2. Data sources for metabolic models

David Fell

OXFORD BROOKES UNIVERSITY

C1net gas fermentation

email: dfell@brookes.ac.uk

http://mudshark.brookes.ac.uk

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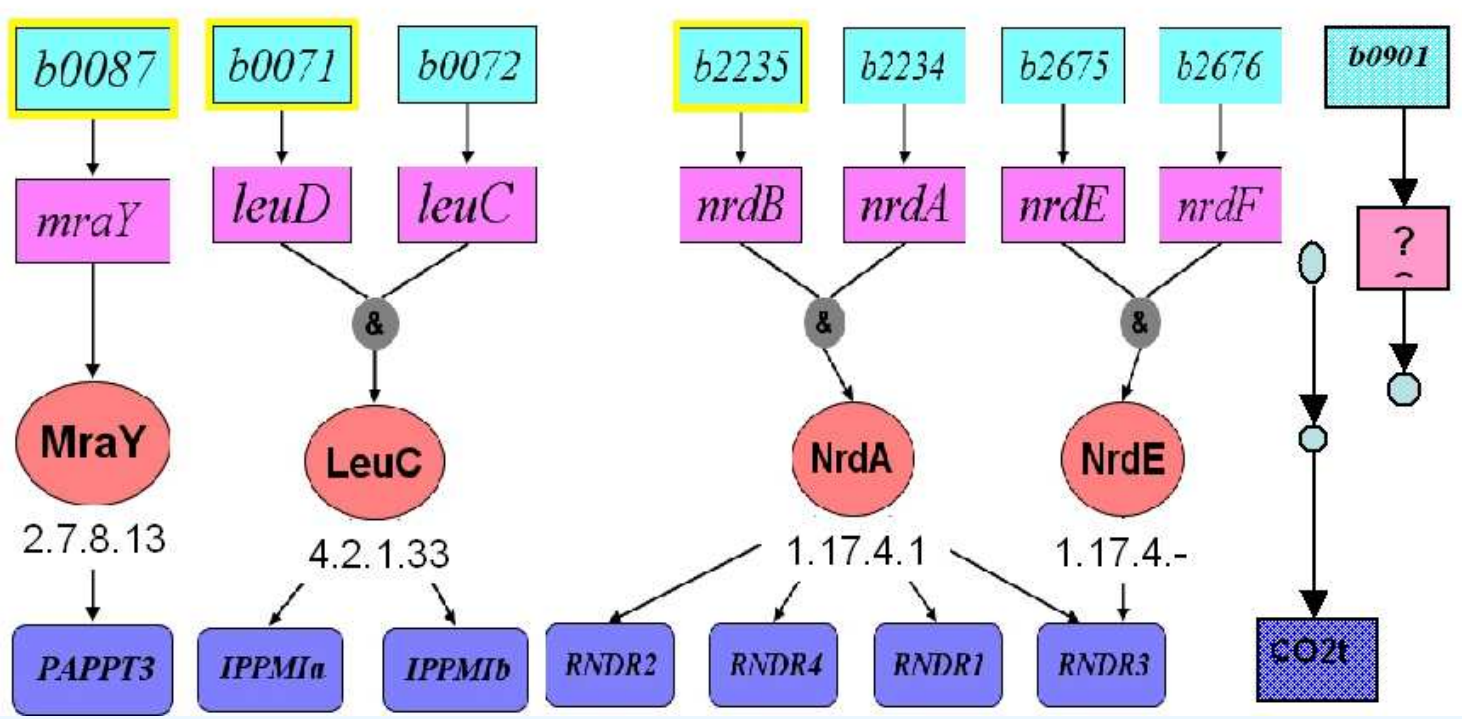
Genes to Reactions

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



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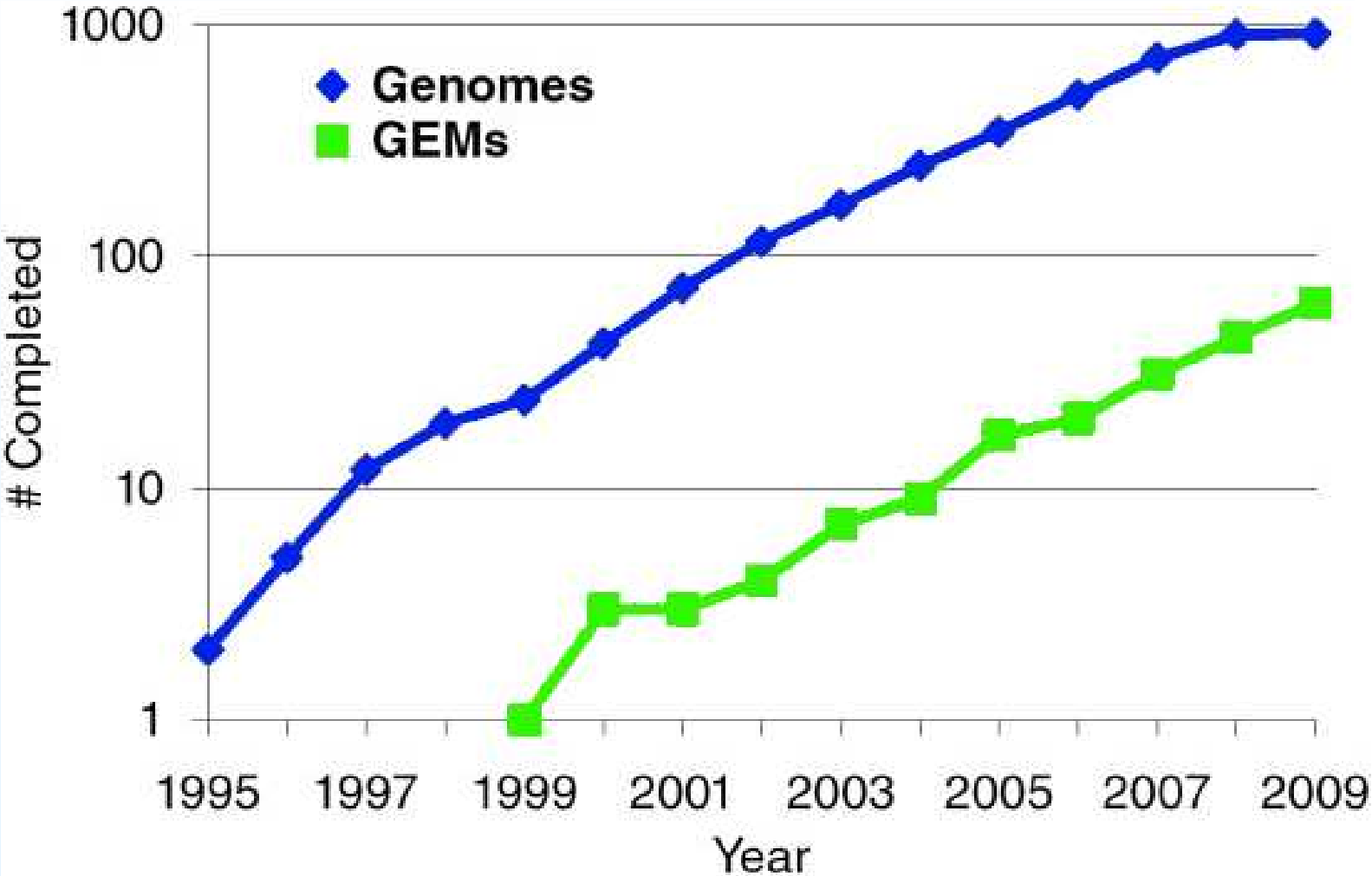

Milne et al (2009) Biotech. J, **4**, 1653-1670

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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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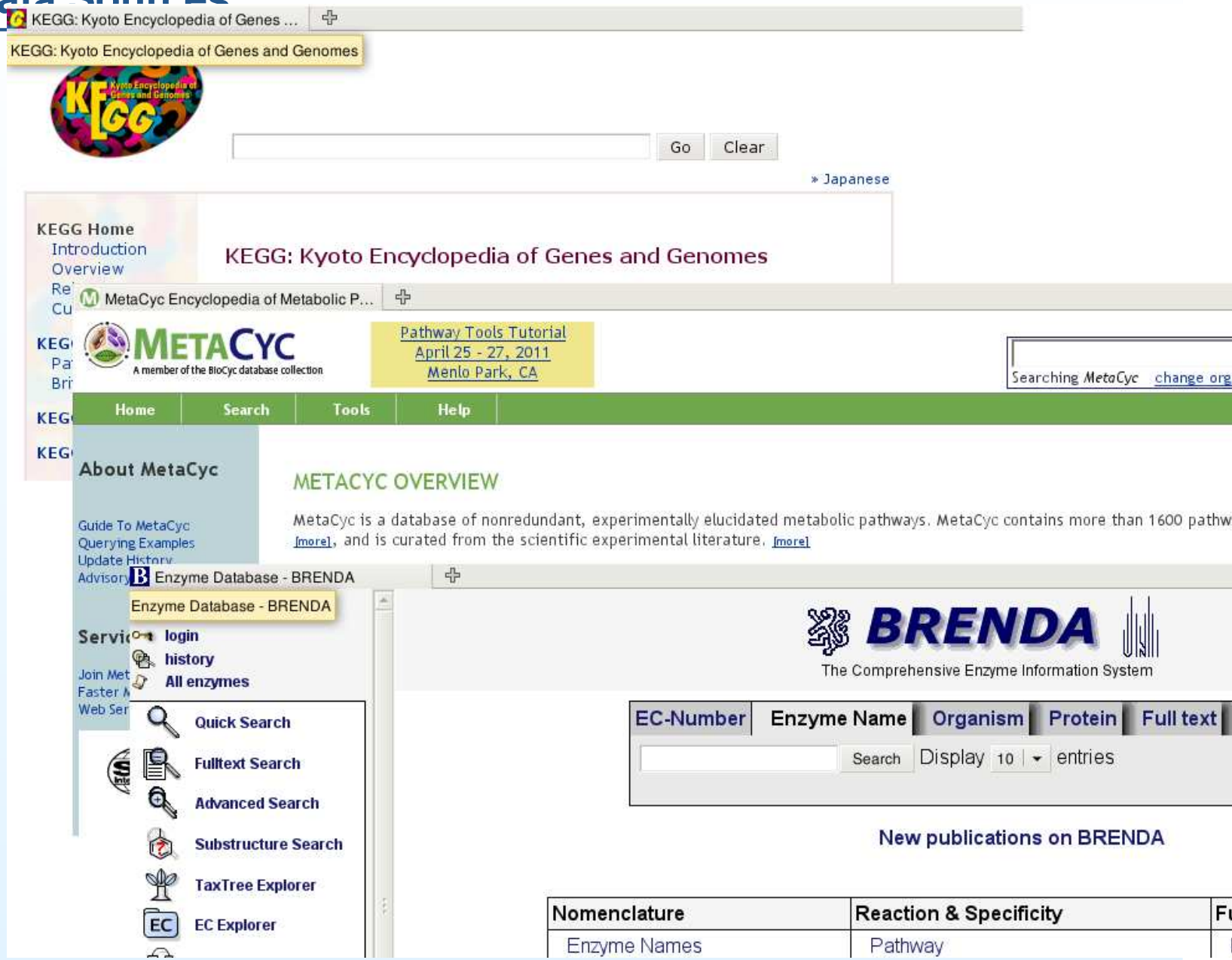

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http://biocyc.org/

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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IntEnz at http://www.ebi.ac.uk/intenz/

Example entry: Pyruvate kinase

Expasy Enzyme

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

Example entry: Pyruvate kinase; 2.7.1.40

BRENDA

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Brenda: http://www.brenda-enzymes.info/

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.

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