

2. Data sources for metabolic models

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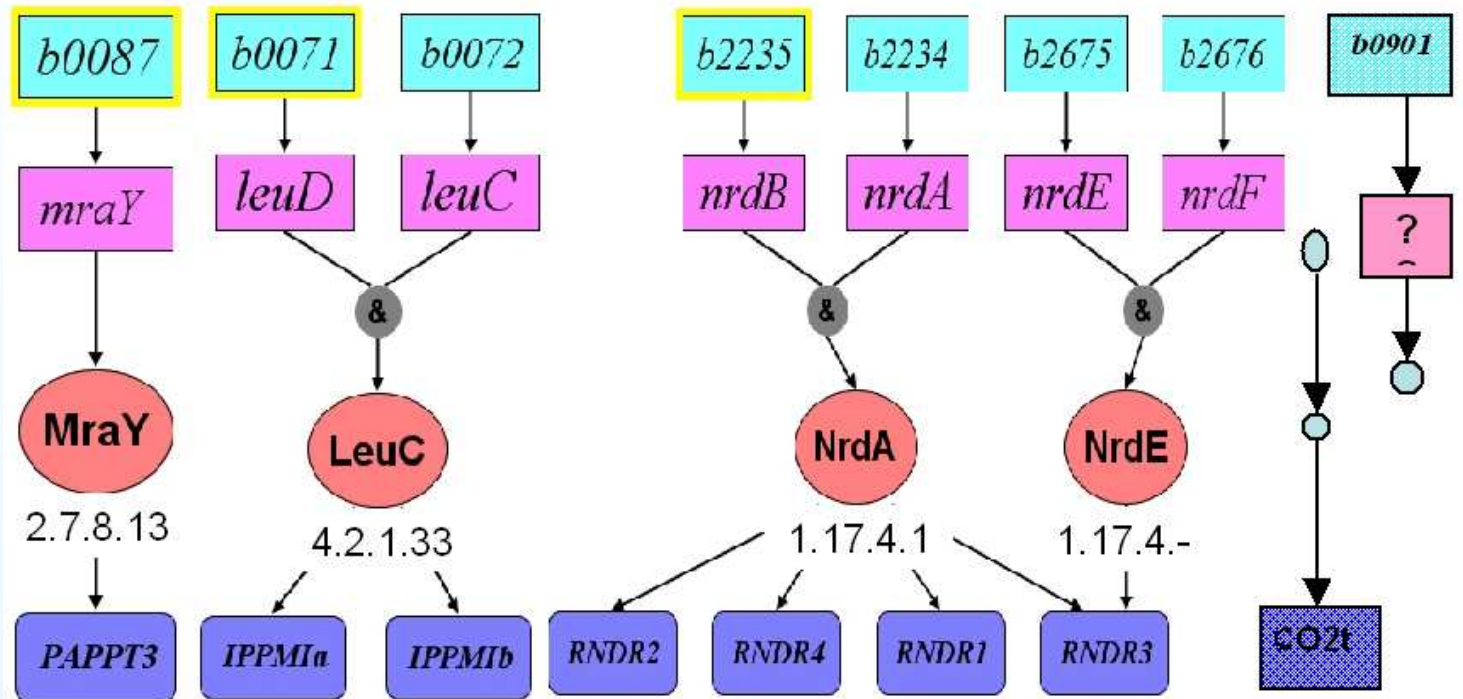
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Genes to Reactions

Genome to reaction mapping

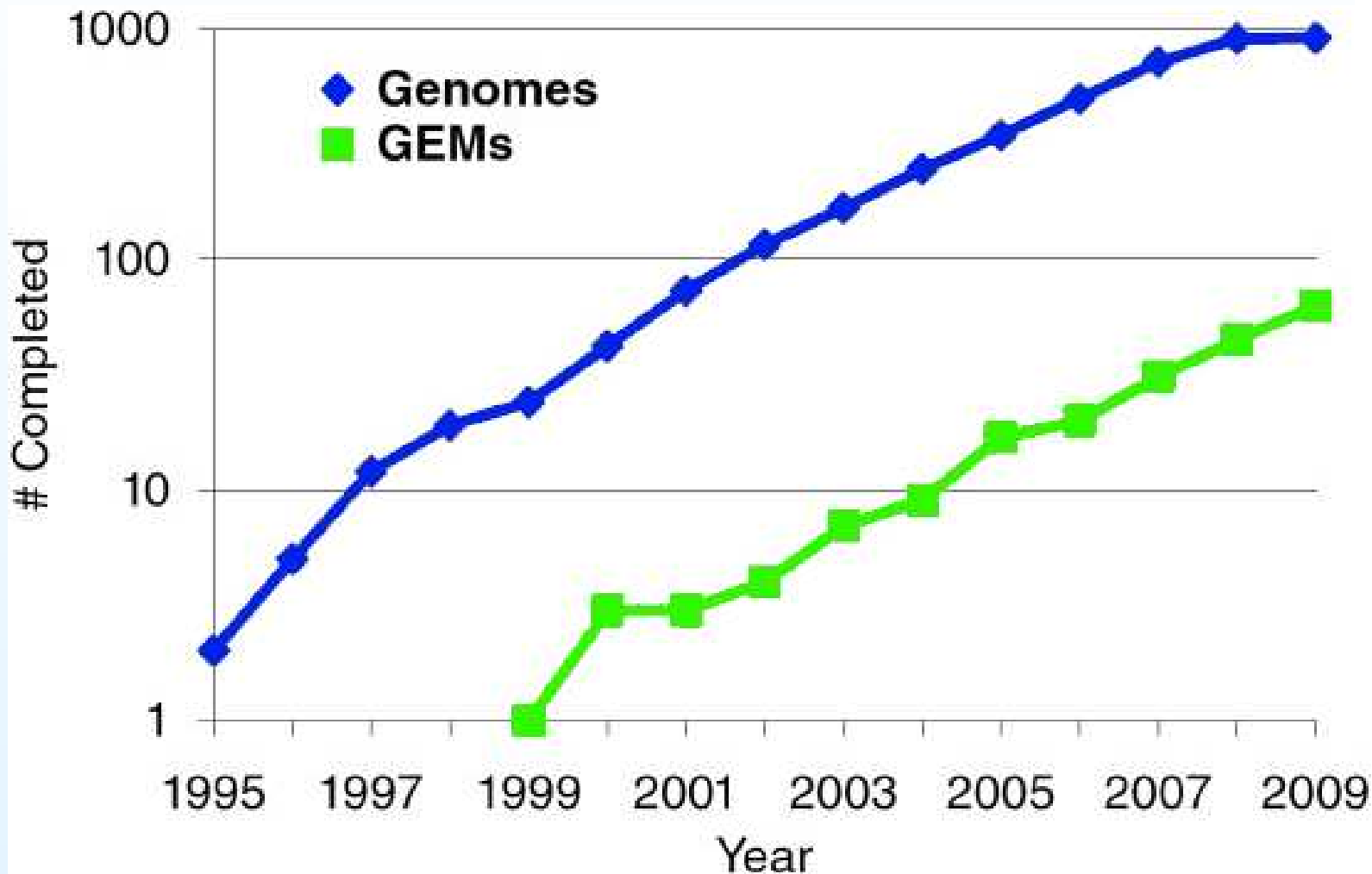
- Genes to Reactions
- The Interpretation Gap
- The Reaction List
- Data Sources
- BioCyc
- KEGG
- IntEnz: Enzymes at EBI
- Expaty Enzyme
- BRENDA
- Other Resources
- Requirements for a Structural Model



The Interpretation Gap

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Milne et al (2009) Biotech. J, 4, 1653-1670

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Where does the data for writing the reaction list for a metabolic model come from?

- Biochemical literature: books, reviews, journal articles.
- Genome databases plus annotation plus enzyme database.
 - BioCyc: <http://biocyc.org/>
 - KEGG: <http://www.genome.jp/kegg/>
 - IntEnz at <http://www.ebi.ac.uk/intenz/> (now the primary source) or EXPASY Enzyme: <https://enzyme.expasy.org/>
 - Brenda: <http://www.brenda-enzymes.info>

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KEGG: Kyoto Encyclopedia of Genes and Genomes



Go Clear

» Japanese

KEGG Home
Introduction
Overview

KEGG: Kyoto Encyclopedia of Genes and Genomes

MetaCyc Encyclopedia of Metabolic Pathways

Pathway Tools Tutorial
April 25 - 27, 2011
Menlo Park, CA

Searching MetaCyc change org

Home Search Tools Help

KEGG

KEGG

About MetaCyc

METACYC OVERVIEW

MetaCyc is a database of nonredundant, experimentally elucidated metabolic pathways. MetaCyc contains more than 1600 pathways, and is curated from the scientific experimental literature. [more](#)


Enzyme Database - BRENDA

Enzyme Database - BRENDA

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[history](#)
[All enzymes](#)

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Web Services

Quick Search
Fulltext Search
Advanced Search
Substructure Search
TaxTree Explorer
EC Explorer

 **BRENDA**
The Comprehensive Enzyme Information System

EC-Number Enzyme Name Organism Protein Full text

Search Display 10 entries

New publications on BRENDA

Nomenclature	Reaction & Specificity	Full text
Enzyme Names	Pathway	

BioCyc

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<http://biocyc.org/>

Example entry: **Pyruvate kinase**

KEGG

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Kyoto Encyclopaedia of Genes and Genomes

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

Example entry: **TCA cycle**

IntEnz: Enzymes at EBI

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ENZYME database at <https://enzyme.expasy.org/>

Example entry: Pyruvate kinase; 2.7.1.40

BRENDA

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Example entry: **Pyruvate kinase**

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Alternatives to reciprocal BLAST homology searching

(Deficiencies: Chinese whispers; failure to detect bi- or multifunctional- enzymes.)

Enzyme-finding tools based on sequence signatures:

- PRIAM
- theSEED (part of KBASE: <http://kbase.us>)
- EfiCAZ

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A valid structural model requires a reaction list in which:

- Every internal metabolite is both produced and consumed, either by an enzyme or a transporter.
- The metabolites that exchange with the environment or between compartments, usually via transporters, can be identified.
- Every enzyme/transporter in the list has a role in at least one pathway.
- Arguably, the metabolic network should form a single connected component.

Requirements for a Structural Model

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