Metabolic Databases
MetaCyc and AraCyc: Curation of Plant Metabolism

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Carnegie Institution
Outline

- MetaCyc
  - Goals and application
  - Curation Progress
  - MetaCyc – main functions
  - Pathway tools

- AraCyc
  - Build of AraCyc
  - Curation progress
  - Introduction to the database
  - Omics viewer
MetaCyc

http://www.metacyc.org


MetaCyc: a multiorganism database of metabolic pathways and enzymes

What is MetaCyc?

- MetaCyc is a multi-organism database that collects any known pathways across all kingdoms.

- MetaCyc is a curated, literature-based biochemical pathways database.

- Collaboration between SRI International and Carnegie Institution.
Goal and Applications

Goal

- Universal repository of metabolic pathways
  - Up-to-date, literature-curated catalogue of commented enzymes and pathways for use in research, metabolic engineering and education

Applications

- Database of reference used to generate predicted Pathway/Genome DataBases (PGDBs)
The Content of MetaCyc

- Pathways from primary and secondary (specialized) metabolism
  - Reactions with compound structures
    - Proteins
    - Genes
  - Does not contain sequence information
Curation Team

- PhD-level curators

- Extract data from literature
  - experimentally verified data
  - ideally protein information

- Follow MetaCyc Curator’s guide
MetaCyc Version 11.1
released May 25th, 2007

<table>
<thead>
<tr>
<th>Year</th>
<th>Metabolites</th>
<th>Pathways</th>
<th>Enzymes</th>
<th>Reactions</th>
<th>Chemicals</th>
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<td>115</td>
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</table>

Note: The statistics for each year pertain to the last MetaCyc version released in that year.
The Taxonomic Distribution in MetaCyc

- Mostly from microorganism and plant kingdoms, and several animal pathways
- Plants: 219 species from 69 plant families
- Share about 220 pathways involved in primary metabolism and 180 pathways of secondary (specialized) metabolism
Taxonomy/Metabolism Ratio in MetaCyc

- Plant families with the highest number of annotated pathways:
  - Brassicaceae (*Arabidopsis thaliana*)
  - Legumes (*Glycine max*)
  - Poaceae (*Zea mays*)
  - Solanaceae (*Solanum tuberosum, Nicotiana tabacum*)

- Plant families with the highest number of contributing species:
  - Legumes (36)  Solanaceae (16)
  - Poaceae (12)  Brassicaceae (10)
Explore class hierarchy of pathways, compounds, reactions, genes and cell components.
Explore class hierarchy of pathways, compounds, reactions, genes and cell components.
MetaCyc – Discover the Metabolic Universe

Query the database (pathways, reactions, compounds, genes)
MetaCyc – Query Page

Type your search term and click submit

Molybdenum
MetaCyc – Query Result Page
The pathway diagram shows compounds, reactions and metabolic links.
Pathway commentary comprises general and specific information about the pathway.
Extend or collapse the detail level of the pathway detail page
In depth information about reaction, EC number, enzymes, genes, regulatory aspects, and metabolic links to related pathways.
MetaCyc – More Detail (cont’d)
More detail reveals structural information about compounds.
MetaCyc – Reaction Detail Page

NiceZyme View of ENZYME: EC 1.14.13.21

**Official Name**: Phospho-D-xylosidase.
**Alternative Names**: Phospho-D-Xylosidase.
**Reaction Catalyzed**: 
A D-xylose + NaHPO₄ + H₂O → D-xylopyranose + Na₃PO₄ + H₂O
**Comments**: 
- Acts on a number of substrates, including xylans and dithioxylysines.
- Does not act on 4-coumaric-OH or 4-carboxyphenyl.

**Cross-references**:
- ChEMBL
- PUMA/C
- Model organism-specific profiles
- Rice University LEAM (Name or database)
- KEMB Enzyme Nomenclature
- RICE
- MEDLINE
- MetaCyc
- Local Protein (Protein Files)
MetaCyc – Enzymes and Genes

Contains enzyme commentary, references, and physico-chemical properties of the enzyme
MetaCyc – Enzymes and Genes (cont’d)
Variants, Related Pathways and Links

- Pathway variants are created as separate pathways
  - *IAA biosynthesis I* (tryptophane-dependent)
  - *IAA biosynthesis II* (tryptophane-independent)

- Links are added between interconnected pathways

- Related pathways are grouped into superpathways
  - *e.g. superpathway of choline biosynthesis*
Creation of a Superpathway

choline biosynthesis III

- phosphoryl-choline
- CDP-choline-choline
- a phosphatidylcholine

- choline

Superpathway biosynthesis

- L-serine
- ethanolamine

- phosphoryl-ethanolamine
- N-methylethanolamine phosphate
- N-dimethylethanolamine phosphate
- phosphoryl-choline

choline biosynthesis II

- ethanolamine
- N-monomethylethanolamine
- N-dimethylethanolamine

- choline

choline biosynthesis I

- choline

 META CYC

TAIR
Applications: Pathways Prediction

Goal

- Universal repository of metabolic pathways
  - Up-to-date, literature-curated catalogue of commented enzymes and pathways for use in research, metabolic engineering and education

Applications

- Database of reference used to generate predicted Pathway/Genome DataBases (PGDBs)
Pathway Tools Software Suite

- Software for generating, curating, querying, displaying PGDBs

- Developed by Peter Karp and team
  - PathoLogic – Infers pathways from genome or transcripts sequencing
  - Pathway/Genome Editors – Curation interface
  - Pathway/Genome Navigator – Query, visualization, analysis and Web publishing
  - OMICS Viewer
The Family of Species-specific Databases

Annotated Genome
Arabidopsis thaliana

PathoLogic Software

Pathway/Genome Database (AraCyc)

Pathways

Reactions

Compounds

Gene products

Genes

Reference Pathway Database (MetaCyc)

tair
AraCyc
META CYC™
AraCyc:
The *Arabidopsis thaliana* specific metabolic database

http://www.arabidopsis.org/tools/aracyc

Zhang P, Foerster H, Tissier CP, Mueller L, Paley S, Karp PD, Rhee SY
*MetaCyc and AraCyc. Metabolic pathway databases for plant research*
AraCyc – Birth of the *A. thaliana* Specific Database
The Computational Build of AraCyc

- In 2004, the *Arabidopsis* genome contained 7900 genes annotated to the GO term ‘catalytic activity’.

- 4900 loci in small molecule metabolism (19% of the total genome).

- PathoLogic inferred 219 pathways and mapped 940 (19% enzyme-coding) genes to the pathways.
Cleaning of a Newborn Database

- PathoLogic errs on the side of over-prediction
- First round of curation to remove false-positives
- Add missing pathways
- Improve the quality of information
  - Introduce new pathways
  - Increase number of pathway and protein comments
  - Refine computational assignment of protein
Pathway Validation Criteria

- A pathway that is described in the *Arabidopsis* literature
- A pathway whose crucial metabolites are described in the *Arabidopsis* literature
- A pathway that contains unique reactions and having genes assigned to those unique reactions
Validation Procedure

- Delete non-plant pathways:
  - Pathway variants of bacteria-origin
  - Pathways not operating in plants at all (e.g. glycogen biosynthesis)

- Add new plant-specific pathways:
  - Pathway variants of plant-origin
  - Plant-specific metabolites (e.g. plant hormones)
  - Plant-specific metabolism (e.g. xanthophyll cycle)
## AraCyc - Curation Progress

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<th>AraCyc (2.1) April 2005</th>
<th>AraCyc (2.5) October 2005</th>
<th>AraCyc (2.6) May 2006</th>
<th>AraCyc (3.5) February 2007</th>
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<td>71 (32%)</td>
<td>170 (86%)</td>
<td>201 (88%)</td>
<td>233 (89%)</td>
<td>285 (100%)</td>
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</table>
How to Link to AraCyc

From the TAIR home page click on the link to AraCyc pathways
AraCyc – The Home Page

Paint data from high-throughput experiments on the metabolic map

Browse pathways, enzymes, genes, compounds

Display of the Arabidopsis metabolic network

User submission form
AraCyc – All the Help you Can Get

QuickTime Movies

The following movies illustrate some of the features of AraCyc described in this tutorial.

To view the movies you will need to have Quicktime installed on your computer.

Tutorial Demo: Searching and Browsing AraCyc

This Quicktime movie demonstrates how to use the simple search and browse features to query AraCyc.

Tutorial Demo: AraCyc Metabolic Map Overview

This Quicktime movie demonstrates how to browse pathways in AraCyc starting from the metabolic pathway overview diagram.

Tutorial Demo: Using the Omics Viewer

This Quicktime movie demonstrates how to use the Omics viewer to overlay gene expression data onto the pathway overview.
AraCyc’s Content

AraCyc Pathway: flavonol biosynthesis
Evidence Codes

Evidence codes provide assessment of data quality, i.e. the affirmation for the existence of an pathway.

Inferred by curator. An assertion was inferred by a curator from relevant information such as other assertions in a database.

Evidence codes provide assessment of data quality, i.e. the affirmation for the catalytic activity of an enzyme.

Intuitive icons
Evidence Codes (cont’d)

Evidence

This following evidence codes describe evidence that this protein validates this reaction or facilitates this process. For more information about Pathway Tools evidence codes and the Pathway Tools evidence ontology, click on: [Pathway Tools evidence ontology](https://www.aracyc.org/tair/tools/evidence.html)

**Experimental Evidence**

- Evidence code: D-EXP-DA-FARFRED-PROTEIN Source [Link1](https://example.com)

- Evidence code: D-EXP-DA-FARFRED-PROTEIN Source [Link2](https://example.com)

- Evidence code: D-EXP-DA-FARFRED-PROTEIN Source [Link3](https://example.com)

- Evidence code: D-EXP-DA-FARFRED-PROTEIN Source [Link4](https://example.com)

**References**

- [Kwon, S., & Kim, J. (2002). Additional evidence for the role of bacterial enzyme (E. coli)](https://example.com)
### AraCyc Pathway: flavonol biosynthesis

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<tr>
<th>Gene ID</th>
<th>Gene name</th>
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<th>Reaction EC</th>
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**Note:**

AraCyc: Metabolic Map

This section compiles a series of links which provides you with a brief history of the creation of AraCyc, information on its current data content, access to the database and ways to submit new pathways/enzyme or updates to improve AraCyc.

Search AraCyc This link allows you to search or browse the information (Pathways, Compounds, Enzymes...) contained in the AraCyc database.

Introduction You will find here all the information you need concerning the creation of AraCyc and the current status of its content. A recommended short read.

Metabolic Map The Metabolic map provides you with a 'bird's eye' view of Arabidopsis metabolism currently stored in AraCyc. (Note: This page may take a moment to load). For more info, visit the Tutorial (contains QuickTime demo).

Pathway Data Submission Form Your input is invaluable! This preformatted Excel Form allows you to send us your suggestions: pathway updates (comments, enzymes...), new pathways or even to point out mistakes.

Release Notes What's new in the latest AraCyc release? You will find it here along with comprehensive lists of pathways that have been added to and deleted from AraCyc over time.

Troubleshooting
Generation of precursor metabolites and energy > Calvin cycle

Degradation/Utilization/Assimilation > C1 compounds

Related pathways are grouped together

Compound: GA9
Reaction: GA12 + O2 + NADPH = GA9 + CO2 + NADP+

AraCyc: Metabolic Map (cont’d)
AraCyc: OmicsViewer

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Troubleshooting
OMICS Viewer

- Part of the Pathway Tools Software Suite

- Displays bird-eye view of the Metabolic Overview diagram for a single organism
  - KEGG pathways are ‘superpathways’ without consideration of species specificity and pathway variants

- Allows to paint data values from the user's high-throughput onto the Metabolic Overview diagram
  - Microarray Expression Data
  - Proteomics Data
  - Metabolomics Data
The Pathway Tools Omics Viewer (formerly the Pathway Tools Expression Viewer) paints data values from the user's high-throughput and other experiments onto the Metabolic Overview diagram for an organism.

The Omics Viewer can be used for:

- **Microarray Expression Data**: Reaction lines (and protein icons, where present) are color-coded according to the relative or absolute expression level of the gene that codes for the enzyme that catalyzes that reaction step. The Omics Viewer allows a scientist to interpret the results of gene-expression experiments in a pathway context.

- **Proteomics Data**: Reaction lines (and protein icons, where present) are color-coded and provide information about your data.

**Step 1**: Select a dataset:
- Arabidopsis thaliana CO

**Step 2**: File containing experimental data (NOT a URL):
- C:\Documents and Settings\Browse...

Do you want to display absolute or relative data values?
- Relative

**Sample data file** (text tab-delimited):

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<tr>
<th>time_point_1</th>
<th>time_point_2</th>
<th>time_point_3</th>
<th>time_point_4</th>
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<td>-1.55</td>
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<td>-0.3</td>
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</table>
The Pathway Tools Omics Viewer (formerly the Pathway Tools Expression Viewer) paints data values from the user’s high-throughput and other experiments onto the Metabolic Overview diagram for an organism.

The Omics Viewer can be used for:

- Microarray Expression Data: Reaction lines (and protein icons, where present) are color-coded according to the relative or absolute expression level of the gene that codes for the enzyme that catalyzes that reaction step. The Omics Viewer allows a scientist to interpret the results of gene-expression experiments in a pathway context.
- Proteomics Data: Reaction lines (and protein icons, where present) are color-coded according to the concentration of the enzyme that catalyzes that reaction step.
- Metabolomics Data: Compound icons

Step 3
Choose relative or absolute values
Check the box if you have log values or negative fold change numbers

Step 4
Choose to display a single or multiple step experiment

Step 5
Select the type of data you want to display (refers to your loading file)

Step 6
The items in the first (zeroth) column of your datafile are

- Genes
- Proteins
- Compounds
- Reactions
- Any of the above

Note: By selecting Any of the above, combine, for example, gene expression and metabolite names may be ambiguous if it is not known if the gene codes for a protein or metabolite. In addition, data values from different kinds of experiments may not be directly comparable.
The Omics Viewer takes as input a tab-delimited data file that is stored on your local computer. The file contains relative or absolute data for a set of genes, proteins, reactions, metabolites, or some combination. Each row of the file contains data for a single gene, protein, reaction, or metabolite, and begins with the object name, ID or EC number. You may choose to display either data from a single column, the ratio of two columns, or a time series animation of multiple columns. Data assigned to genes, proteins, reactions or metabolites can be viewed in a pathway context using the Omics Viewer.

More information about the Omics Viewer, including sample datafiles and displays.

For single/multiple or the ratio of time points add the corresponding column number(s).

To display an animated time series, enter a list of column numbers (with each column number corresponding to a single timepoint), one per line, in the first column number field below. If you wish to include a denominator column for a ratio calculation, you can enter either a single column number (in which case the same data column will be used as the denominator for all timepoints), or one column number for each numerator column number. Note that zoomed views of individual pathways are not available with animations.

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<td>0.73</td>
<td>1.05</td>
<td>1.15</td>
</tr>
</tbody>
</table>

If using two columns, denominator data column:

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3</td>
<td>4</td>
</tr>
</tbody>
</table>

Data column (numerator in ratios):

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>

Note: For column numbering purposes, the first column, which contains the gene name, is column number 0. The first potential data column is column number 1.

Step 7
OmicsViewer Submission Page (cont’d)

Choose your cutoff to visualize your expression values

Choose a color scheme:
- Full color spectrum, computed from data provided (default)
- Full color spectrum with a maximum cutoff: [ ]
- Three color display with specified threshold: [ ]

Display Type

By default, data values are painted on the cellular overview chart. However, an alternative display is to generate a table containing all individual pathways which have one or more data values that exceed some threshold (or are less than the inverse of that threshold). To select this alternative display, choose the corresponding option below and specify the threshold.
- Paint data on overview chart (default)
- Generate a table of individual pathways exceeding threshold: [ ]
- Combine both displays (not yet implemented for animations)

Submit

Note that this request will take several minutes to complete (possibly longer for large datasets).
reactions (lines) are color-coded according to the gene expression level

compounds (icons) are color-coded according to the concentration of compounds
The statistics for the expression map (single time points only) is provided at the bottom of the page.
Saving Results
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