reactant pairs (substrates and products) or uncharacterized reactions, and a web-server named E-zyme as an application. This technology is based on our original biochemical ...

Cited by 14 - Related articles - All 10 versions

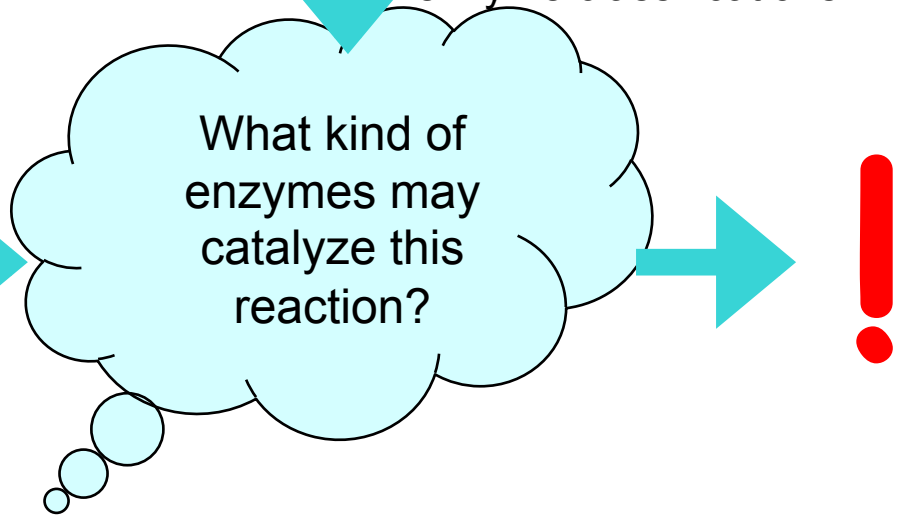




Known correspondence between RDM patterns and enzyme classifications



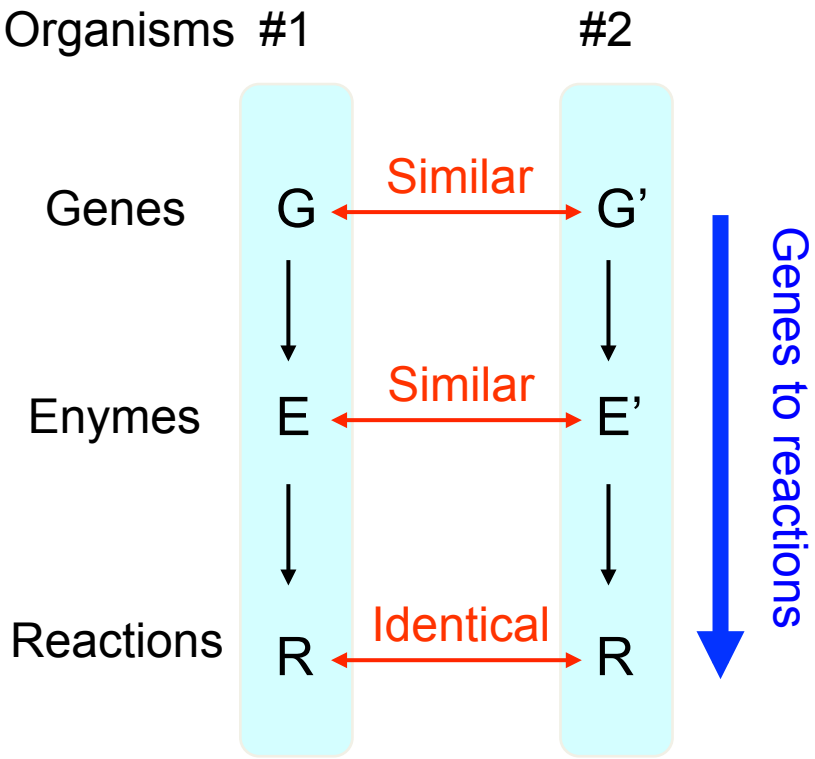
RDM chemical transformation pattern



Genome annotation with chemical point of view

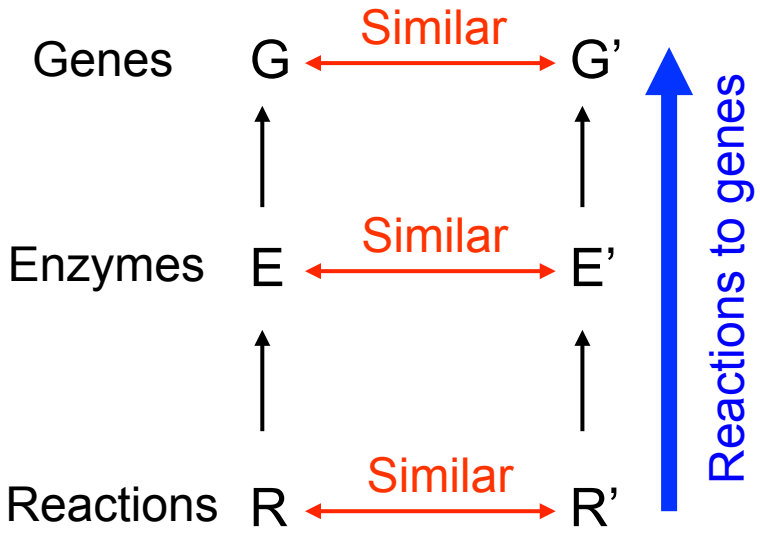
KEGG Orthology (KO)

Sequence similarity groups



Reaction Class (RC)

Reaction similarity groups



What is meant by being “similar”?

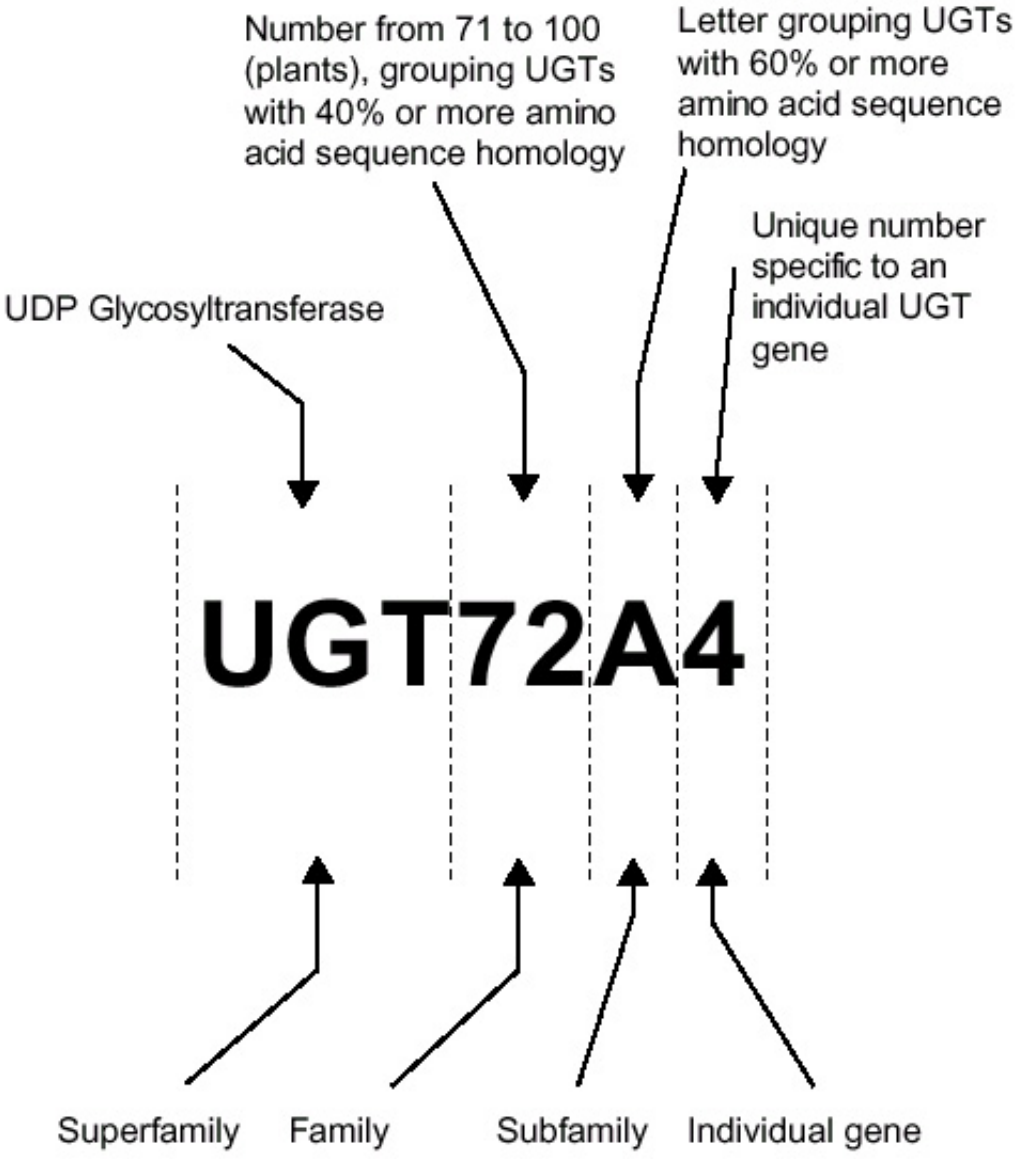
- Enzyme “proteins” are similar
- Enzyme “reactions” are similar

	Sequence	3D
Globally	Full-length	Fold
Locally	Motif	Cavity

	Reaction	Substrates
Globally	?	?
Locally	?	?

Sequence similarity-based enzyme classifications

- Cyt P450
  - EC 1.14
- Glycosyltransferases
  - EC 2.4



[PDF] **Higher plant glycosyltransferases**
J Ross, Y Li, EK Lim, DJ Bowles - Genome Biol, 2001 - biome
Uridine diphosphate (UDP) glycosyltransferases (UGTs) media
from activated nucleotide sugars to acceptor molecules (aglyc
of the acceptors such as their bioactivity, solubility and transp
引用元 110 - 関連記事 - HTMLバージョン - 全 11 バージョン

EC classification criteria

Class	Subclass	Sub-subclass	Remarks
1. Oxidoreductases	Functional groups of reductants	Oxidants	Which compounds are reductants, or oxidants?
2. Transferases	Transferred groups	Transferred groups in detail	From where to where?
3. Hydro-lases	Hydrolyzed bond	Hydrolyzed bond in detail	Nucleases and peptidases are classified in much more detail.
4. Lyases	Digested bond	Types of products	Some hydrolase-like reactions
5. Isomerases	Types of isomeration (RS, EZ, Redox, Transfer, Elimation)	Types of reacting bonds, or products	Any one-molecular reactions.
6. Ligases	Generated bond	Types of substrate	Multi-step reactions

[PDF] **SCOPEC: a database of protein catalytic domains**
RA George, RV Spriggs, JM Thornton, B Al- ... - ..., 2004 - Oxford Univ Press
Page 1. BIOINFORMATICS Vol. 20 Suppl. 1 2004, pages i130–i136 DOI: 10.1093/bioinformatics/bth948 SCOPEC: a database of protein catalytic domains Richard A. George 1,2,* , Ruth V. Spriggs 1,2 , Janet M. Thornton 2 , Bissan Al-Lazikani 1 and Mark B. Swindells 1 ...
引用元 25 - 関連記事 - 全 8 バージョン

Thioesterase domain of polypeptide, polyketide and fatty acid synthases

Aspartate aminotransferase-like domain

NAD(P)-binding Rossmann-fold domain

Hydro-lyase

Phosphotransferases on alcohol groups

Alkyl or aryl transferase

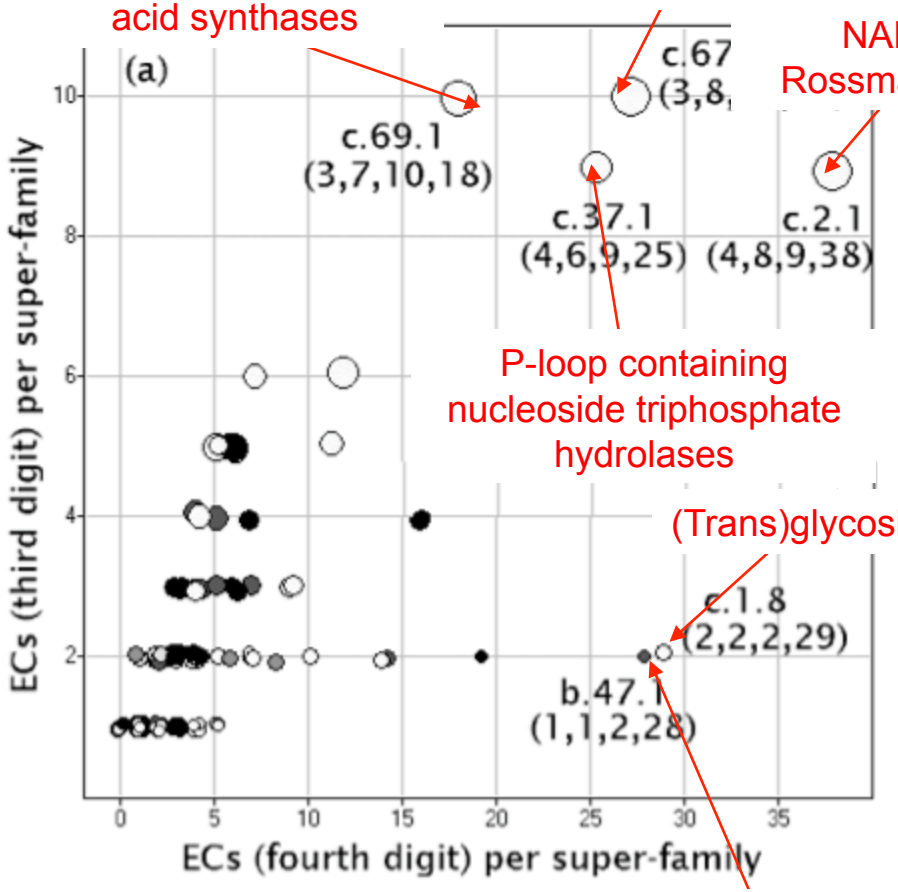
P-loop containing nucleoside triphosphate hydrolases

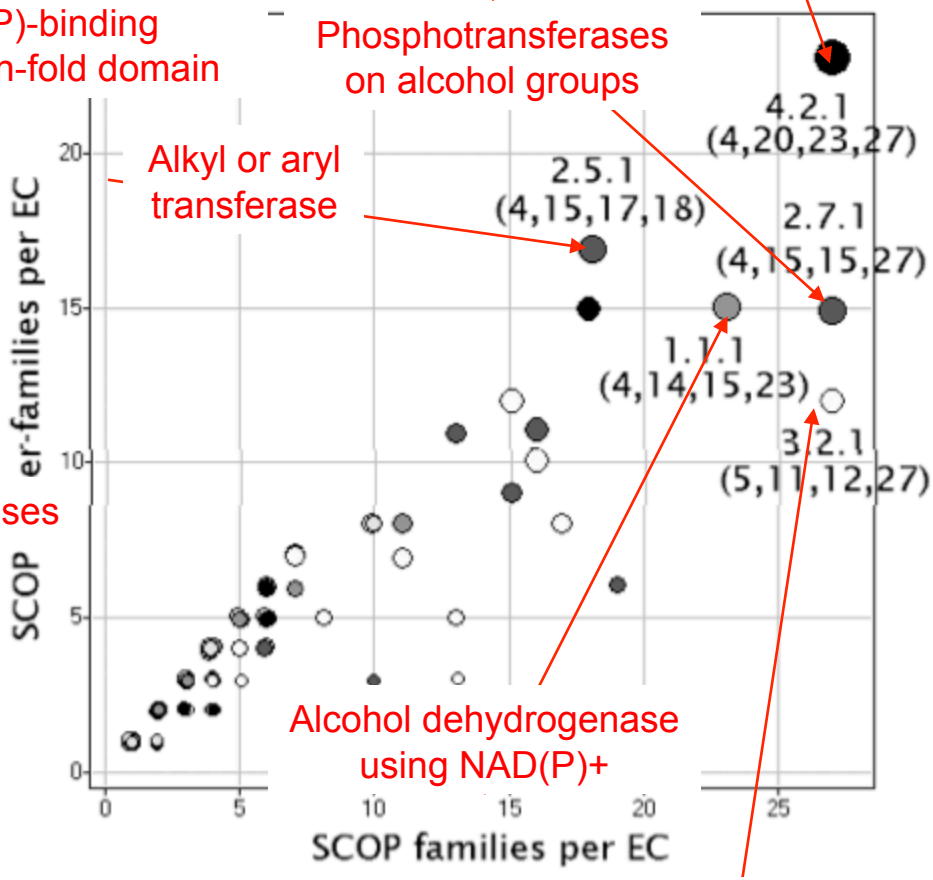
(Trans)glycosidases

Alcohol dehydrogenase using NAD(P)+

Trypsin-like serine proteases

O- or S-glycosidases



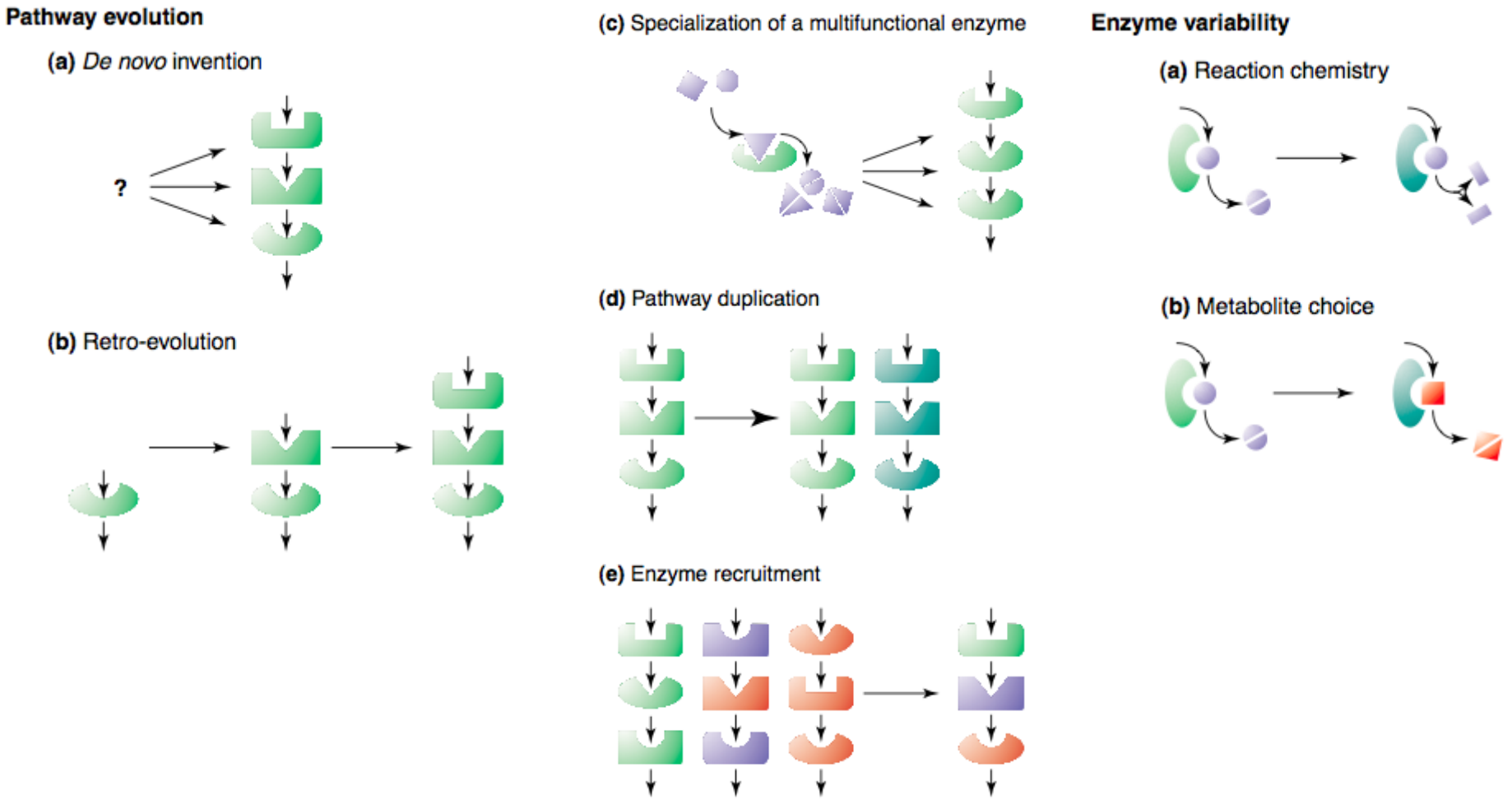


Metabolites: a helping hand for pathway evolution?

…, S Sunyaev, P **Bork**, T **Dandekar** - Trends in biochemical …, 2003 - Elsevier

The evolution of enzymes and pathways is under debate. Recent studies show that recruitment of single enzymes from different pathways could be the driving force for pathway evolution. Other mechanisms of evolution, such as pathway duplication, enzyme ...

Cited by 91 - Related articles - All 12 versions



Evolution of a metabolic pathway for degradation of a toxic xenobiotic: the **patchwork** approach
SD **Copley** - Trends in Biochemical Sciences, 2000 - Elsevier
The pathway for degradation of the xenobiotic pesticide pentachlorophenol in Sphingomonas chlorophenolica probably evolved in the past few decades by the recruitment of enzymes from two other catabolic pathways. The first and third enzymes in ...
Cited by 117 - Related articles - BL Direct - All 10 versions

The **evolution** and structural anatomy of the small molecule **metabolic pathways** in Escherichia coli1
SA Teichmann, SCG Rison, JM **Thornton**... - Journal of Molecular ..., 2001 - Elsevier
The 106 small molecule **metabolic** (SMM) **pathways** in Escherichia coli are formed by the protein products of 581 genes. We can define 722 domains, nearly all of which are homologous to proteins of known structure, that form all or part of 510 of these proteins. ...
Cited by 102 - Related articles - BL Direct - All 24 versions

Small-molecule metabolism: an **enzyme mosaic**
SA Teichmann, SCG Rison, JM **Thornton**... - TRENDS in ..., 2001 - Elsevier
Escherichia coli has been a popular organism for studying metabolic pathways. In an attempt to find out more about how these pathways are constructed, the enzymes were analysed by defining their protein domains. Structural assignments and sequence ...
Cited by 44 - Related articles - All 20 versions

Pathway evolution, structurally speaking
..., JM **Thornton** - Current opinion in structural biology, 2002 - Elsevier
Small-molecule metabolism forms the core of the metabolic processes of all living organisms. As early as 1945, possible mechanisms for the **evolution** of such a complex metabolic system were considered. The problem is to explain the appearance and ...
Cited by 53 - Related articles - All 9 versions

おまけ演習

1. KEGG Mapper を使ってみよう
   - パスウェイマッピングツール
2. KegArray を使ってみよう
   - マイクロアレイ解析にも使えるマッピングツール
3. SIMCOMP を使ってみよう
   - 化合物類似構造検索ツール
4. KegDrawを使ってみよう
   - 化合物描画ツール
5. PathPred を使ってみよう
   - 化合物代謝予測ツール
6. KEGG API を使ってみよう
   - KEGGでプログラミングする

KEGG Mapperを使ってみよう

1. http://www.genome.jp/kegg/mapper.html にアクセス
2. 「Search Pathway」をクリック
3. データを貼付けて「Exec」
   - サンプルデータは http://web.kuicr.kyoto-u.ac.jp/~kot/enshu/ の list*.txt
4. パスウェイの色づけを眺めてみる
   - どんな化合物が多いか考えてみましょう

KEGG Mapper

http://www.genome.jp/kegg/mapper.html

KEGG Mapper: Overview

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

KEGG Mapper

KEGG Mapper is a collection of KEGG mapping tools, both for KEGG pathway mapping and BRITE mapping (ontology enrichment). Two pathway mapping tools, "Search Pathway" and "Color Pathway", were made available from the beginning of the KEGG project. Although the naming of these tools is somewhat misleading since both involve searching and coloring procedures, similar naming was introduced to BRITE mapping as well. With the release of the third BRITE mapping tool, Join Brite, the collection of five tools shown below is now called KEGG Mapper.

Pathway mapping tools

- Search Pathway - basic pathway mapping tool where mapped objects are marked in red
- Color Pathway - modified pathway mapping tool where mapped objects are marked in any color

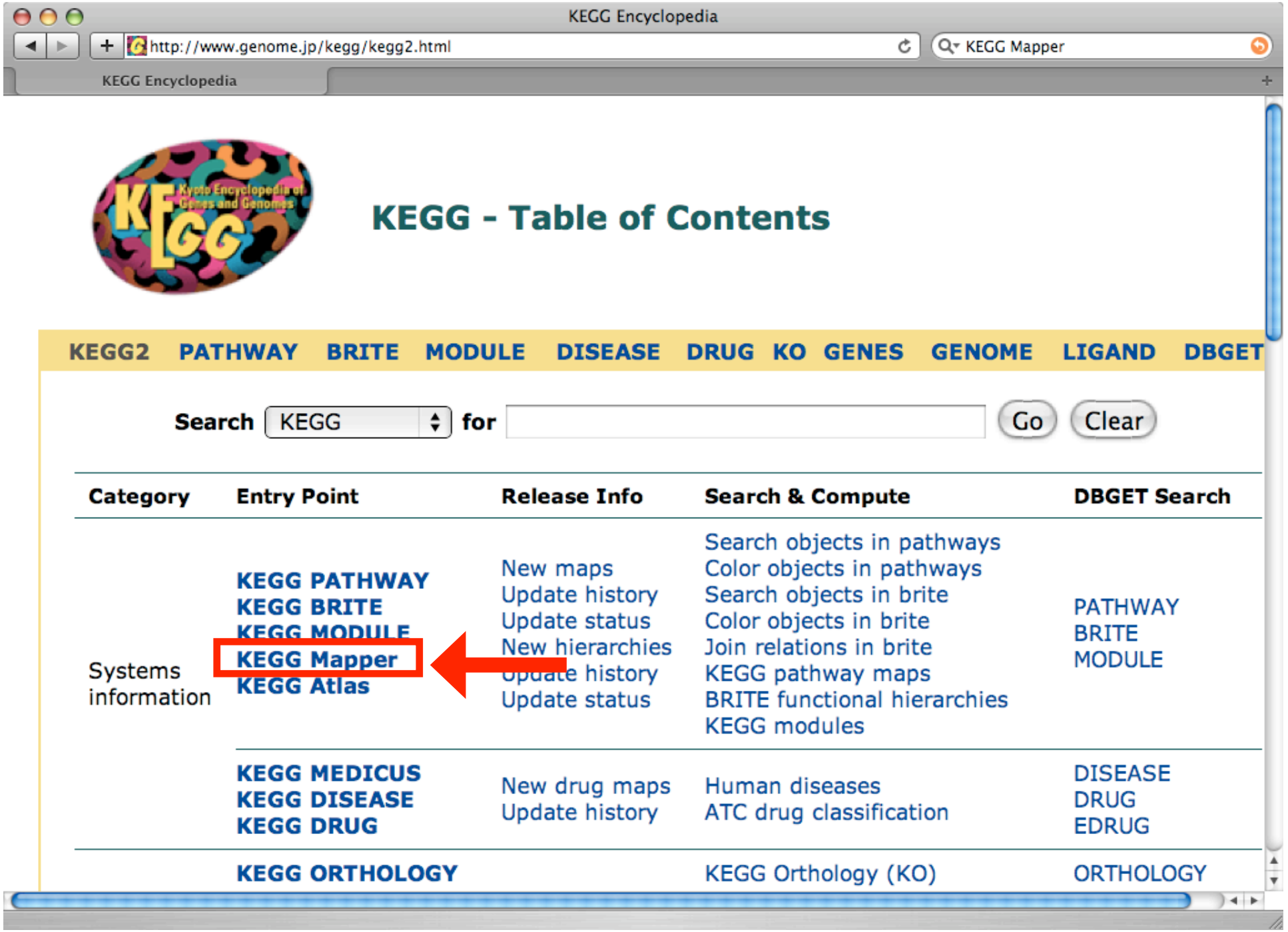
Brite mapping tools

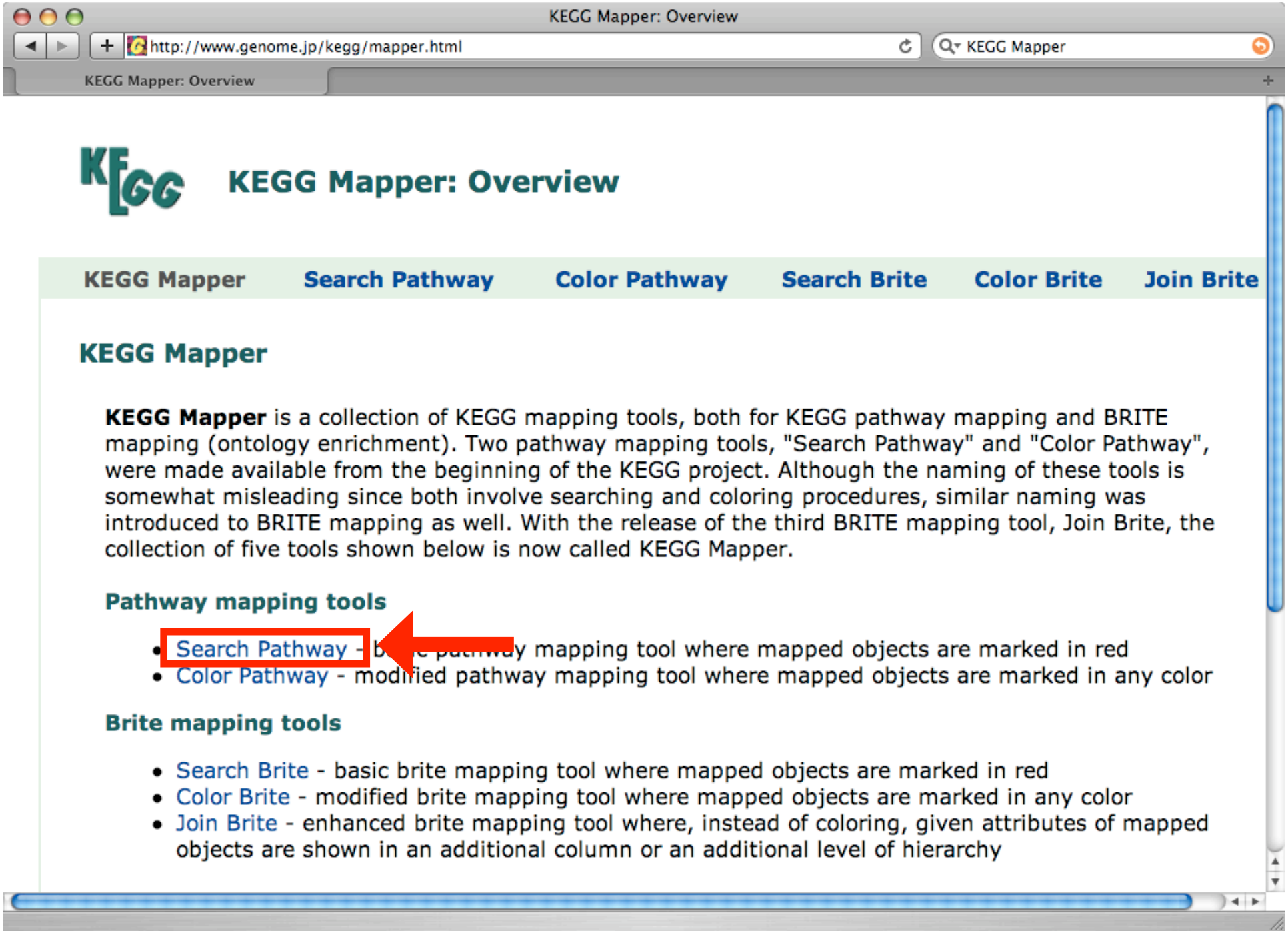
- Search Brite - basic brite mapping tool where mapped objects are marked in red
- Color Brite - modified brite mapping tool where mapped objects are marked in any color
- Join Brite - enhanced brite mapping tool where, instead of coloring, given attributes of mapped objects are shown in an additional column or an additional level of hierarchy

feb27-1.ath.1.txt

C08578
C08650
C15525
C16404
C16405
C16406
C16408
C16417
C01709
C05911
C09099
C09614
C09789
C16419
C16422
C16492
C00389
C00616
C01265
C03897
C04443
C04444

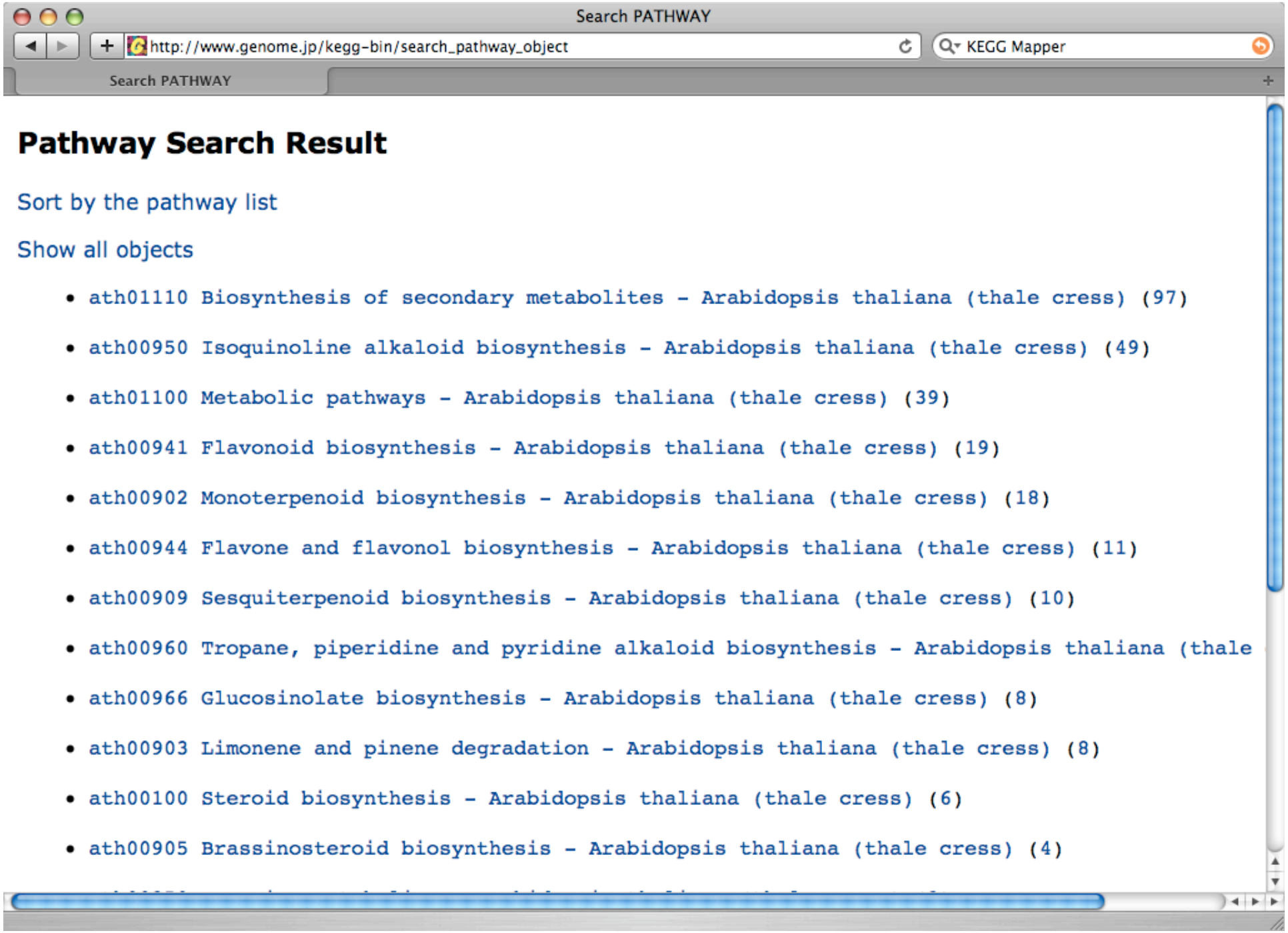
化合物のIDリスト


KEGG Encyclopedia
http://www.genome.jp/kegg/kegg2.html
KEGG Mapper
KEGG Encyclopedia
KEGG - Table of Contents
KEGG2 PATHWAY BRITE MODULE DISEASE DRUG KO GENES GENOME LIGAND DBGET
Search KEGG for Go Clear
Category
Entry Point
Release Info
Search & Compute
DBGET Search
Systems information
KEGG PATHWAY
KEGG BRITE
KEGG MODULE
KEGG Mapper
KEGG Atlas
New maps
Update history
Update status
New hierarchies
Update history
Update status
Search objects in pathways
Color objects in pathways
Search objects in brite
Color objects in brite
Join relations in brite
KEGG pathway maps
BRITE functional hierarchies
KEGG modules
PATHWAY
BRITE
MODULE
KEGG MEDICUS
KEGG DISEASE
KEGG DRUG
New drug maps
Update history
Human diseases
ATC drug classification
DISEASE
DRUG
EDRUG
KEGG ORTHOLOGY
KEGG Orthology (KO)
ORTHOLOGY


KEGG Mapper: Overview
http://www.genome.jp/kegg/mapper.html
KEGG Mapper
KEGG Mapper: Overview
KEGG Mapper: Overview
KEGG Mapper
Search Pathway
Color Pathway
Search Brite
Color Brite
Join Brite
KEGG Mapper
KEGG Mapper is a collection of KEGG mapping tools, both for KEGG pathway mapping and BRITE mapping (ontology enrichment). Two pathway mapping tools, "Search Pathway" and "Color Pathway", were made available from the beginning of the KEGG project. Although the naming of these tools is somewhat misleading since both involve searching and coloring procedures, similar naming was introduced to BRITE mapping as well. With the release of the third BRITE mapping tool, Join Brite, the collection of five tools shown below is now called KEGG Mapper.
Pathway mapping tools
Search Pathway - b e pathway mapping tool where mapped objects are marked in red
Color Pathway - modified pathway mapping tool where mapped objects are marked in any color
Brite mapping tools
Search Brite - basic brite mapping tool where mapped objects are marked in red
Color Brite - modified brite mapping tool where mapped objects are marked in any color
Join Brite - enhanced brite mapping tool where, instead of coloring, given attributes of mapped objects are shown in an additional column or an additional level of hierarchy


KEGG Mapper: Search Objects in KEGG Pathways
http://www.genome.jp/kegg/tool/search_pathway.html
KEGG Mapper
KEGG Mapper: Search Objects in ...
KEGG Mapper: Search Objects in KEGG Pathways
KEGG Mapper
Search Pathway
Color Pathway
Search Brite
Color Brite
Join Brite
Search against:
Reference pathway (KO)
Enter objects:
Examples:
(Reference pathway (KO))
ko:K01803 cpd:C00111 cpd:C00118
K00134 C00236
(Homo sapiens pathway)
hsa:7167 hsa:GPI cpd:C00118
ALDOA 1.2.1.12 C00236
Alternatively, enter the file name containing the data:
ファイルを選択
ファイルが選...ていません


KEGG Mapper: Search Objects in KEGG Pathways
http://www.genome.jp/kegg/tool/search_pathway.html
KEGG Mapper
KEGG Mapper: Search Objects in ...
KEGG Mapper: Search Objects in KEGG Pathways
KEGG Mapper
Search Pathway
Color Pathway
Search Brite
Color Brite
Join Brite
Search against:
Arabidopsis thaliana (thale cress)
Enter objects:
Examples:
(Reference pathway (KO))
ko:K01803 cpd:C00111 cpd:C00118
K00134 C00236
(Homo sapiens pathway)
hsa:7167 hsa:GPI cpd:C00118
ALDOA 1.2.1.12 C00236
Alternatively, enter the file name containing the data:
ファイルを選択
feb27-1.ath.1.txt

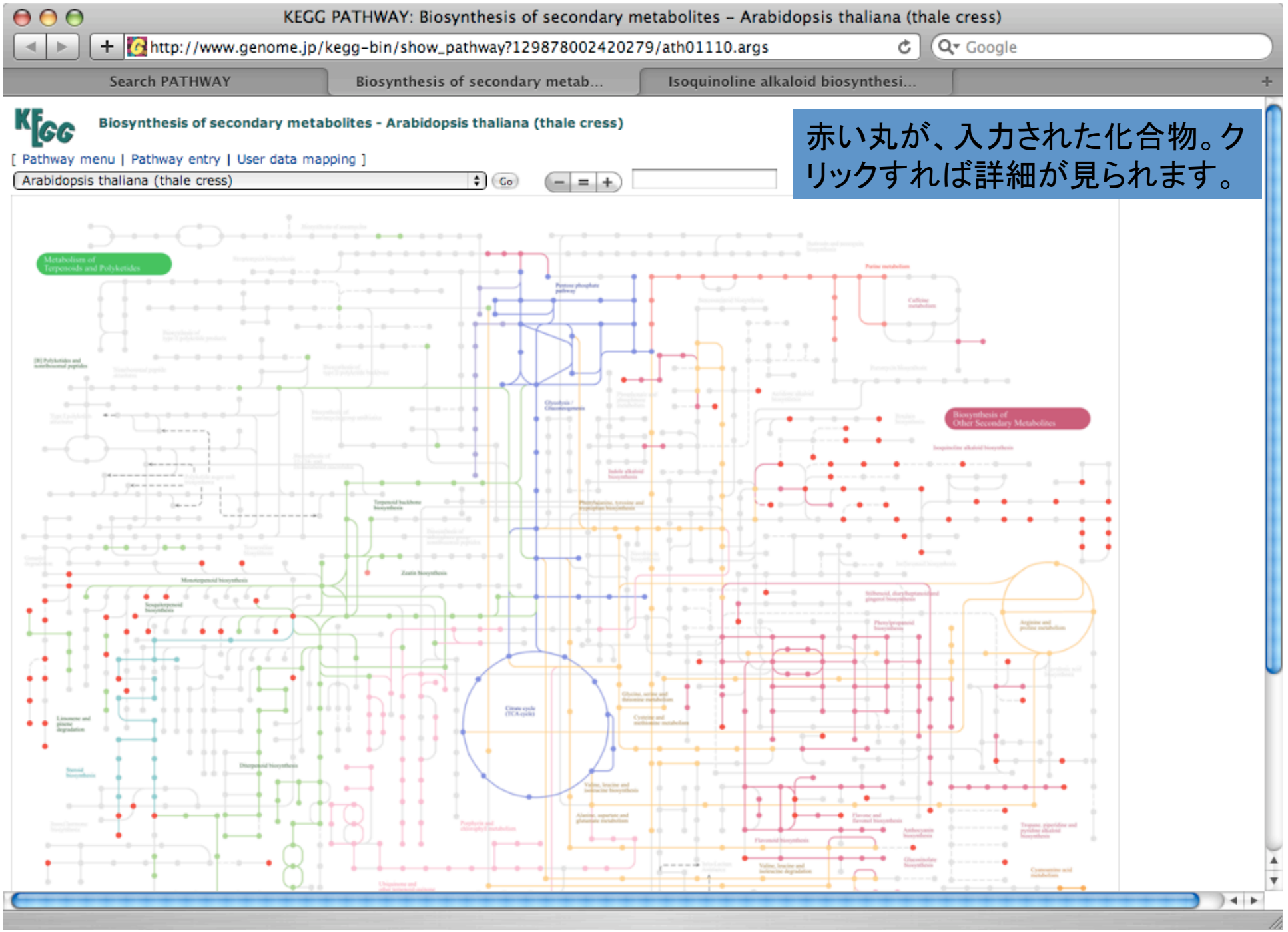


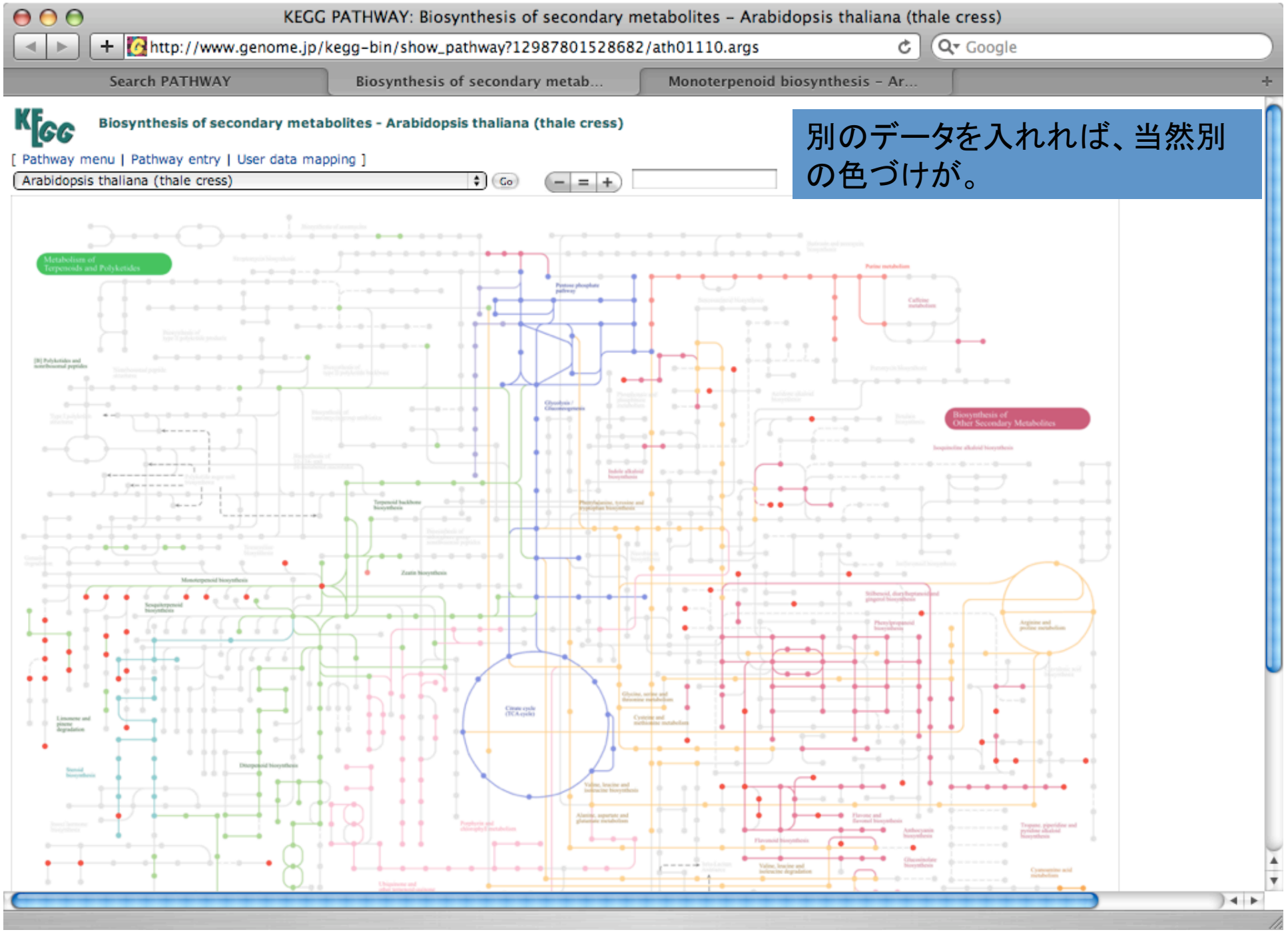
Pathway Search Result

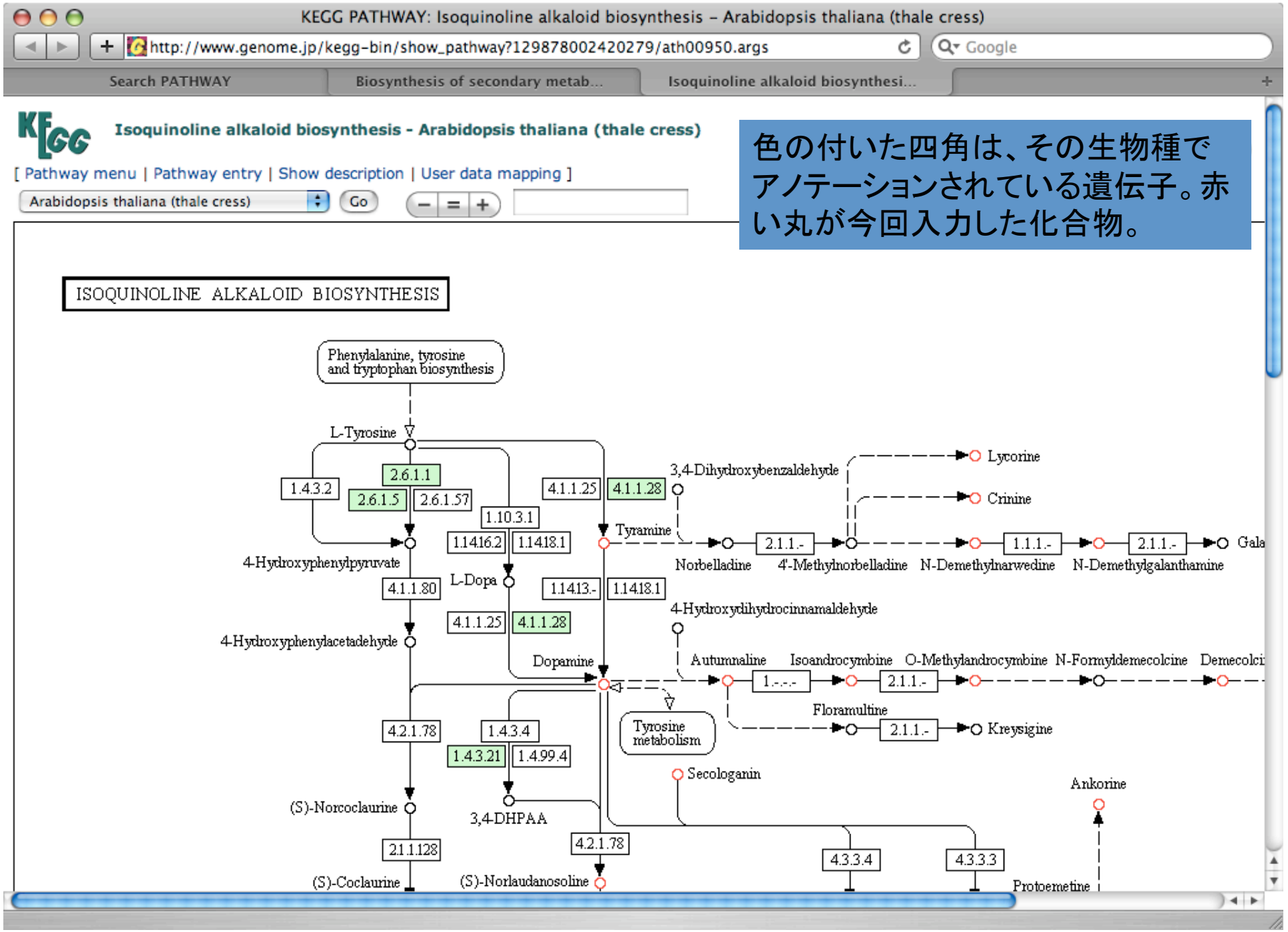
Sort by the pathway list

Show all objects

- ath01110 Biosynthesis of secondary metabolites - Arabidopsis thaliana (thale cress) (97)
- ath00950 Isoquinoline alkaloid biosynthesis - Arabidopsis thaliana (thale cress) (49)
- ath01100 Metabolic pathways - Arabidopsis thaliana (thale cress) (39)
- ath00941 Flavonoid biosynthesis - Arabidopsis thaliana (thale cress) (19)
- ath00902 Monoterpenoid biosynthesis - Arabidopsis thaliana (thale cress) (18)
- ath00944 Flavone and flavonol biosynthesis - Arabidopsis thaliana (thale cress) (11)
- ath00909 Sesquiterpenoid biosynthesis - Arabidopsis thaliana (thale cress) (10)
- ath00960 Tropane, piperidine and pyridine alkaloid biosynthesis - Arabidopsis thaliana (thale
- ath00966 Glucosinolate biosynthesis - Arabidopsis thaliana (thale cress) (8)
- ath00903 Limonene and pinene degradation - Arabidopsis thaliana (thale cress) (8)
- ath00100 Steroid biosynthesis - Arabidopsis thaliana (thale cress) (6)
- ath00905 Brassinosteroid biosynthesis - Arabidopsis thaliana (thale cress) (4)

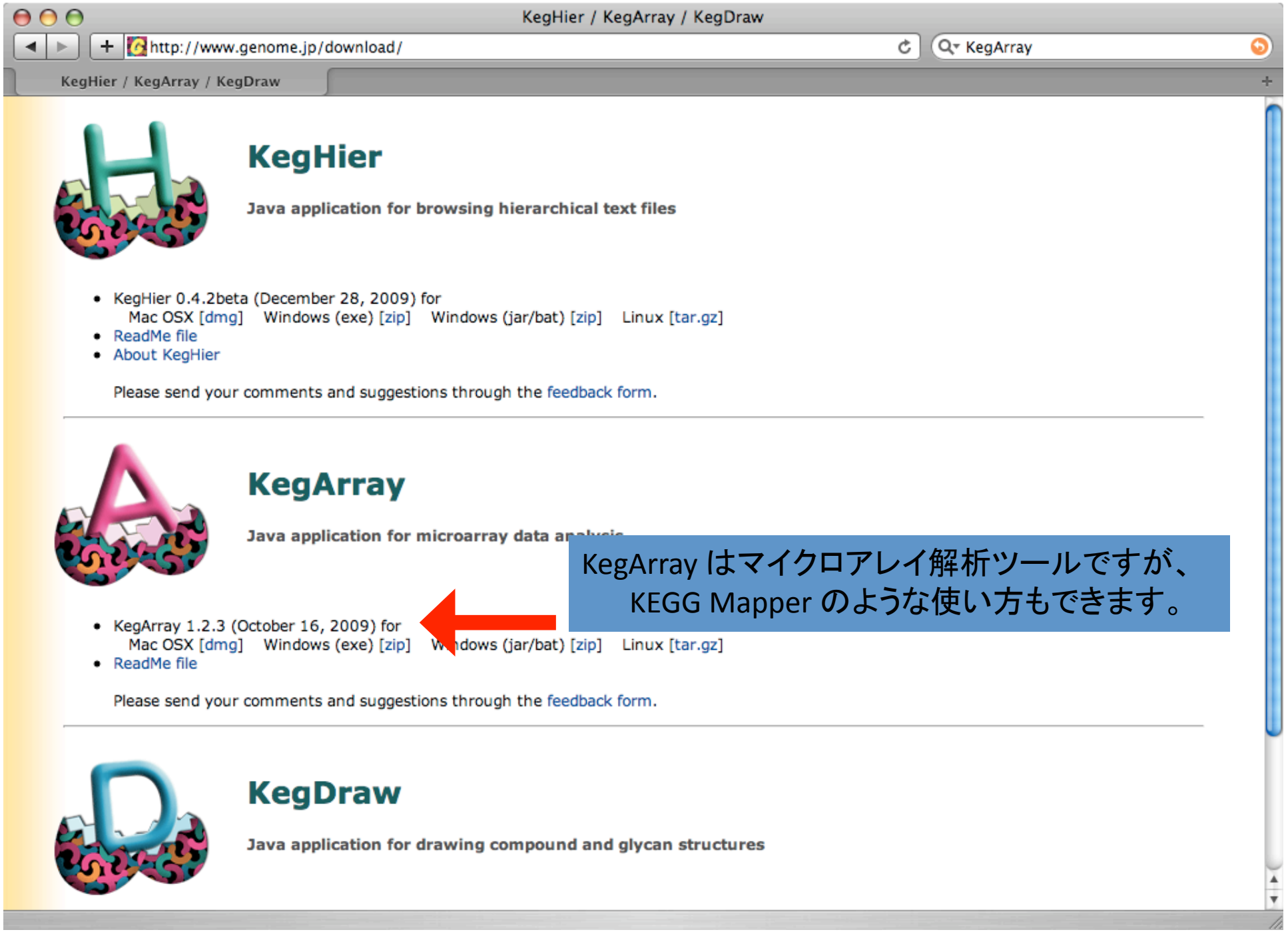

KEGG PATHWAY: Biosynthesis of secondary metabolites – Arabidopsis thaliana (thale cress)
http://www.genome.jp/kegg-bin/show_pathway?129878002420279/ath01110.args
Google
Search PATHWAY
Biosynthesis of secondary metab...
Isoquinoline alkaloid biosynthesi...
KEGG
Biosynthesis of secondary metabolites - Arabidopsis thaliana (thale cress)
[Pathway menu | Pathway entry | User data mapping]
Arabidopsis thaliana (thale cress)
Go
赤い丸が、入力された化合物。クリックすれば詳細が見られます。

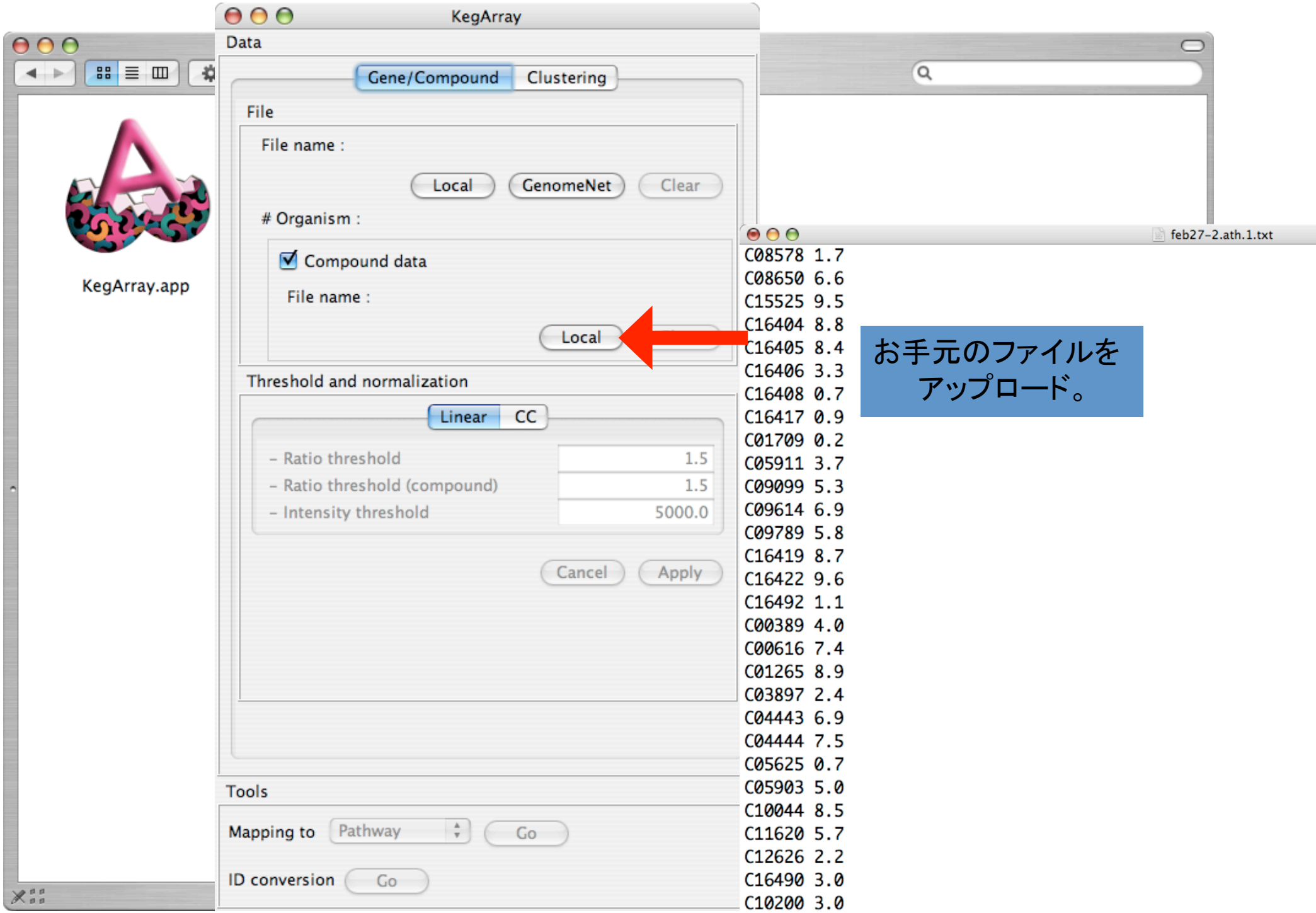

KEGG PATHWAY: Biosynthesis of secondary metabolites – Arabidopsis thaliana (thale cress)
http://www.genome.jp/kegg-bin/show_pathway?12987801528682/ath01110.args
Google
Search PATHWAY
Biosynthesis of secondary metab...
Monoterpenoid biosynthesis – Ar...
Biosynthesis of secondary metabolites - Arabidopsis thaliana (thale cress)
[Pathway menu | Pathway entry | User data mapping]
Arabidopsis thaliana (thale cress)
Go
別のデータを入れれば、当然別の色づけが。

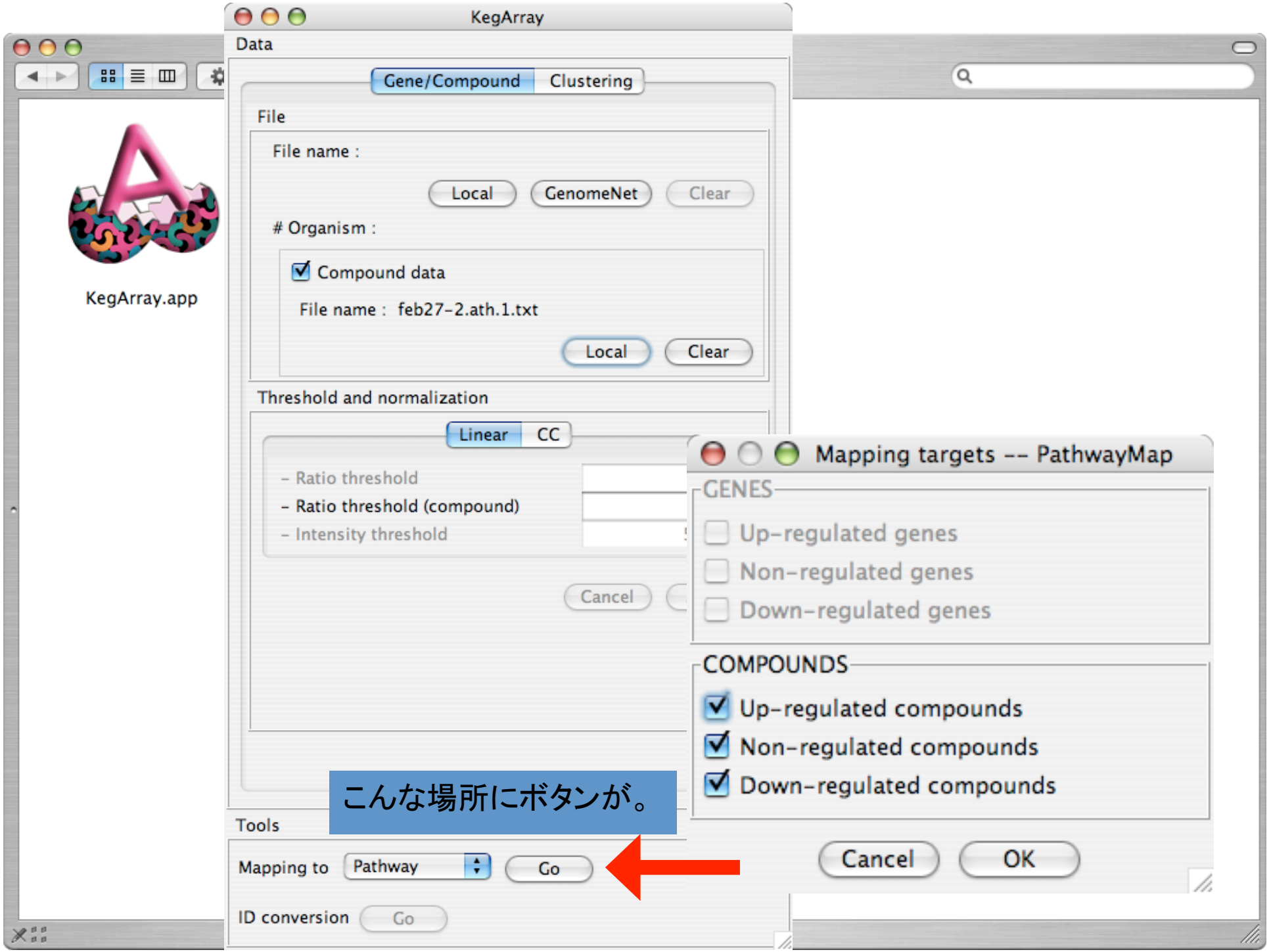

KEGG PATHWAY: Isoquinoline alkaloid biosynthesis – Arabidopsis thaliana (thale cress)
http://www.genome.jp/kegg-bin/show_pathway?129878002420279/ath00950.args
Search PATHWAY
Biosynthesis of secondary metab...
Isoquinoline alkaloid biosynthesi...
Isoquinoline alkaloid biosynthesis - Arabidopsis thaliana (thale cress)
[Pathway menu | Pathway entry | Show description | User data mapping]
Arabidopsis thaliana (thale cress)
Go
色の付いた四角は、その生物種でアノテーションされている遺伝子。赤い丸が今回入力した化合物。
ISOQUINOLINE ALKALOID BIOSYNTHESIS
Phenylalanine, tyrosine and tryptophan biosynthesis
L-Tyrosine
1.4.3.2
2.6.1.1
2.6.1.5
2.6.1.57
1.10.3.1
1.14.16.2
1.14.18.1
4-Hydroxyphenylpyruvate
4.1.1.80
4-Hydroxyphenylacetadehyde
L-Dopa
1.14.13.-
1.14.18.1
4.1.1.25
4.1.1.28
Dopamine
4.2.1.78
1.4.3.4
1.4.3.21
1.4.99.4
(S)-Norcoclaurine
3,4-DHPAA
2.1.1.128
(S)-Coclaurine
4.2.1.78
(S)-Norlaudanosoline
3,4-Dihydroxybenzaldehyde
4.1.1.25
4.1.1.28
Tyramine
2.1.1.-
Norbelladine
4'-Methylnorbelladine
Lycorine
Crinine
1.1.1.-
N-Demethylnarwedine
2.1.1.-
N-Demethylgalanthamine
Gala
4-Hydroxydihydrocinnamaldehyde
Autumnaline
1.-.-.-
Isoandrocymbine
2.1.1.-
O-Methylandrocymbine
N-Formyldemecolcine
Demecolci
Floramultine
2.1.1.-
Kreysigine
Tyrosine metabolism
Secologanin
Ankorine
4.3.3.4
4.3.3.3
Protoemetine

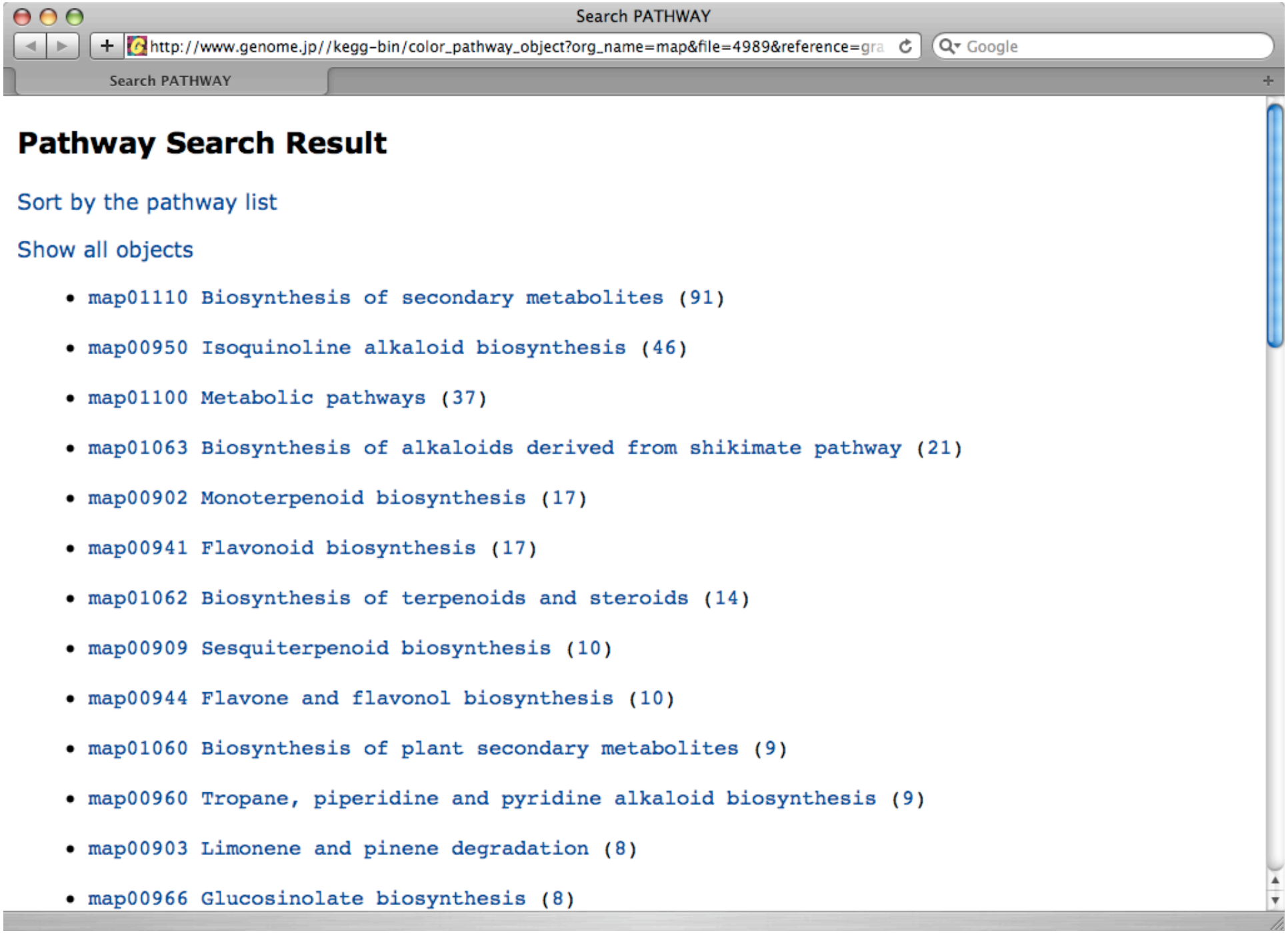
KegArray を使ってみよう

1. http://www.genome.jp/download/ にアクセス
2. KegArray 1.2.3 の Mac OSX [dmg] をクリックしてダウンロード
3. データをロード
   - サンプルデータは http://web.kuicr.kyoto-u.ac.jp/~kot/enshu/ の list_with_values*.txt
4. パスウェイにマッピング
   - どんなパスウェイが活性化されているか考えてみましょう


KegHier / KegArray / KegDraw
http://www.genome.jp/download/
KegArray
KegHier / KegArray / KegDraw
KegHier
Java application for browsing hierarchical text files
KegHier 0.4.2beta (December 28, 2009) for
Mac OSX [dmg] Windows (exe) [zip] Windows (jar/bat) [zip] Linux [tar.gz]
ReadMe file
About KegHier
Please send your comments and suggestions through the feedback form.
KegArray
Java application for microarray data analysis
KegArray はマイクロアレイ解析ツールですが、
KEGG Mapper のような使い方もできます。
KegArray 1.2.3 (October 16, 2009) for
Mac OSX [dmg] Windows (exe) [zip] Windows (jar/bat) [zip] Linux [tar.gz]
ReadMe file
Please send your comments and suggestions through the feedback form.
KegDraw
Java application for drawing compound and glycan structures


KegArray
Data
Gene/Compound
Clustering
File
File name :
Local
GenomeNet
Clear
Organism :
Compound data
File name :
Local
Threshold and normalization
Linear
CC
- Ratio threshold
1.5
- Ratio threshold (compound)
1.5
- Intensity threshold
5000.0
Cancel
Apply
Tools
Mapping to
Pathway
Go
ID conversion
Go
KegArray.app
feb27-2.ath.1.txt
C08578 1.7
C08650 6.6
C15525 9.5
C16404 8.8
C16405 8.4
C16406 3.3
C16408 0.7
C16417 0.9
C01709 0.2
C05911 3.7
C09099 5.3
C09614 6.9
C09789 5.8
C16419 8.7
C16422 9.6
C16492 1.1
C00389 4.0
C00616 7.4
C01265 8.9
C03897 2.4
C04443 6.9
C04444 7.5
C05625 0.7
C05903 5.0
C10044 8.5
C11620 5.7
C12626 2.2
C16490 3.0
C10200 3.0
お手元のファイルを
アップロード。


KegArray.app
KegArray
Data
Gene/Compound
Clustering
File
File name :
Local
GenomeNet
Clear
Organism :
Compound data
File name : feb27-2.ath.1.txt
Local
Clear
Threshold and normalization
Linear
CC
- Ratio threshold
- Ratio threshold (compound)
- Intensity threshold
Cancel
Tools
Mapping to
Pathway
Go
ID conversion
Go
こんな場所にボタンが。
Mapping targets -- PathwayMap
GENES
Up-regulated genes
Non-regulated genes
Down-regulated genes
COMPOUNDS
Up-regulated compounds
Non-regulated compounds
Down-regulated compounds
Cancel
OK

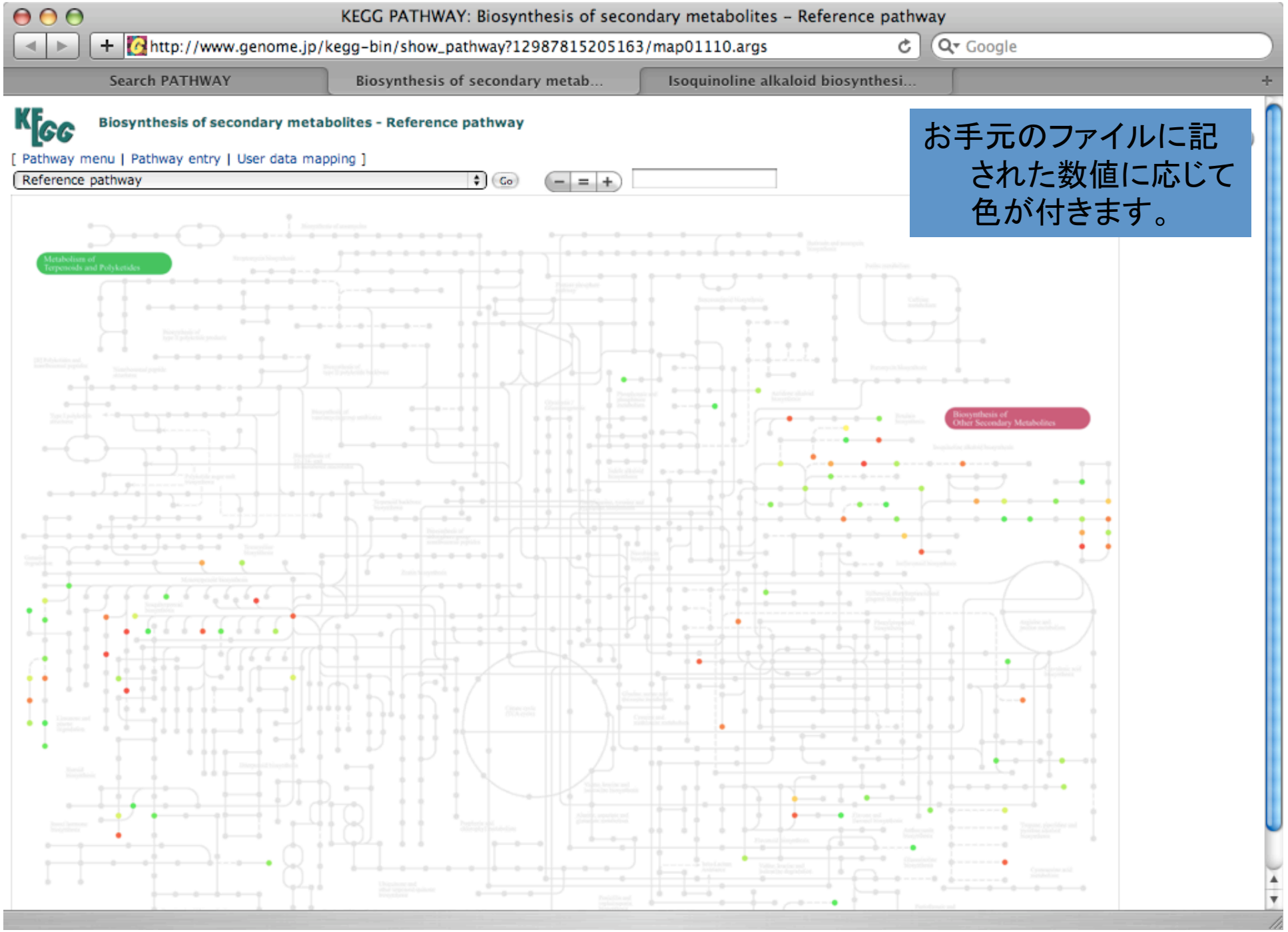


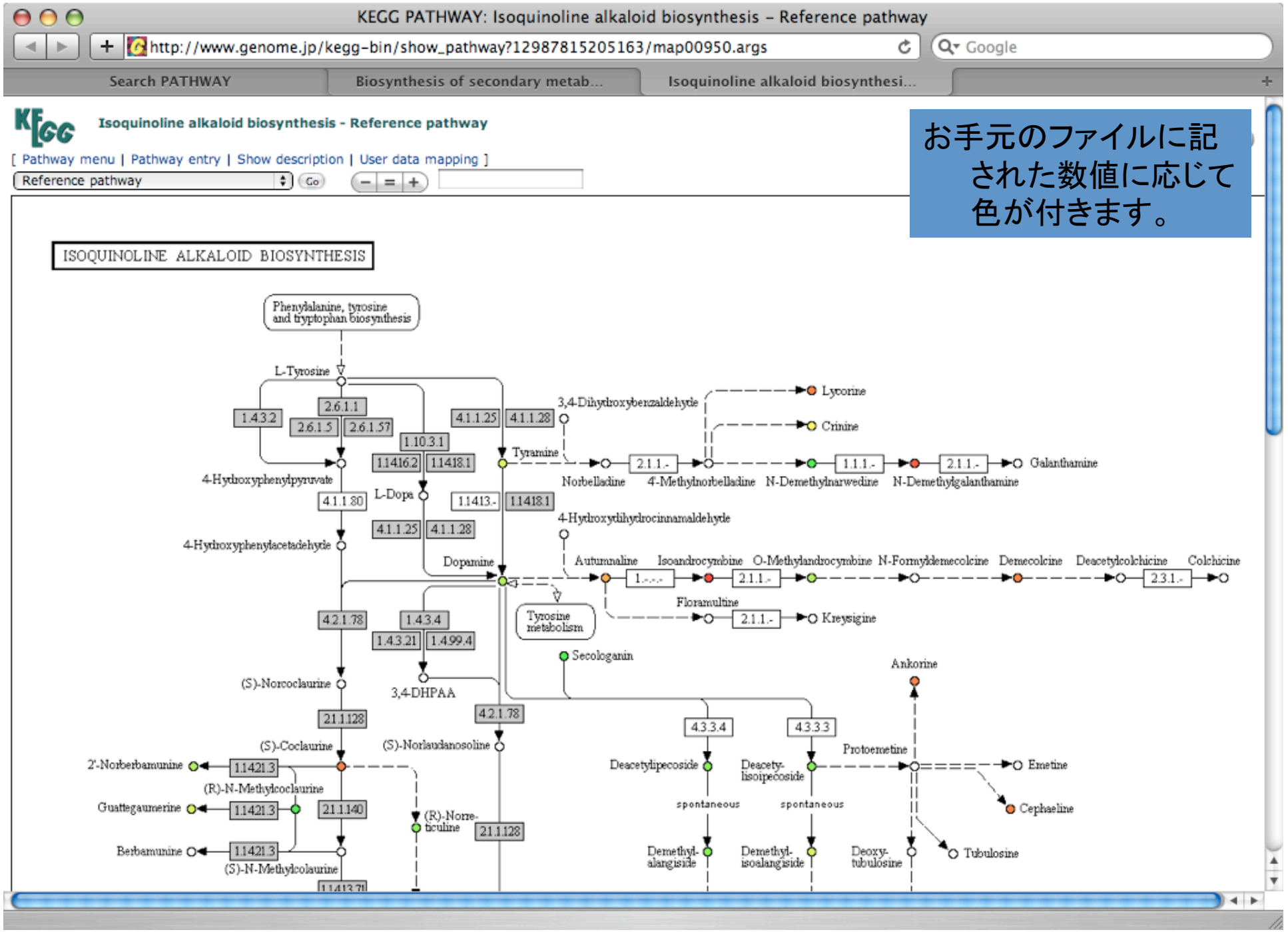
Pathway Search Result

Sort by the pathway list

Show all objects

- map01110 Biosynthesis of secondary metabolites (91)
- map00950 Isoquinoline alkaloid biosynthesis (46)
- map01100 Metabolic pathways (37)
- map01063 Biosynthesis of alkaloids derived from shikimate pathway (21)
- map00902 Monoterpenoid biosynthesis (17)
- map00941 Flavonoid biosynthesis (17)
- map01062 Biosynthesis of terpenoids and steroids (14)
- map00909 Sesquiterpenoid biosynthesis (10)
- map00944 Flavone and flavonol biosynthesis (10)
- map01060 Biosynthesis of plant secondary metabolites (9)
- map00960 Tropane, piperidine and pyridine alkaloid biosynthesis (9)
- map00903 Limonene and pinene degradation (8)
- map00966 Glucosinolate biosynthesis (8)


KEGG PATHWAY: Biosynthesis of secondary metabolites – Reference pathway
http://www.genome.jp/kegg-bin/show_pathway?12987815205163/map01110.args
Google
Search PATHWAY
Biosynthesis of secondary metab...
Isoquinoline alkaloid biosynthesi...
KEGG
Biosynthesis of secondary metabolites - Reference pathway
[Pathway menu | Pathway entry | User data mapping]
Reference pathway
Go
お手元のファイルに記
された数値に応じて
色が付きます。
Metabolism of
Terpenoids and Polyketides
Biosynthesis of
Other Secondary Metabolites


KEGG PATHWAY: Isoquinoline alkaloid biosynthesis - Reference pathway
http://www.genome.jp/kegg-bin/show_pathway?12987815205163/map00950.args
Search PATHWAY
Biosynthesis of secondary metab...
Isoquinoline alkaloid biosynthesi...
Isoquinoline alkaloid biosynthesis - Reference pathway
[Pathway menu | Pathway entry | Show description | User data mapping]
Reference pathway
Go
お手元のファイルに記
された数値に応じて
色が付きます。
ISOQUINOLINE ALKALOID BIOSYNTHESIS
Phenylalanine, tyrosine and tryptophan biosynthesis
L-Tyrosine
Tyramine
3,4-Dihydroxybenzaldehyde
Lycorine
Crinine
Norbelladine
4'-Methylnorbelladine
N-Demethylnarwedine
N-Demethylgalanthamine
Galanthamine
4-Hydroxyphenylpyruvate
L-Dopa
4-Hydroxyphenylacetadehyde
Dopamine
4-Hydroxydihydrocinnamaldehyde
Autumnaline
Isoandrocymbine
O-Methylandrocymbine
N-Formyldemecolcine
Demecolcine
Deacetylcolchicine
Colchicine
Floramultine
Kreysigine
Tyrosine metabolism
Secologanin
Ankorine
(S)-Norcoclaurine
3,4-DHPAA
(S)-Coclaurine
(S)-Norlaudanosoline
2'-Norberbamunine
(R)-N-Methylcoclaurine
Guattegaumerine
Berbamunine
(S)-N-Methylcolaurine
(R)-Norre-ticuline
Deacetylipecoside
Deacety-lisoipecoside
spontaneous
Demethyl-alangiside
Demethyl-isoalangiside
Protoemetine
Emetine
Cephaeline
Deoxy-tubulosine
Tubulosine

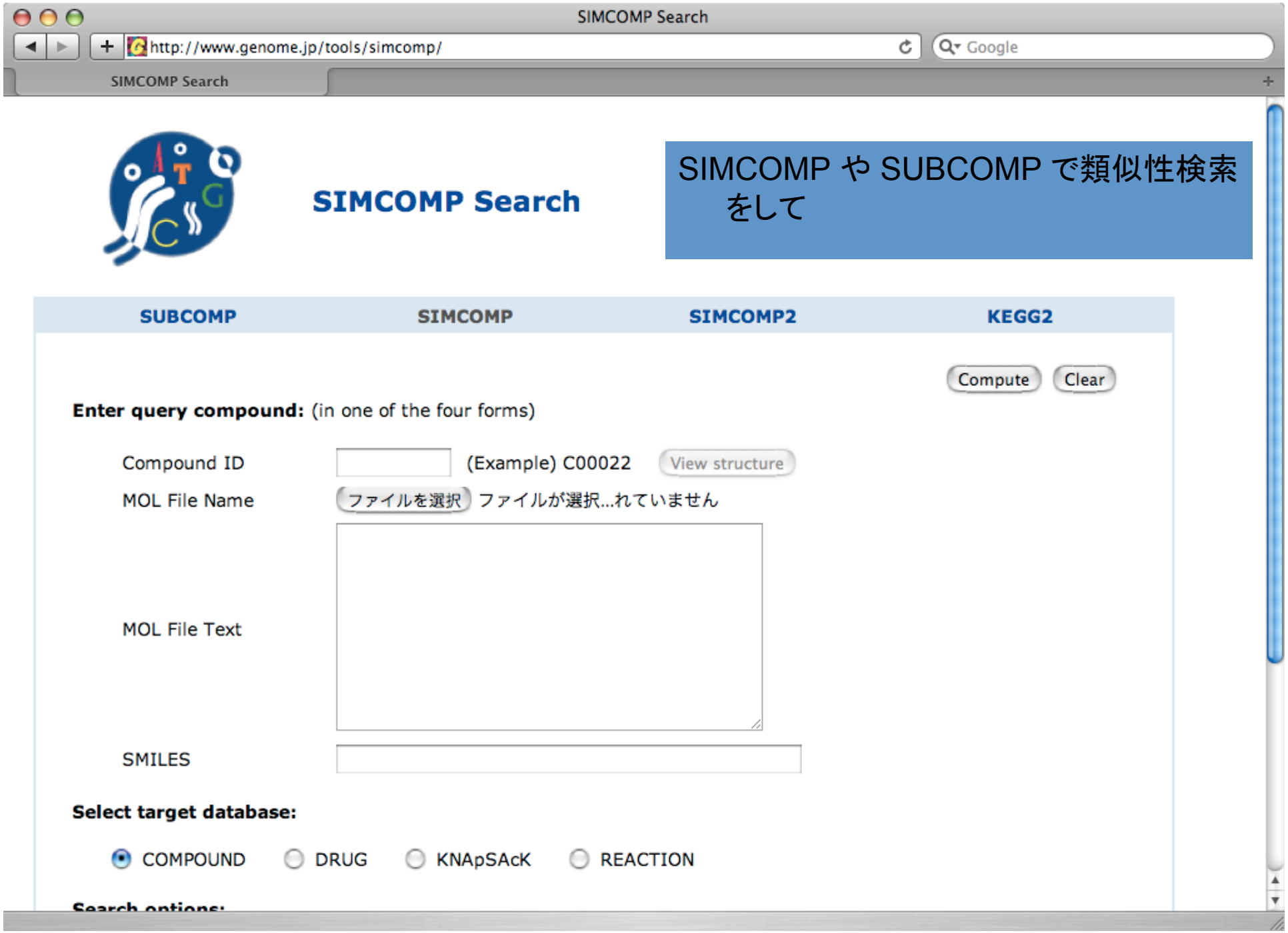
SIMCOMP を使ってみよう

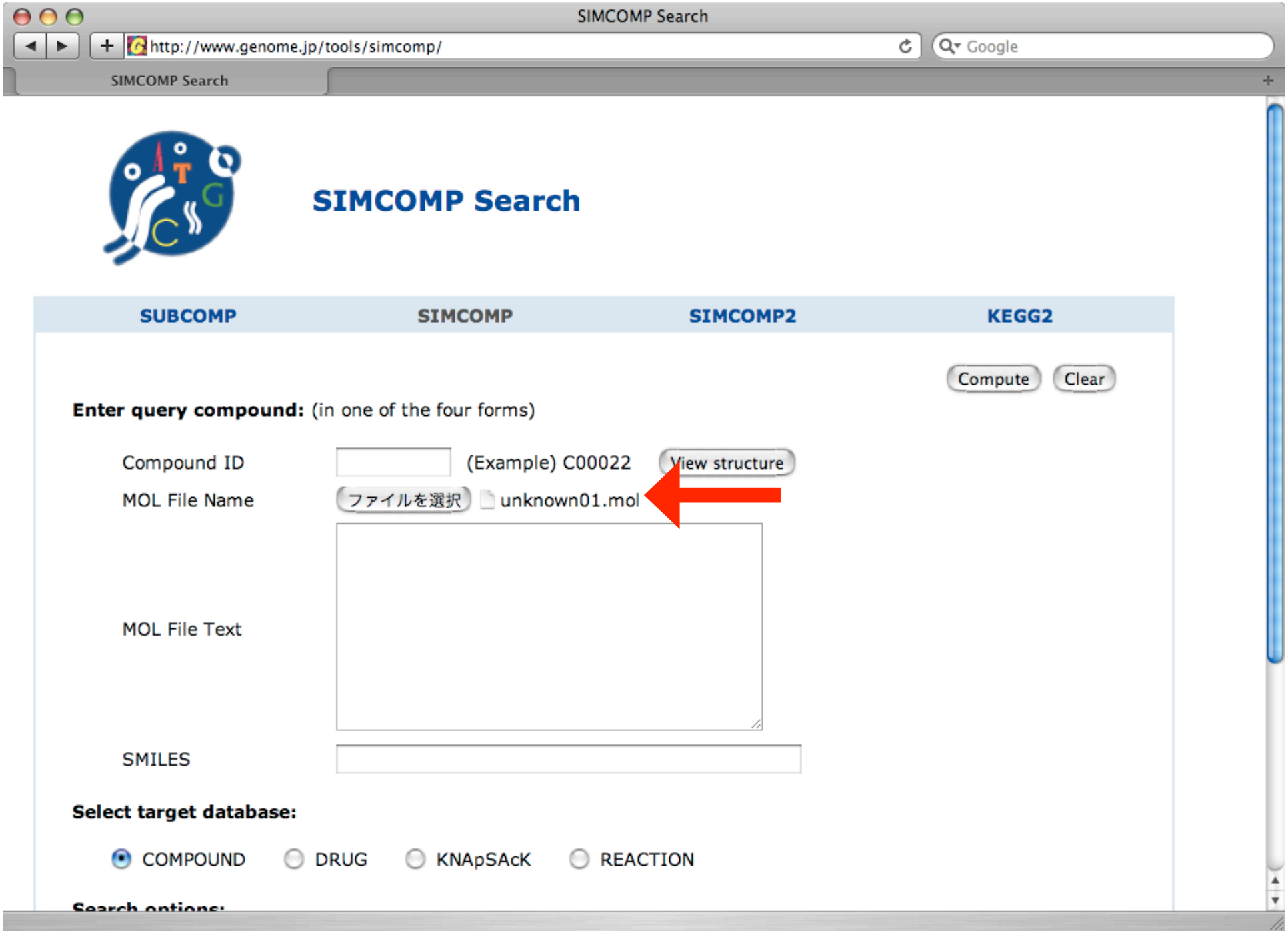
1. http://www.genome.jp/tools/simcomp/ にアクセス
2. データを貼付けて「View Structure」をクリック
   - サンプルデータは http://web.kuicr.kyoto-u.ac.jp/~kot/enshu/ のenshu*.mol
3. さらに「Compute」をクリック
4. 結果が出たら、「Map to Pathway」または「Map to BRITE」を選択して「Exec」
   - 入力した化合物がどの分類に属するのか、どのパスウェイで合成されそうか、考えてみましょう。

unknown01.mol

```
34 37  0  0  0  0  0  0  0  0999 V2000
  25.1677  -15.1324    0.0000 C   0  0  3  0  0  0  0  0  0  0  0  0
  26.3800  -15.8434    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  25.1736  -13.7280    0.0000 C   0  0  3  0  0  0  0  0  0  0  0  0
  23.9497  -15.8317    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  27.5863  -15.1383    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  26.3624  -17.2420    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  23.9614  -13.0286    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  26.3800  -13.0229    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  22.7377  -15.1207    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  28.7984  -15.8493    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  27.5746  -17.9413    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  22.7434  -13.7221    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  27.5921  -13.7221    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  21.5313  -15.8259    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  28.7926  -17.2537    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  30.0164  -15.1499    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  21.5313  -13.0229    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  20.3250  -15.1207    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  30.0047  -17.9530    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  20.3250  -13.7221    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  19.1070  -15.8259    0.0000 C   0  0  3  0  0  0  0  0  0  0  0  0
  17.8949  -15.1207    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  19.1129  -17.2246    0.0000 C   0  0  3  0  0  0  0  0  0  0  0  0
  16.6827  -15.8317    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  17.9007  -17.9238    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  20.3250  -17.9180    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  16.6827  -17.2246    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  15.4706  -15.1266    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  17.9007  -19.3224    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  15.4764  -17.9180    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  14.2643  -15.8317    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  14.2643  -17.2246    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  15.4764  -19.3224    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  13.0463  -15.1266    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
1  2  1  0     0  0
1  3  1  0     0  0
1  4  1  0     0  0
```

mol ファイルか SDF ファイルさえ手に入れば、、、


SIMCOMP Search
http://www.genome.jp/tools/simcomp/
Google
SIMCOMP Search
SIMCOMP Search
SIMCOMP や SUBCOMP で類似性検索をして
SUBCOMP
SIMCOMP
SIMCOMP2
KEGG2
Compute
Clear
Enter query compound: (in one of the four forms)
Compound ID
(Example) C00022
View structure
MOL File Name
ファイルを選択
ファイルが選択...れていません
MOL File Text
SMILES
Select target database:
COMPOUND
DRUG
KNApSAcK
REACTION


SIMCOMP Search
http://www.genome.jp/tools/simcomp/
Google
SIMCOMP Search
SIMCOMP Search
SUBCOMP
SIMCOMP
SIMCOMP2
KEGG2
Compute
Clear
Enter query compound: (in one of the four forms)
Compound ID
(Example) C00022
View structure
MOL File Name
ファイルを選択
unknown01.mol
MOL File Text
SMILES
Select target database:
COMPOUND
DRUG
KNApSAcK
REACTION
Search options:

SIMCOMP Search

http://www.genome.jp/tools-bin/strsearch_view_compound?pid=32495

Google

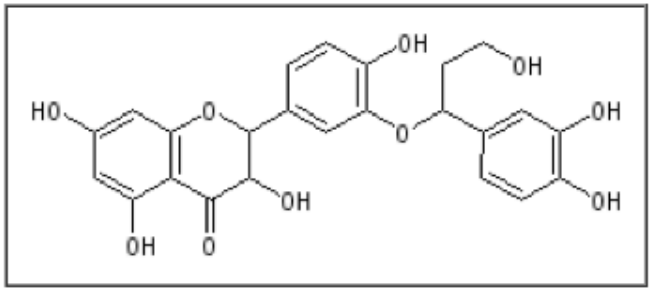
SIMCOMP Search

SIMCOMP Search

SUBCOMP | SIMCOMP | SIMCOMP2 | KEGG2

Compute Return

Structure



Database ◉ COMPOUND ○ DRUG ○ KNApSAcK ○ REACTION

Options ◉ Global search ○ Local search ○ Customized search

▶ Option details

Feedback KEGG GenomeNet Kyoto University Bioinformatics Center

SIMCOMP Search

http://www.genome.jp/tools-bin/search_list?DATABASE=compound&TARGET=STR&PID=32499&SH

Google

SIMCOMP Search

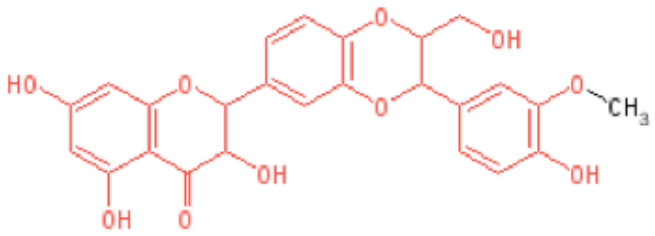
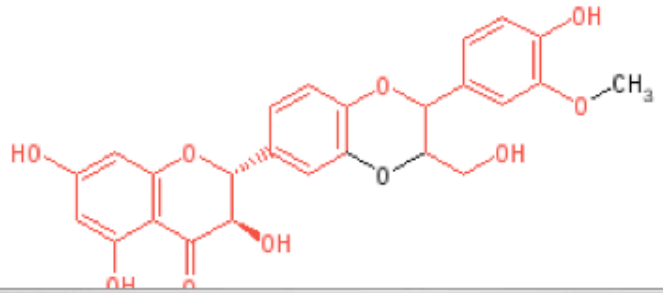
SIMCOMP Search Result

Database : KEGG COMPOUND

Number of entries in a page 20 Hide structure

Page : 1 Go of 29 Items : 1 - 20 of 567 Top Previous Next Bottom

Top 10 Clear Select operation Exec

No	Entry	Structure	Name
1	C07610	 Similarity-Score : 0.92	Silymarin Silibinin Silybin
2	C16808		Isosilybin

SIMCOMP Search

http://www.genome.jp/tools-bin/search_list?DATABASE=compound&TARGET=STR&PID=32499&SH

Google

SIMCOMP Search

SIMCOMP Search Result

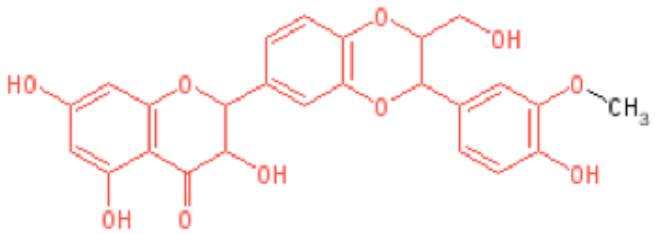
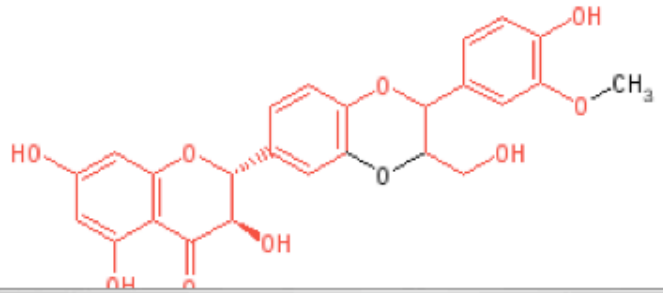
引っかかって来た化合物をマッピングできます。

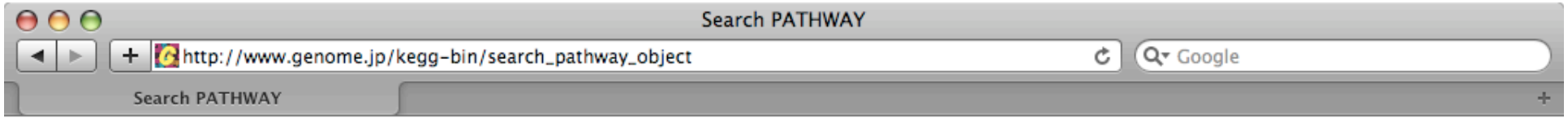
Database : KEGG COMPOUND

Number of entries in a page 20 Hide structure

Page : 1 Go of 29 Items : 1 - 20 of 567 Top Previous Next Bottom

Top 50 Clear Map to Pathway Exec

No	Entry	Structure	Name
1	C07610	 Similarity-Score : 0.92	Silymarin Silibinin Silybin
2	C16808		Isosilybin



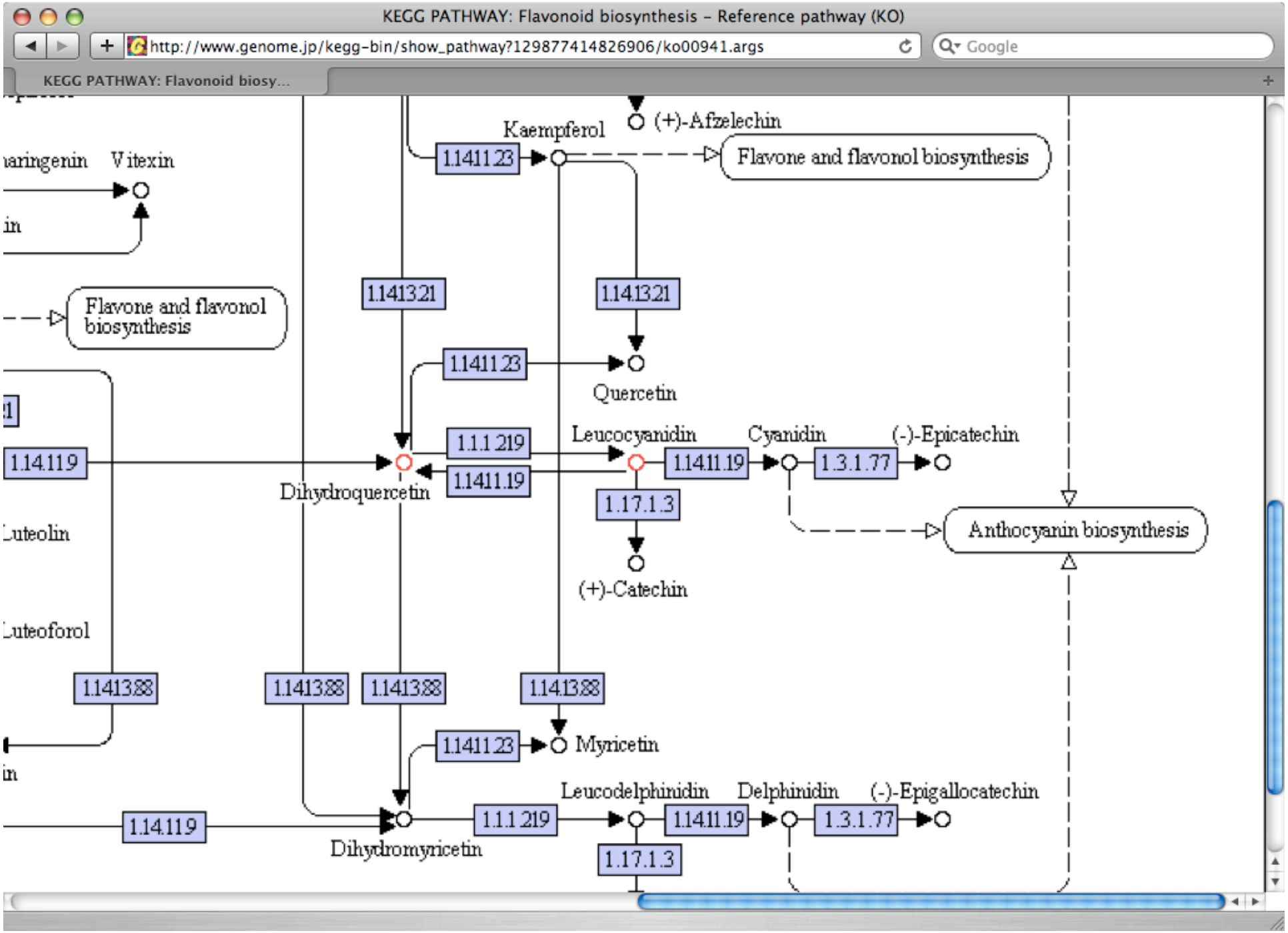
Pathway Search Result

Following object(s) was/were not found cpd:C03430 cpd:C07610 cpd:C08600 cpd:C08717 cpd:C09731 cpd:C09758 cpd:C09763 cpd:C10179 cpd:C10217 cpd:C10221 cpd:C10238 cpd:C12316 cpd:C16808 cpd:C17639 cpd:C17640 cpd:C17775 cpd:C17776

Sort by the pathway list

Show all objects

- ko00941 Flavonoid biosynthesis (3)
- ko01110 Biosynthesis of secondary metabolites (2)
- ko01100 Metabolic pathways (1)


KEGG PATHWAY: Flavonoid biosynthesis - Reference pathway (KO)
http://www.genome.jp/kegg-bin/show_pathway?129877414826906/ko00941.args
Google
KEGG PATHWAY: Flavonoid biosy...
Kaempferol
(+)-Afzelechin
1.14.11.23
Flavone and flavonol biosynthesis
aringenin
Vitexin
in
Flavone and flavonol biosynthesis
1.14.13.21
1.14.13.21
1.14.11.23
Quercetin
1.14.11.9
1.1.1.219
1.14.11.19
Dihydroquercetin
Leucocyanidin
Cyanidin
(-)-Epicatechin
1.14.11.19
1.3.1.77
1.17.1.3
Anthocyanin biosynthesis
(+)-Catechin
Luteolin
Luteoforol
1.14.13.88
1.14.13.88
1.14.13.88
1.14.13.88
1.14.11.23
Myricetin
in
Leucodelphinidin
Delphinidin
(-)-Epigallocatechin
1.14.11.9
1.1.1.219
1.14.11.19
1.3.1.77
Dihydromyricetin
1.17.1.3

KegDraw を使ってみよう

1. http://www.genome.jp/download/ にアクセス
2. KegDraw 0.1.11beta の Mac OSX [dmg] をクリックしてダウンロード
3. データをロード
   - サンプルデータは http://web.kuicr.kyoto-u.ac.jp/~kot/enshu/ のenshu*.mol
4. 結合を消してみたり、新たに書き加えたりしてみましょう
5. そして「Tools」メニューから「Search Structure」→「SIMCOMP」
   - あとはさっきと同じ。

KegHier / KegArray / KegDraw

http://www.genome.jp/download/

KegArray

KegHier / KegArray / KegDraw

KegHier

Java application for browsing hierarchical text files

- KegHier 0.4.2beta (December 28, 2009) for
  Mac OSX [dmg] Windows (exe) [zip] Windows (jar/bat) [zip] Linux [tar.gz]
- ReadMe file
- About KegHier

Please send your comments and suggestions through the feedback form.

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

Please send your comments and suggestions through the feedback form.

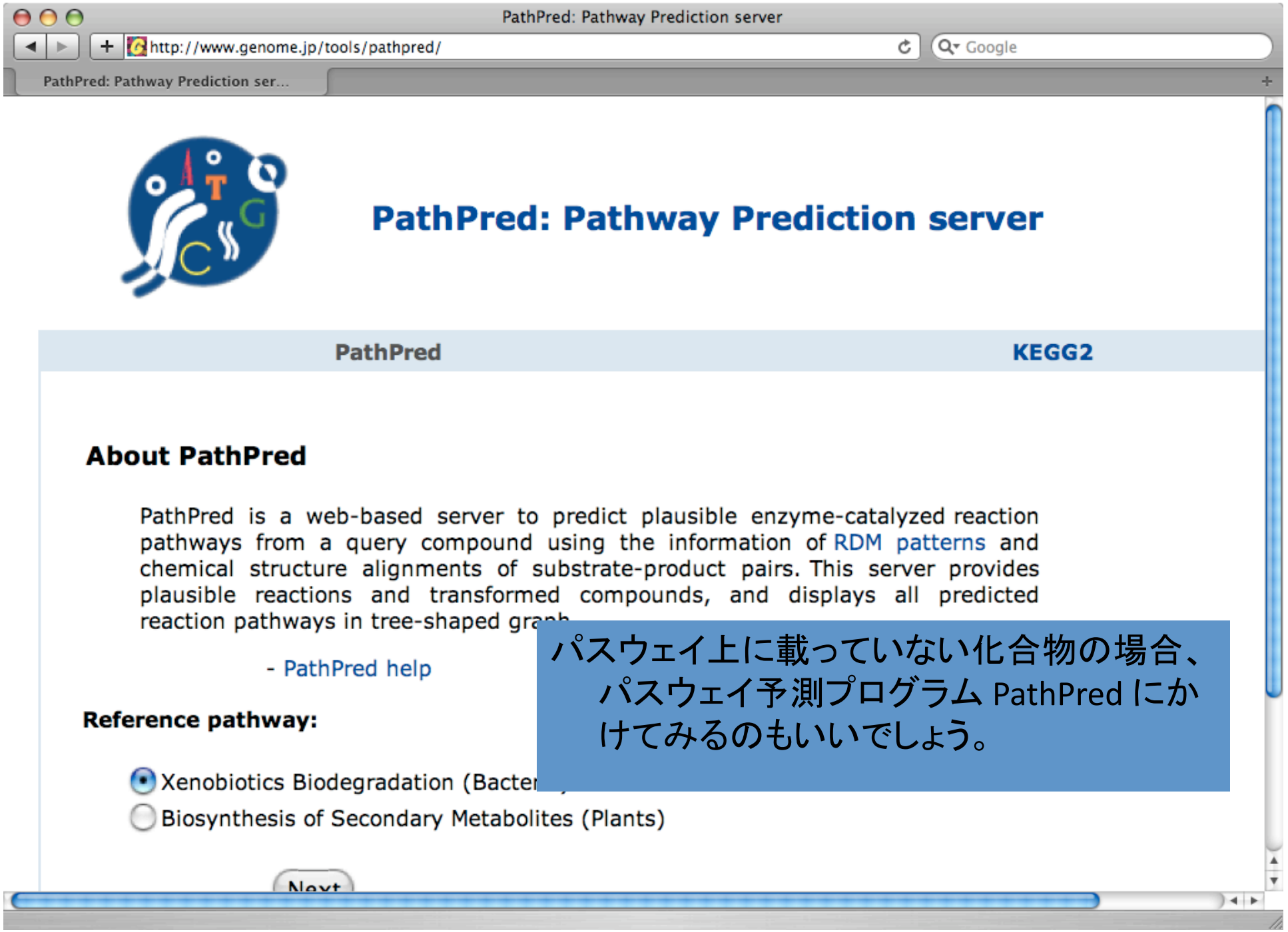
KegDraw

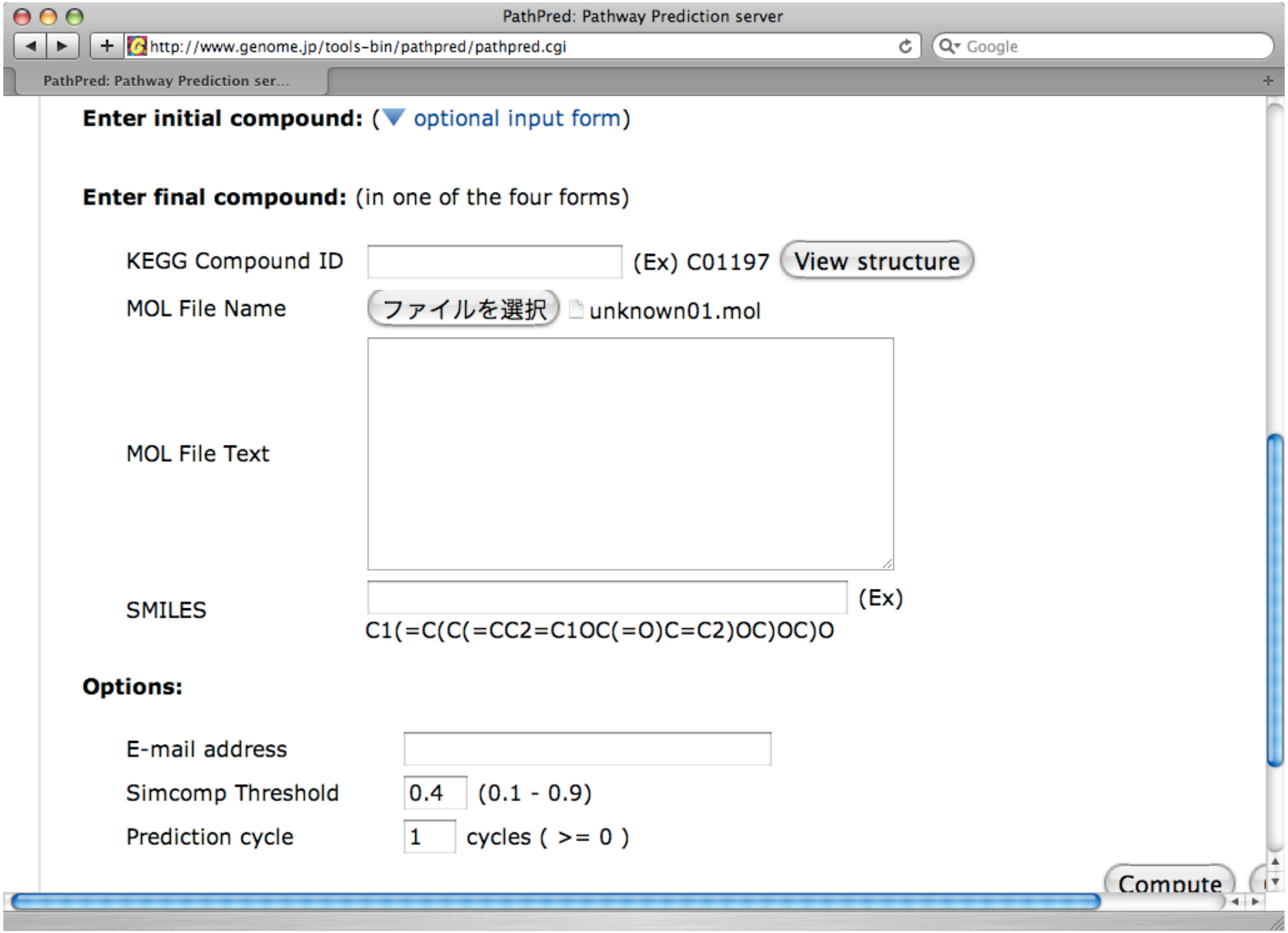
Java application for drawing compound and glycan structures

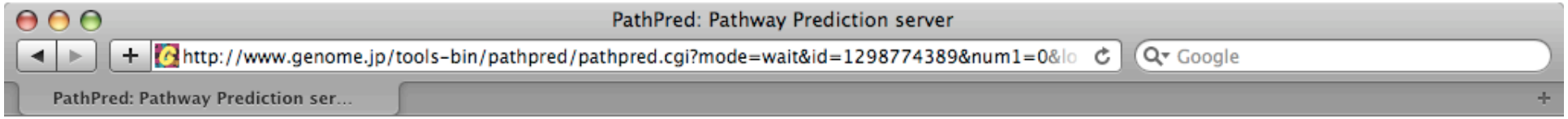
KegDraw は化合物／糖鎖構造描画ツールで、
SIMCOMP 検索にも対応してます。

PathPred を使ってみよう

1. http://www.genome.jp/tools/pathpred/ にアクセス
2. 「Biosynthesis of Secondary Metabolites (plants)」をチェックし「Next」をクリック
3. データを貼付けて「View Structure」をクリック
   - サンプルデータは http://web.kuicr.kyoto-u.ac.jp/~kot/enshu/ のenshu*.mol
4. さらに「Compute」をクリック
5. 結果が出たら、画面中程にある<show all path>をクリック
   - CXで始まる化合物は予測された中間体、Cで始まる化合物はKEGGに登録されている（存在の知られている）化合物


PathPred: Pathway Prediction server
http://www.genome.jp/tools/pathpred/
Google
PathPred: Pathway Prediction ser...
PathPred: Pathway Prediction server
PathPred
KEGG2
About PathPred
PathPred is a web-based server to predict plausible enzyme-catalyzed reaction pathways from a query compound using the information of RDM patterns and chemical structure alignments of substrate-product pairs. This server provides plausible reactions and transformed compounds, and displays all predicted reaction pathways in tree-shaped gra
- PathPred help
Reference pathway:
Xenobiotics Biodegradation (Bacte
Biosynthesis of Secondary Metabolites (Plants)
Next
パスウェイ上に載っていない化合物の場合、
パスウェイ予測プログラム PathPred にか
けてみるのもいいでしょう。


PathPred: Pathway Prediction server
http://www.genome.jp/tools-bin/pathpred/pathpred.cgi
Google
PathPred: Pathway Prediction ser...
Enter initial compound: (▼ optional input form)
Enter final compound: (in one of the four forms)
KEGG Compound ID
(Ex) C01197
View structure
MOL File Name
ファイルを選択
unknown01.mol
MOL File Text
SMILES
(Ex)
C1(=C(C(=CC2=C1OC(=O)C=C2)OC)OC)O
Options:
E-mail address
Simcomp Threshold
0.4
(0.1 - 0.9)
Prediction cycle
1
cycles (>= 0)
Compute



Please wait a few minutes, or access to result page later.

..... 0% of computation has completed.

Pathway Prediction

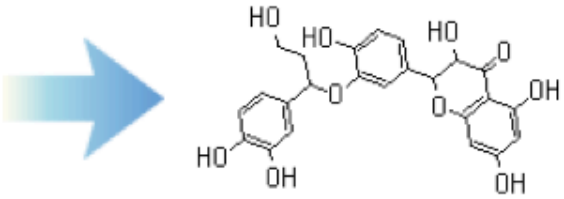
http://www.genome.jp/tools-bin/pathpred/view.cgi?id=1298774389&file=0000

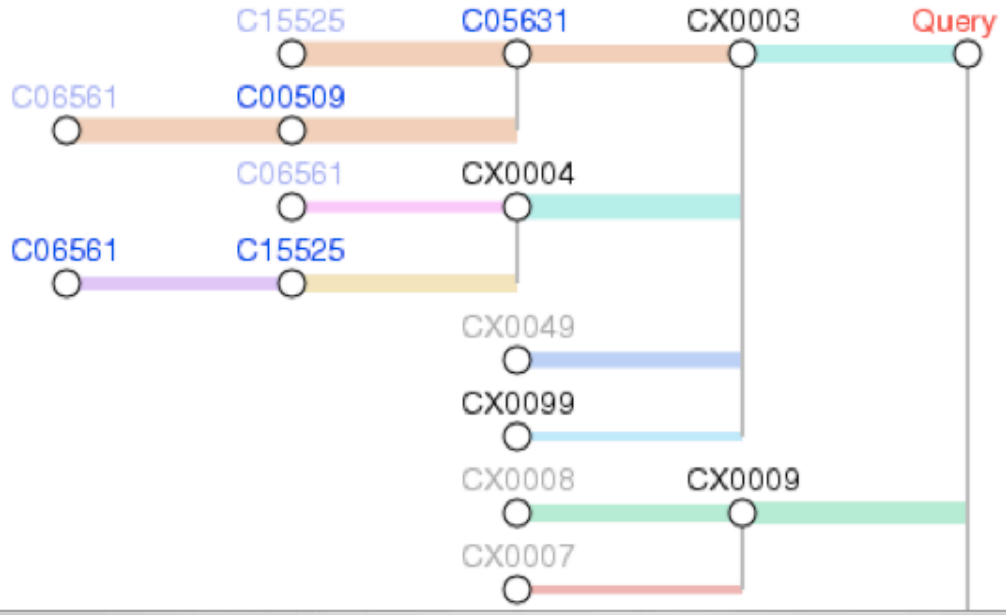
Google

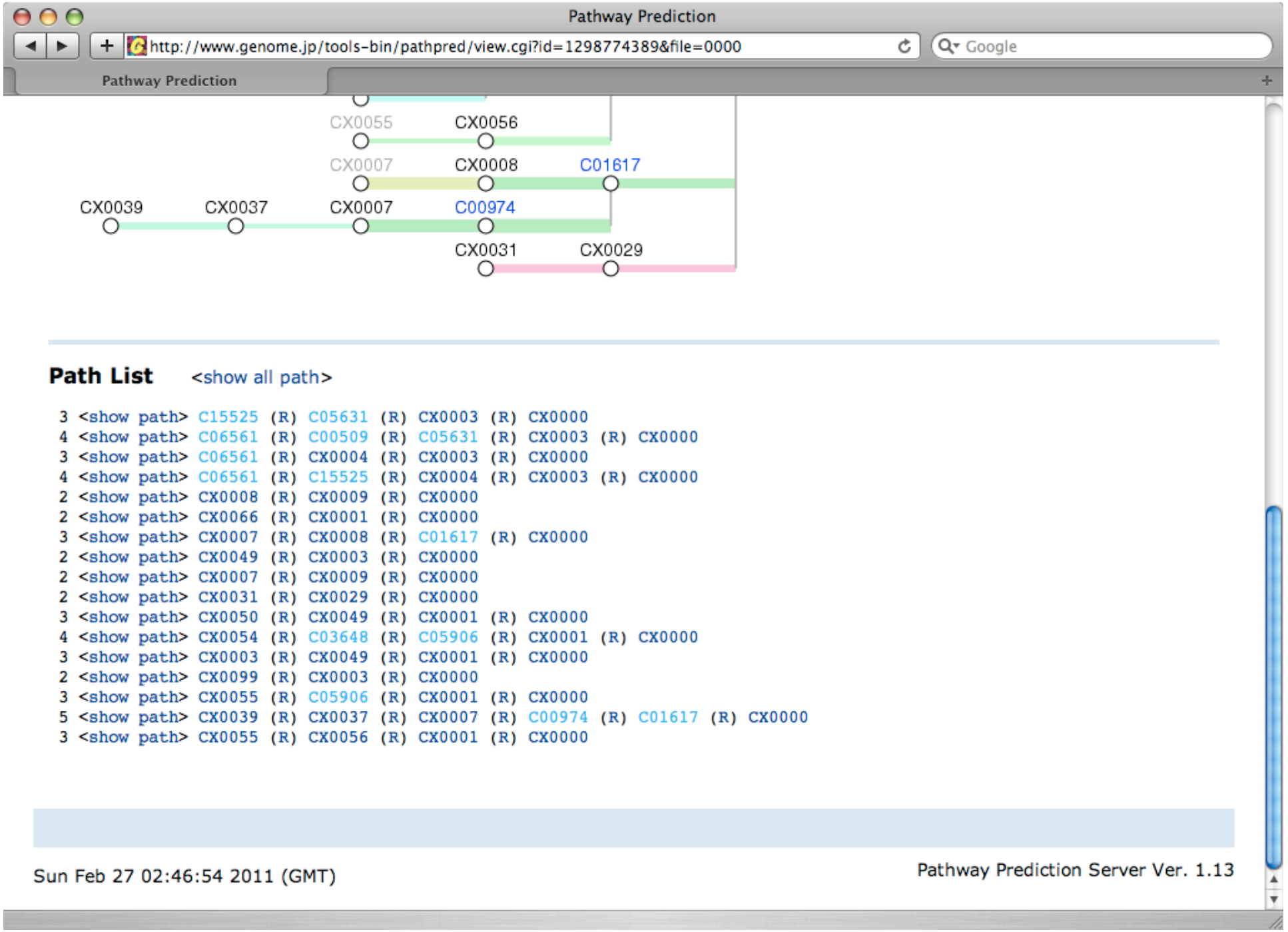
Pathway Prediction

Pathway Prediction Result

[Top] [Help]







Path List <show all path>

```
3 <show path> C15525 (R) C05631 (R) CX0003 (R) CX0000
4 <show path> C06561 (R) C00509 (R) C05631 (R) CX0003 (R) CX0000
3 <show path> C06561 (R) CX0004 (R) CX0003 (R) CX0000
4 <show path> C06561 (R) C15525 (R) CX0004 (R) CX0003 (R) CX0000
2 <show path> CX0008 (R) CX0009 (R) CX0000
2 <show path> CX0066 (R) CX0001 (R) CX0000
3 <show path> CX0007 (R) CX0008 (R) C01617 (R) CX0000
2 <show path> CX0049 (R) CX0003 (R) CX0000
2 <show path> CX0007 (R) CX0009 (R) CX0000
2 <show path> CX0031 (R) CX0029 (R) CX0000
3 <show path> CX0050 (R) CX0049 (R) CX0001 (R) CX0000
4 <show path> CX0054 (R) C03648 (R) C05906 (R) CX0001 (R) CX0000
3 <show path> CX0003 (R) CX0049 (R) CX0001 (R) CX0000
2 <show path> CX0099 (R) CX0003 (R) CX0000
3 <show path> CX0055 (R) C05906 (R) CX0001 (R) CX0000
5 <show path> CX0039 (R) CX0037 (R) CX0007 (R) C00974 (R) C01617 (R) CX0000
3 <show path> CX0055 (R) CX0056 (R) CX0001 (R) CX0000
```

Sun Feb 27 02:46:54 2011 (GMT)

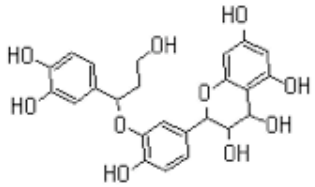
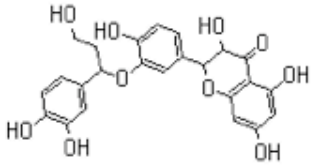
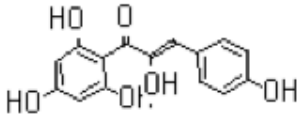
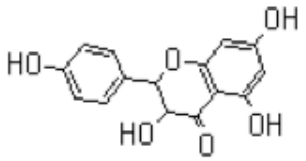
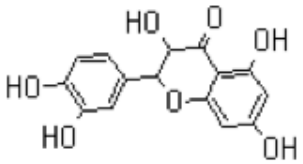
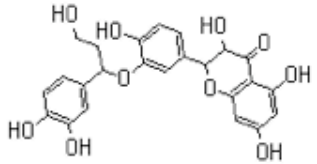
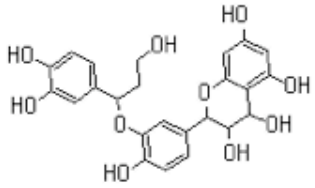
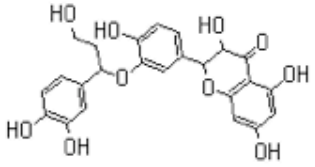
Pathway Prediction Server Ver. 1.13

Pathway Prediction

http://www.genome.jp/tools-bin/pathpred/view.cgi?id=1298774389&file=0000&mode=all

Google

Pathway Prediction

RP11588 RP09097 RP09080 RP09422 0.5814	 CX0001 1.4120	RP00701 RP11788 RP02776 RP11308 0.7143	 CX0000 0.0000				
RP11825 0.3056	 CX0007 1.0689	RP02223 0.8837	 C00974 1.1614	RP02219 0.9667	 C01617 1.3562	RP11588 RP09080 RP09422 0.6585	 CX0000 0.0000
RP11789 RP09082 RP02223 RP11808 RP11729 RP11589 0.5833		RP00701 RP11788 RP02776 RP11308 0.7143					

KEGG API を使ってみよう

- 自作プログラム等からKEGGを利用するためのウェブサービス
- Ruby / Perl / Python / Java など他言語に対応

KEGG API

getpdb.rb

```
#!/usr/bin/env ruby

require 'soap/wsdlDriver'

wsdl = "http://soap.genome.jp/KEGG.wsdl"
serv = SOAP::WSDLDriverFactory.new(wsdl).create_rpc_driver
serv.generate_explicit_type = true

offset = 1
limit = 5
cpd = ARGV.shift || 'cpd:C00345'
organism = ARGV.shift || 'eco'

top5_enz = serv.get_enzymes_by_compound(cpd)
top5_enz.each do |enz|
  puts enz
  genes = serv.get_genes_by_enzyme(enz, organism)
  genes.each do |gene|
        print "¥t", gene, "¥n"
        if links = serv.get_linkdb_by_entry(gene, 'pdb', offset, limit)
                links.each do |link|
                        print "¥t¥t"
                        puts link.entry_id2
                end
        end
  end
end
```

サンプルプログラム：化合物「C00345」を基質とする大腸菌（eco）の酵素の中で、PDBにエントリがあるものを列挙する。

result.txt

```
ec:1.1.1.43
ec:1.1.1.44
        eco:b2029
                pdb:2ZYA
                pdb:2ZYD
                pdb:3FWN
ec:2.7.1.12
        eco:b3437
                pdb:1KNQ
                pdb:1KO1
                pdb:1KO4
                pdb:1KO5
                pdb:1KO8
        eco:b4268
ec:3.1.1.31
        eco:b0767
                pdb:1RI6
ec:4.2.1.12
        eco:b1851
```

KEGG API

サンプルプログラム；大腸菌（eco）から採取した複数の化合物に対し、それらを基質としうる酵素の遺伝子のリストを得て、また、それらの遺伝子をパスウェイ上にマッピングする。

getpathway.rb

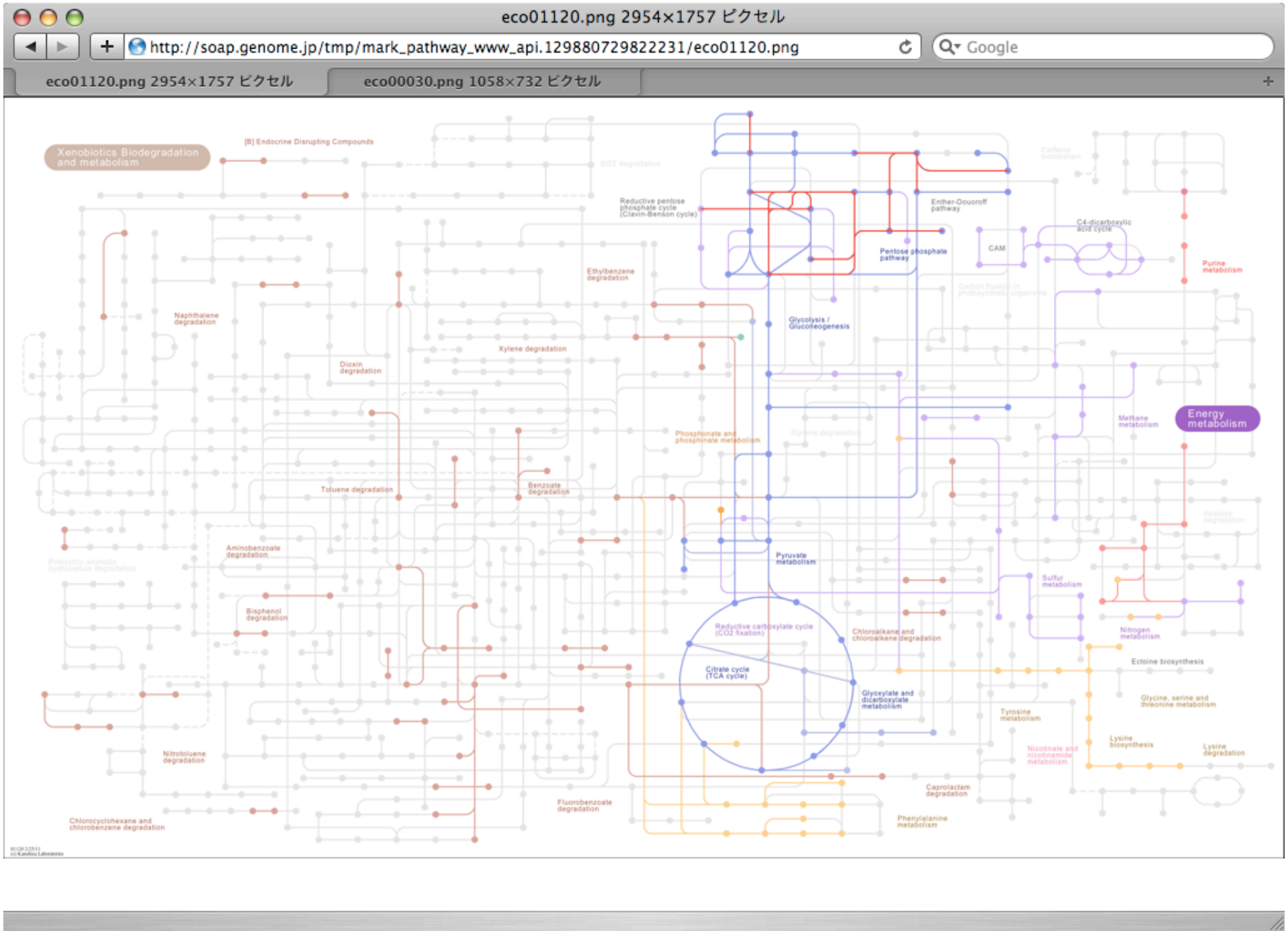
```
#!/usr/bin/env ruby

require 'soap/wsdlDriver'

wsdl = "http://soap.genome.jp/KEGG.wsdl"
serv = SOAP::WSDLDriverFactory.new(wsdl).create_rpc_driver
serv.generate_explicit_type = true

offset = 1
limit = 5
cpds = ['cpd:C00345', 'cpd:C00117']
organism = ARGV.shift || 'eco'

genes = Array.new
cpds.each do |cpd|
  if top5_enz = serv.get_enzymes_by_compound(cpd)
    top5_enz.each do |enz|
      if tmp_genes = serv.get_genes_by_enzyme(enz, organism)
        genes += tmp_genes
      end
    end
  end
end

pathway2genes = Hash.new
genes.uniq.each do |gene|
  if tmp_pathways = serv.get_pathways_by_genes([gene])
    tmp_pathways.each do |pathway|
      pathway2genes[pathway] ||= Array.new
      pathway2genes[pathway] << gene
    end
  end
end

pathway2genes.each do |pathway, genes|
  fg_list = Array.new
  bg_list = Array.new
  genes.each do |gene|
    fg_list << "#ff0000"
    bg_list << "#ff6666"
  end
  url = serv.color_pathway_by_objects(pathway, genes, fg_list, bg_list)
  puts url
  print "¥t", genes.join(" "), "¥n"
end
```

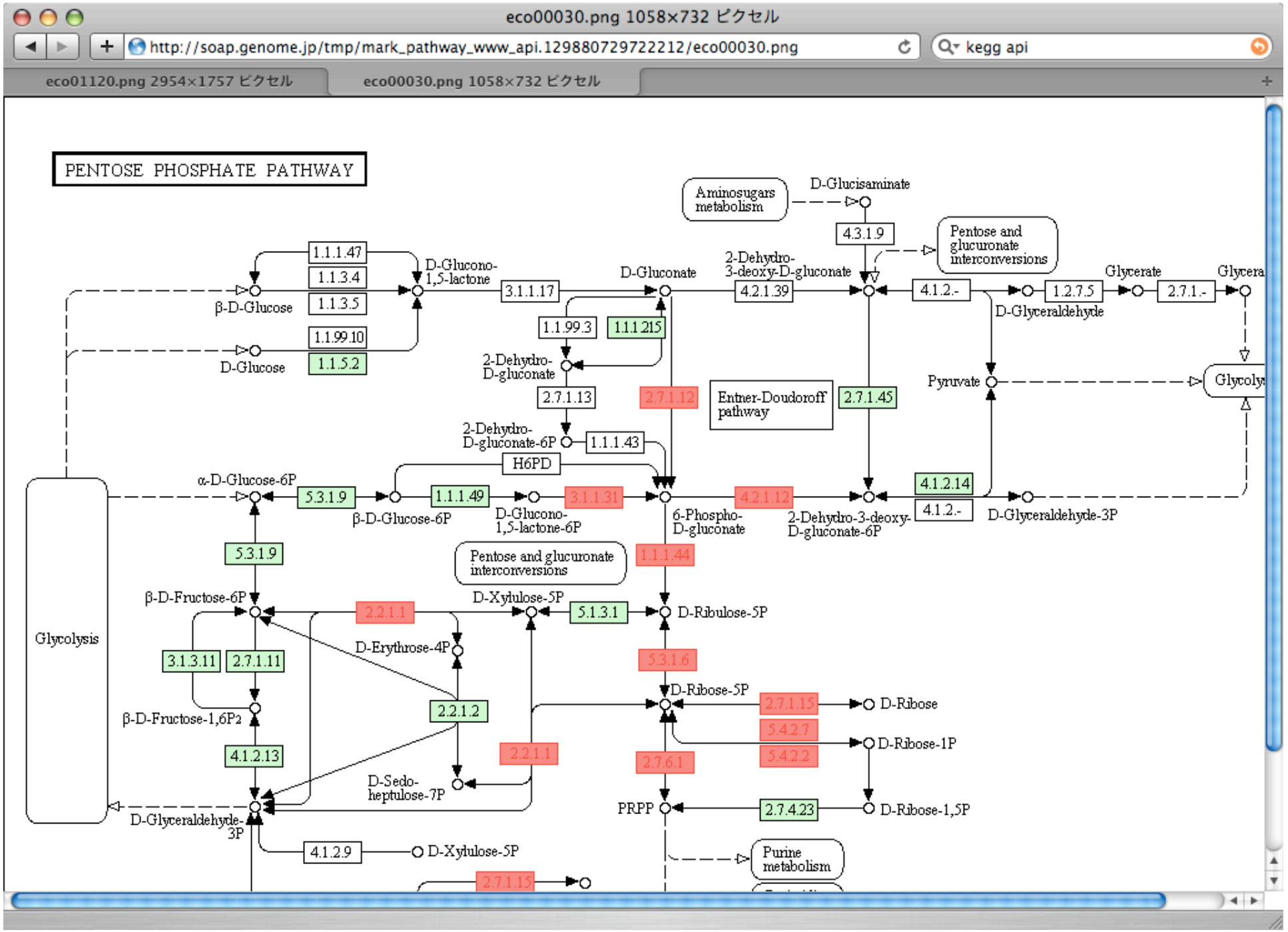
KEGG API

出力結果

retult2.txt

```
http://soap.genome.jp/tmp/mark_pathway_www_api.129880728622096/eco00520.png
        eco:b0688
http://soap.genome.jp/tmp/mark_pathway_www_api.129880728922117/eco00521.png
        eco:b0688
http://soap.genome.jp/tmp/mark_pathway_www_api.129880729122127/eco00500.png
        eco:b0688
http://soap.genome.jp/tmp/mark_pathway_www_api.129880729322159/eco00480.png
        eco:b2029
http://soap.genome.jp/tmp/mark_pathway_www_api.129880729522201/eco00052.png
        eco:b0688
http://soap.genome.jp/tmp/mark_pathway_www_api.129880729722212/eco00030.png
        eco:b2029 eco:b3437 eco:b4268 eco:b0767 eco:b1851 eco:b2465 eco:b2935 eco:b3752 eco:b1207 eco:b2914 eco:b4090
eco:b0688 eco:b4383
http://soap.genome.jp/tmp/mark_pathway_www_api.129880729822231/eco01120.png
        eco:b2029 eco:b3437 eco:b4268 eco:b0767 eco:b1851 eco:b2465 eco:b2935 eco:b1207 eco:b2914 eco:b4090 eco:b0688
http://soap.genome.jp/tmp/mark_pathway_www_api.129880730622310/eco00010.png
        eco:b0688
http://soap.genome.jp/tmp/mark_pathway_www_api.129880730822328/eco00230.png
        eco:b1207 eco:b1982 eco:b3034 eco:b0688 eco:b4383
http://soap.genome.jp/tmp/mark_pathway_www_api.129880731122338/eco01110.png
        eco:b2029 eco:b3437 eco:b4268 eco:b0767 eco:b2465 eco:b2935 eco:b1207 eco:b2914 eco:b4090 eco:b0688
http://soap.genome.jp/tmp/mark_pathway_www_api.129880732022370/eco01100.png
        eco:b2029 eco:b3437 eco:b4268 eco:b0767 eco:b1851 eco:b2465 eco:b2935 eco:b1207 eco:b2914 eco:b4090 eco:b0688
```


eco01120.png 2954×1757 ピクセル
http://soap.genome.jp/tmp/mark_pathway_www_api.129880729822231/eco01120.png
Google
eco01120.png 2954×1757 ピクセル
eco00030.png 1058×732 ピクセル
Xenobiotics Biodegradation and metabolism
[B] Endocrine Disrupting Compounds
DDT degradation
Reductive pentose phosphate cycle (Calvin-Benson cycle)
Ether-Dousroff pathway
Caffeine metabolism
C4-dicarboxylic acid cycle
CAM
Pentose phosphate pathway
Purine metabolism
Ethylbenzene degradation
Carbon fixation in photosynthetic organisms
Glycolysis / Gluconeogenesis
Naphthalene degradation
Xylene degradation
Dioxin degradation
Methane metabolism
Energy metabolism
Phosphonate and phosphinate metabolism
Styrene degradation
Toluene degradation
Benzoate degradation
Aminobenzoate degradation
Pyruvate metabolism
Sulfur metabolism
Polycyclic aromatic hydrocarbon degradation
Bisphenol degradation
Reductive carboxylate cycle (CO2 fixation)
Chloroalkane and chloroalkene degradation
Nitrogen metabolism
Citrate cycle (TCA cycle)
Ectoine biosynthesis
Glyoxylate and dicarboxylate metabolism
Glycine, serine and threonine metabolism
Tyrosine metabolism
Nicotinate and nicotinamide metabolism
Lysine biosynthesis
Lysine degradation
Nitrotoluene degradation
Caprolactam degradation
Fluorobenzoate degradation
Phenylalanine metabolism
Chlorocyclohexane and chlorobenzene degradation


eco00030.png 1058×732 ピクセル
http://soap.genome.jp/tmp/mark_pathway_www_api.129880729722212/eco00030.png
kegg api
eco01120.png 2954×1757 ピクセル
eco00030.png 1058×732 ピクセル
PENTOSE PHOSPHATE PATHWAY
Aminosugars metabolism
D-Glucisaminate
4.3.1.9
Pentose and glucuronate interconversions
1.1.1.47
1.1.3.4
1.1.3.5
1.1.99.10
1.1.5.2
β-D-Glucose
D-Glucose
D-Glucono-1,5-lactone
3.1.1.17
D-Gluconate
2-Dehydro-3-deoxy-D-gluconate
4.2.1.39
4.1.2.-
1.2.7.5
Glycerate
2.7.1.-
Glycera
D-Glyceraldehyde
1.1.99.3
1.1.1.215
2-Dehydro-D-gluconate
2.7.1.13
2.7.1.12
Entner-Doudoroff pathway
2.7.1.45
Pyruvate
Glycoly
2-Dehydro-D-gluconate-6P
1.1.1.43
H6PD
α-D-Glucose-6P
5.3.1.9
β-D-Glucose-6P
1.1.1.49
D-Glucono-1,5-lactone-6P
3.1.1.31
6-Phospho-D-gluconate
4.2.1.12
2-Dehydro-3-deoxy-D-gluconate-6P
4.1.2.14
4.1.2.-
D-Glyceraldehyde-3P
Glycolysis
Pentose and glucuronate interconversions
1.1.1.44
β-D-Fructose-6P
2.2.1.1
D-Xylulose-5P
5.1.3.1
D-Ribulose-5P
D-Erythrose-4P
3.1.3.11
2.7.1.11
5.3.1.6
D-Ribose-5P
2.7.1.15
D-Ribose
β-D-Fructose-1,6P2
2.2.1.2
5.4.2.7
5.4.2.2
D-Ribose-1P
4.1.2.13
2.2.1.1
2.7.6.1
D-Sedo-heptulose-7P
PRPP
2.7.4.23
D-Ribose-1,5P
D-Glyceraldehyde-3P
4.1.2.9
D-Xylulose-5P
Purine metabolism
2.7.1.15

レポート課題

1. KEGG PATHWAY データベース を用い、Glycolysis レファレンス・パスウェイ中で *Mycoplasma hominis* の持つ酵素遺伝子群を図示せよ。
2. *Mycoplasma hominis* は Glycolysis の酵素を欠いているため、通常の Glycolysis を行わないと予想されるが、その欠いている酵素とは何か。
3. 通常の Glycolysis を行わないと予想される *Mycoplasma hominis* が α-D-glucose-6-phosphate から glyceraldehyde-3-phosphate を生成するにあたって、どのようなパスウェイで代替していると予想されるか、KEGG PATHWAY データベースを用いて図示せよ。

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- 締切：2011年11月28日（月）