

# PMN, A Unified Resource For Plant Metabolism

Peifen Zhang

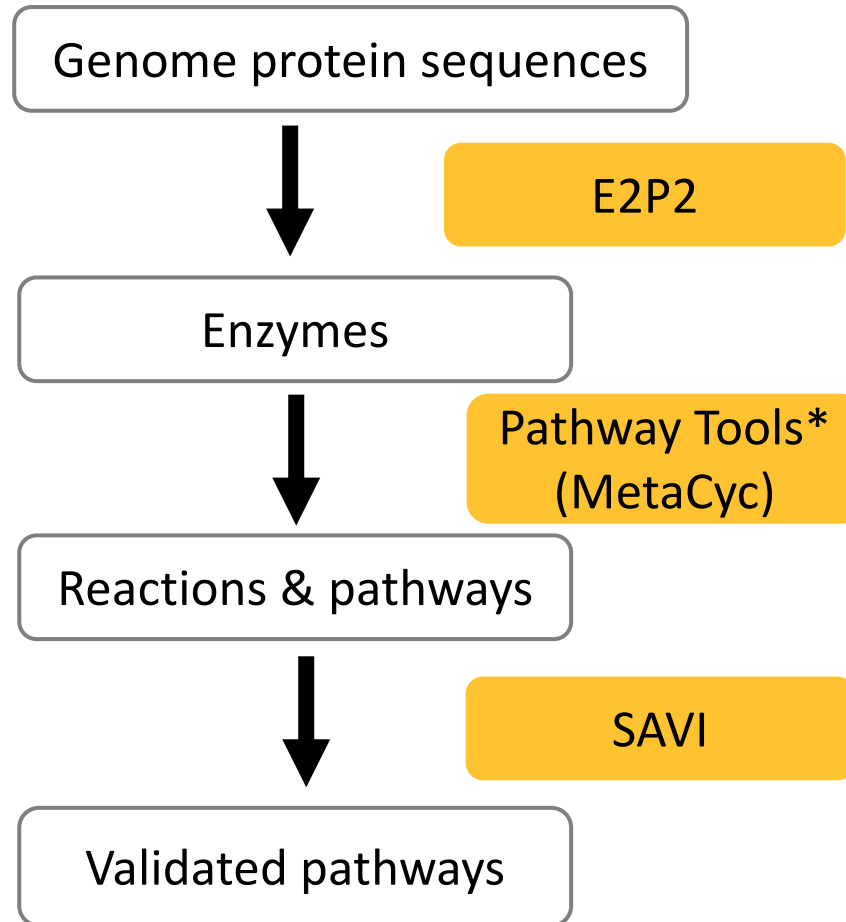
Carnegie Institution for Science

# The PMN Resources

[plantcyc.org](http://plantcyc.org)

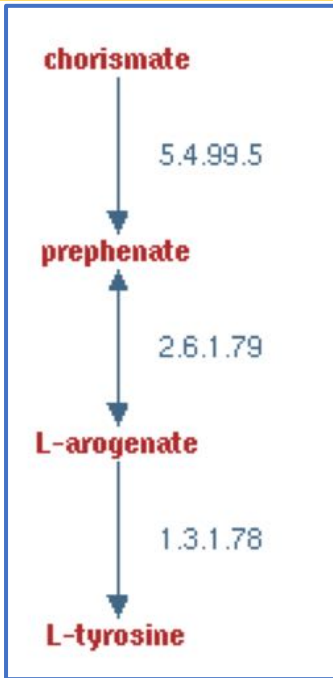
- A pipeline for high quality enzyme function prediction and metabolic pathway inference from sequenced plant genomes

# The PMN Pipeline



# Pathway Inference by Pathway Tools

A curated known pathway in the reference MetaCyc



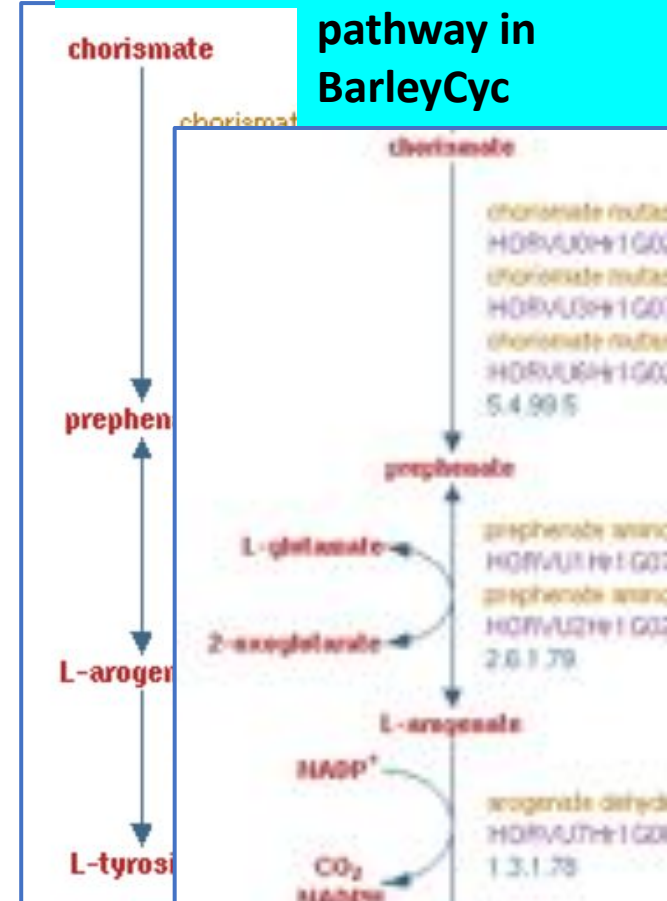
E2P2 enzyme predictions of the Spirodela genome

Gene - reaction ID  
 Gene - reaction ID  
 Gene - reaction ID  
 .....  
 .....



An inferred pathway in SpirodelaCy

An inferred pathway in BarleyCyc



# The PMN Resources

## plantcyc.org

- A pipeline for high quality enzyme function prediction and metabolic pathway inference from sequenced plant genomes
- Metabolic pathway databases inferred for **100** plant genomes



Green alga



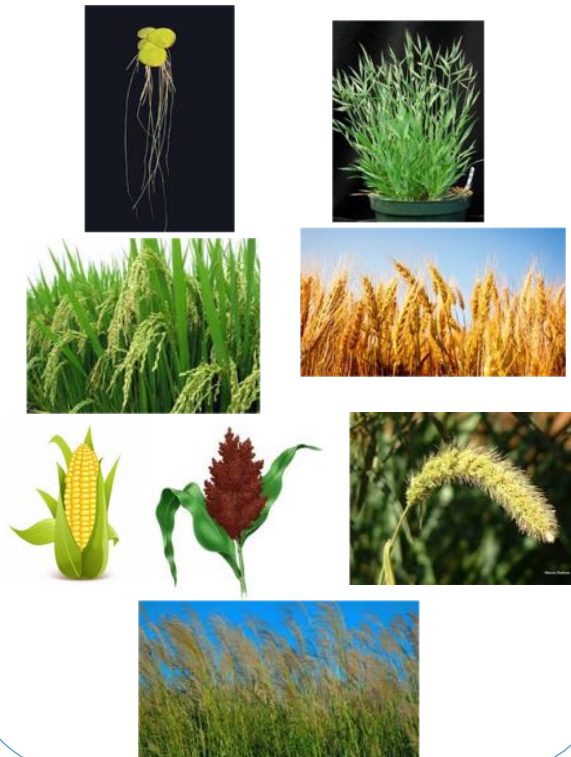
Lower land plant



Dicot



Monocot



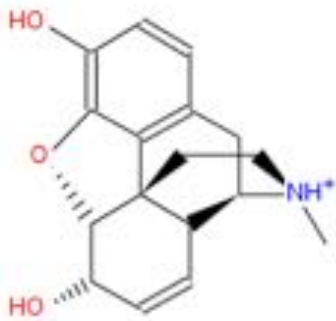
# The PMN Resources

## plantcyc.org

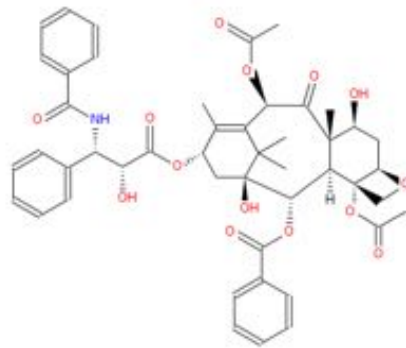
- A pipeline for high quality enzyme function prediction and metabolic pathway inference from sequenced plant genomes
- Metabolic pathway databases inferred for 100 plant genomes
- A pan-plant metabolic pathway database PlantCyc
  - Experimental information of enzymes and pathways for over 400 plant species



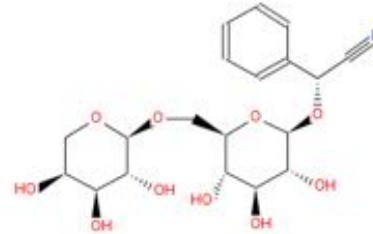
# PlantCyc



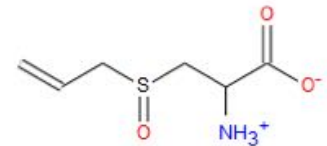
**Morphine**  
(*Papaver somniferum*)



**Taxol**  
(*Taxus brevifolia*)



**Vicianin**  
(*Vicia sativa*)



**Alliin**  
(*Allium sativum*)

# PMN use case-1: my gene

- Search for the gene
  - find reaction
    - find other genes annotated to the same reaction
  - find pathway
    - find upstream and downstream genes

Add to SmartTable

**Zea mays mays Pathway: 2'-deoxymugineic acid phytosiderophore biosynthesis**



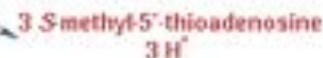
Show Predicted Enzymes More Detail Less Detail

methionine adenosyltransferase:  
Zm00001d024754  
methionine adenosyltransferase:  
Zm00001d009146  
methionine adenosyltransferase:  
Zm00001d008175  
[+ 3 isozymes]  
2.5.1.6



3 H<sub>2</sub>O  
3 ATP → 3 diphosphate  
3 phosphate

nicotianamine synthase:  
Zm00001d047558  
nicotianamine synthase:  
Zm00001d033496  
nicotianamine synthase:  
Zm00001d012829  
[+ 7 isozymes]  
2.5.1.43

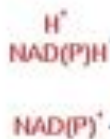


nicotianamine transferase: Zm00001d007462  
nicotianamine transferase: Zm00001d048736  
nicotianamine transferase: Zm00001d053107  
nicotianamine transferase: Zm00001d053281  
nicotianamine transferase: Zm00001d016441  
2.6.1.80



L-glutamate 2-oxoglutarate

deoxymugineic acid synthase: ZmDMAS1  
3'-deamino-3'-oxonicotianamine reductase: Zm00001d025528  
3'-deamino-3'-oxonicotianamine reductase: Zm00001d028360  
[+ 5 isozymes]  
1.1.1.285



gene  
**Zm00001d00006d**  
*Zea mays mays*

Accession IDs



Add to

Superclasses:

EC Number: 1.

Enzymes and C

- Zm00001d
- Zm00001d
- Zm00001d
- Zm00001d
- Zm00001d
- Zm00001d
- Zm00001d
- Zm00001d
- deoxymug

In Pathway: 2'





Use case-2: given a list of genes, find enrichment of pathways

[SmartTables directory](#) [SmartTables Help](#)
**SmartTable: New SmartTable - 2018-07-13T11:50:37-07:00**
[Click to add description](#)

31 rows of all-genes from AraCyc: col

Owner: Peifen Zhang, Created: 13-Jul-2018 11:50:37, Source: FILE

ADD TRANSFORM COLUMN

ADD PROPERTY COLUMN

ENRICHMENTS

1 2 Next Show all

	column 1
<input type="checkbox"/>	1 BAM3
<input type="checkbox"/>	2 AT3G51240
<input type="checkbox"/>	3 SUS1
<input type="checkbox"/>	4 AT3G30775
<input type="checkbox"/>	5 TPPG
<input type="checkbox"/>	6 FLS
<input type="checkbox"/>	7 BAM3
<input type="checkbox"/>	8 BAM3
<input type="checkbox"/>	9 AT3G55120
<input type="checkbox"/>	10 APR2
<input type="checkbox"/>	11 AT5G17330
<input type="checkbox"/>	12 TPPA
<input type="checkbox"/>	13 PAL2
<input type="checkbox"/>	APR2

**Genes enriched for pathways**

Genes enriched for pathways, transcriptional/translational regulators, and GO (all)

Genes enriched for transcriptional/translational regulators (direct and indirect)

Genes enriched for transcriptional/translational regulators (direct only)

GO terms - genes enriched for GO (biological process)

GO terms - genes enriched for GO (cellular component)

GO terms - genes enriched for GO (molecular-function)

 3 Phenylpropanoid Derivatives Biosynthesis

 4 Trehalose Biosynthesis

 5 Organic Solutes Biosynthesis

2.8146094e-6

4.5745805e-5

3.96993e-4

4.6177022e-4

4.6177022e-4

 FLS  
AT3G5  
AT3G5  
AT5G1  
4CL3

 FLS  
AT3G5  
AT3G5  
AT5G1

 AT2G2  
PAL1  
PAL2  
FLS  
4CL3  
AT3G5  
AT3G5  
AT5G1

 TPPE  
TPPG  
TPPA

 TPPE  
TPPG  
TPPA

# Overlay omics data on pathways

PMN

LOGIN | Why Login? | Cre

Enter a gene, protein, metabolite or pathway... Quick Search

Searching *Arabidopsis thaliana col* change organism database

Home Databases Search Metabolites Analysis SmartTables Help

Cellular Overview / Omics Viewer

Run Metabolic Model

Dead-end Metabolites

Checkpoint Reactions

Metabolic Route Search

Authors: Bo Xue<sup>1</sup>, Pascal Schlappe

<sup>1</sup>Carnegie Institution for Science

Library of *Arabidopsis thaliana*, Strain col, version 16.0

Cellular Overview of *Arabidopsis thaliana col*

For left/right/up/down the entire diagram by holding the left mouse button, click on an object for more info, right-click (ctrl-click for Mac) for menu

Base Layer

Cellular Overview

OPERATIONS

Overlay Experimental Data (Omics Viewer) \*

- Upload Data from File
- Enter/Paste Data from Keyboard
- Import Data from PubLine
- Import Data from GEO

Omics Viewer Control Panel

Control Opacity of Overview

Preferences Remove Omics Data Turn into Group \*

Omics data is overlaid on the metabolic pathway diagram, with a color scale ranging from -8.180 (purple) to +8.180 (red). The scale includes values: +8.180, +6.360, +4.540, +2.720, +0.900, -0.900, -2.720, -4.540, -6.360, -8.180.

# Virtual data integration in PlantCyc





Add to SmartTable

### PlantCyc Pathway: ethylene biosynthesis I (plants)

More Detail Less Detail



PlantCyc

hide

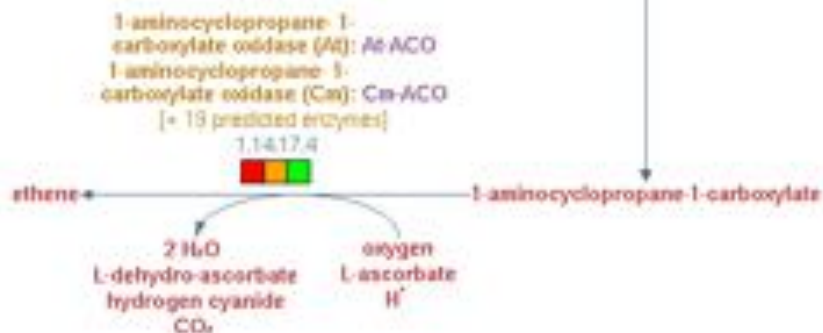
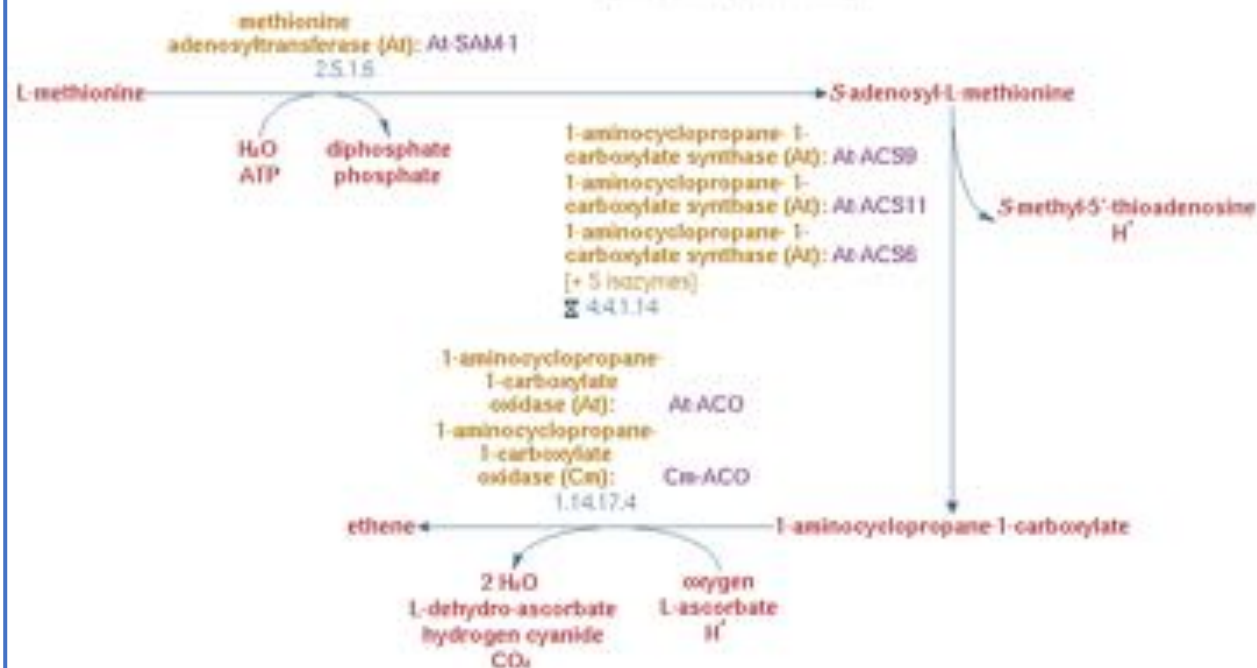
Pathway:  
ethylene biosynthesis I (plants)

#### OPERATIONS

- Customize or Overlay Omics Data on Pathway Diagram
- Generate Pathway Collage
- Download Genes
- BioPax Level 2
- BioPax Level 3
- Select Organisms to Include in Pathway Diagram

#### Comparison Operations

- Show this pathway in another database
- Change organisms/databases for comparison operations
- Search for this pathway in other databases
- Species Comparison



This view shows enzymes only for those organisms listed below, in either the list of selected organisms or the list of taxa known to possess the pathway. If an enzyme name is shown in bold, there is experimental evidence for this enzymatic activity.

Selected Organisms (an organism name in bold means that the pathway is predicted to occur in that organism): *Arabidopsis thaliana* col *Chlamydomonas reinhardtii* *Physcomitrella patens*

# Comparative analysis

Home Databases Search Metabolism Analysis SmartTables Help

Comparative Analysis  
Omics Data Analysis  
Omics Dashboard  
Reports

*Hordeum vulgare* hydroxylated mugineic acid phytosiderophore biosynthesis

Hide Predicted Enzymes More Detail Less Detail

2'-deoxymugineic acid phytosiderophore biosynthesis

2'-deoxymugineate

oxygen 2-oxoglutarate  
CO<sub>2</sub> succinate H<sup>+</sup>

mugineic acid synthase: *Ids3*  
[+ 10 predicted enzymes]  
1.14.11.24

mugineate

oxygen 2-oxoglutarate  
succinate CO<sub>2</sub> H<sup>+</sup>

2'-deoxymugineic acid,2-oxoglutarate:oxygen oxidoreductase (3-hydroxylating): *ids2*  
[+ 1 predicted enzyme]  
1.14.11.25

3-epihydroxy 2'-deoxymugineate

oxygen 2-oxoglutarate


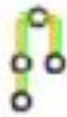




mugineic acid 3-dioxygenase: *ids2*  
mugineic acid,2-

**OPERATIONS**

- Show on Cellular Overview
- Customize or Overlay Omics Data on Pathway Diagram
- Generate Pathway Collage
- Download Genes
- BioPax Level 2
- BioPax Level 3

**Comparison Operations**

- Show this pathway in another database
- Change organism/databases for comparison operations
- Search for this pathway in other databases
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Organism	Evidence Glyph	Enzymes and Genes for hydroxylated mugineic acid phytosiderophore biosynthesis						
AraCyc col		This pathway is not marked as present in this organism. No enzymes or genes have been identified for this pathway						
H. vulgare		<table border="1"> <tr> <td>EC 1.14.11.24</td> <td>mugineic acid synthase: ids3 MLOC_33486.1: MLOC_33486.1 MLOC_80402.1: MLOC_80402.1 MLOC_17126.1: MLOC_17126.1 MLOC_76208.1: MLOC_76208.1 MLOC_48351.2: MLOC_48351.2 MLOC_1079.1: MLOC_1079.1 MLOC_19745.1: MLOC_19745.1</td> </tr> <tr> <td>EC 1.14.11.25</td> <td>mugineic-acid 3-dioxygenase: ids2</td> </tr> <tr> <td>EC 1.14.11.25</td> <td>mugineic-acid 3-dioxygenase: ids-2 mugineic-acid 3-dioxygenase: ids2</td> </tr> </table>	EC 1.14.11.24	mugineic acid synthase: ids3 MLOC_33486.1: MLOC_33486.1 MLOC_80402.1: MLOC_80402.1 MLOC_17126.1: MLOC_17126.1 MLOC_76208.1: MLOC_76208.1 MLOC_48351.2: MLOC_48351.2 MLOC_1079.1: MLOC_1079.1 MLOC_19745.1: MLOC_19745.1	EC 1.14.11.25	mugineic-acid 3-dioxygenase: ids2	EC 1.14.11.25	mugineic-acid 3-dioxygenase: ids-2 mugineic-acid 3-dioxygenase: ids2
EC 1.14.11.24	mugineic acid synthase: ids3 MLOC_33486.1: MLOC_33486.1 MLOC_80402.1: MLOC_80402.1 MLOC_17126.1: MLOC_17126.1 MLOC_76208.1: MLOC_76208.1 MLOC_48351.2: MLOC_48351.2 MLOC_1079.1: MLOC_1079.1 MLOC_19745.1: MLOC_19745.1							
EC 1.14.11.25	mugineic-acid 3-dioxygenase: ids2							
EC 1.14.11.25	mugineic-acid 3-dioxygenase: ids-2 mugineic-acid 3-dioxygenase: ids2							
O. sativa Japonica Group		<table border="1"> <tr> <td>EC 1.14.11.24</td> <td>LOC_Os07g07410.1: LOC_Os07g07410.1</td> </tr> <tr> <td>EC 1.14.11.25</td> <td>None</td> </tr> <tr> <td>EC 1.14.11.25</td> <td>None</td> </tr> </table>	EC 1.14.11.24	LOC_Os07g07410.1: LOC_Os07g07410.1	EC 1.14.11.25	None	EC 1.14.11.25	None
EC 1.14.11.24	LOC_Os07g07410.1: LOC_Os07g07410.1							
EC 1.14.11.25	None							
EC 1.14.11.25	None							
P. patens		This pathway is not marked as present in this organism. No enzymes or genes have been identified for this pathway						
S. bicolor		<table border="1"> <tr> <td>EC 1.14.11.24</td> <td>Sobic.008G109700.1.p: Sobic.008G109700.1.p Sobic.008G109400.1.p: Sobic.008G109400.1.p Sobic.002G046400.1.p: Sobic.002G046400.1.p Sobic.008G109300.1.p: Sobic.008G109300.1.p Sobic.004G348400.1.p: Sobic.004G348400.1.p Sobic.008G109600.1.p: Sobic.008G109600.1.p</td> </tr> <tr> <td>EC 1.14.11.25</td> <td>None</td> </tr> <tr> <td>EC 1.14.11.25</td> <td>None</td> </tr> </table>	EC 1.14.11.24	Sobic.008G109700.1.p: Sobic.008G109700.1.p Sobic.008G109400.1.p: Sobic.008G109400.1.p Sobic.002G046400.1.p: Sobic.002G046400.1.p Sobic.008G109300.1.p: Sobic.008G109300.1.p Sobic.004G348400.1.p: Sobic.004G348400.1.p Sobic.008G109600.1.p: Sobic.008G109600.1.p	EC 1.14.11.25	None	EC 1.14.11.25	None
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EC 1.14.11.25	None							
EC 1.14.11.25	None							
Z. mays mays		<table border="1"> <tr> <td>EC 1.14.11.24</td> <td>GRMZM2G110369_P01: GRMZM2G110369_P01 GRMZM2G146234_P01: GRMZM2G146234_P01 GRMZM2G086231_P01: GRMZM2G086231_P01</td> </tr> <tr> <td>EC 1.14.11.25</td> <td>None</td> </tr> <tr> <td>EC 1.14.11.25</td> <td>None</td> </tr> </table>	EC 1.14.11.24	GRMZM2G110369_P01: GRMZM2G110369_P01 GRMZM2G146234_P01: GRMZM2G146234_P01 GRMZM2G086231_P01: GRMZM2G086231_P01	EC 1.14.11.25	None	EC 1.14.11.25	None
EC 1.14.11.24	GRMZM2G110369_P01: GRMZM2G110369_P01 GRMZM2G146234_P01: GRMZM2G146234_P01 GRMZM2G086231_P01: GRMZM2G086231_P01							
EC 1.14.11.25	None							
EC 1.14.11.25	None							

# Future Development

- Further enhance accuracy of enzyme function predictions
- Annotate transporters and subcellular location of reactions
- Develop genome-scale metabolic models
- Provide online database creation service
- Provide web app for integrated view of metabolism with other information such as gene expression

# Team and Funding Sources

- Sue Rhee (PI)
- Pascal Schlöpfer (Postdoc)
- Jiun Yen (Postdoc)
- Bo Xue (Research Assistant)
- Angela Xu (Research Assistant)
- Kevin Radja (Research Assistant)
- Galyna Vakulenko (Intern)
- Garret Huntress (IT support)
  
- Peter Karp (Collaborator)

