PMN
Plant Metabolic Network

# PMN, A Unified Resource For Plant Metabolism

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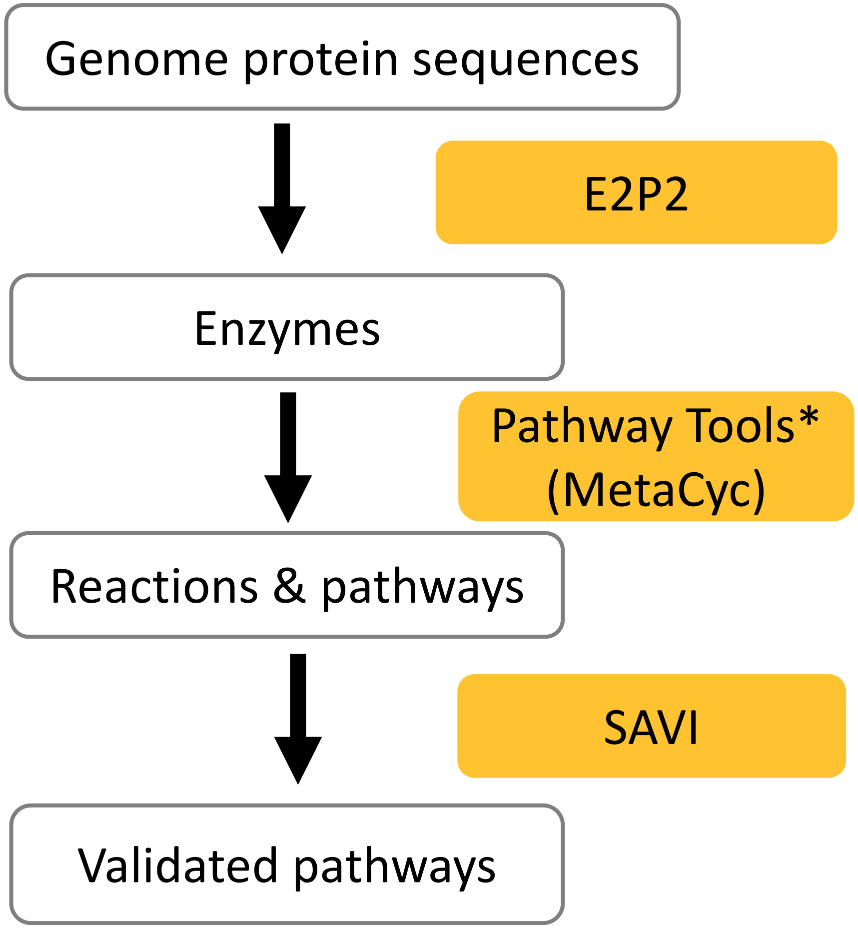
# The PMN Resources
# plantcyc.org

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

# The PMN Pipeline



Genome protein sequences

E2P2

Enzymes

Pathway Tools*
(MetaCyc)

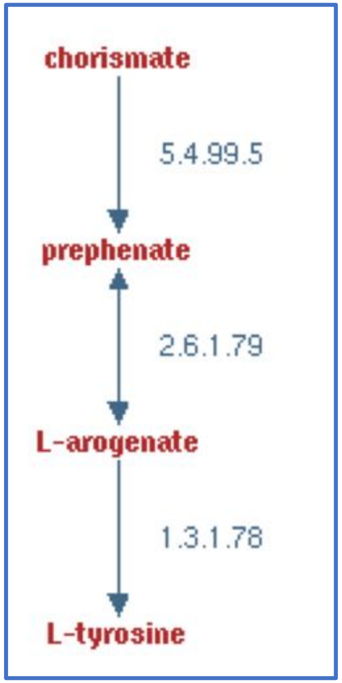
Reactions & pathways

SAVI

Validated pathways

# Pathway Inference by Pathway Tools

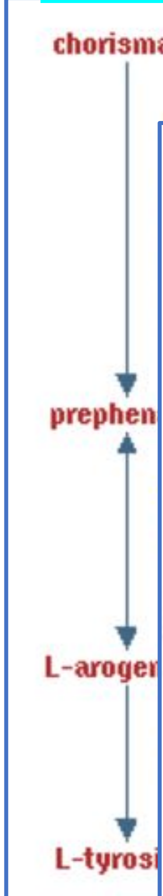
A curated known pathway in the reference MetaCyc



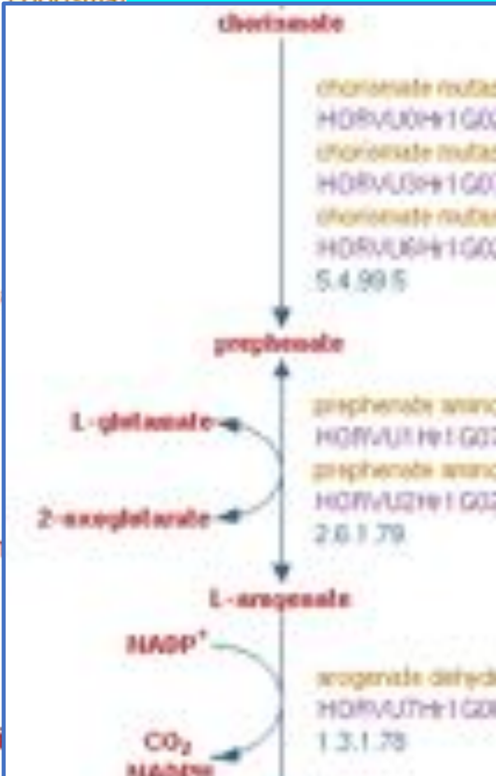
E2P2 enzyme predictions of the Spirodela genome

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

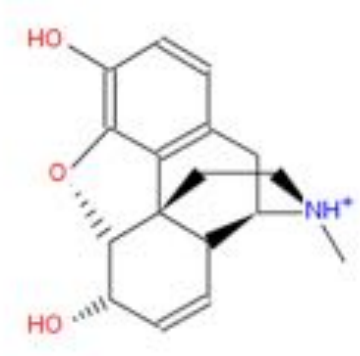
# The PMN Resources
plantcyc.org

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

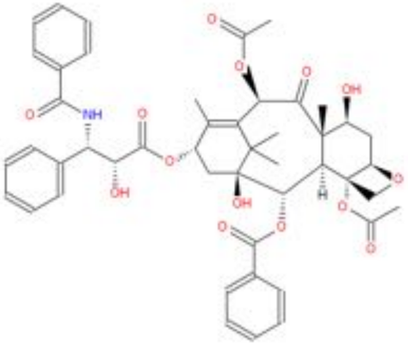
- Metabolic pathway databases inferred for 100 plant genomes

- A pan-plant metabolic pathway database PlantCyc
  - Experimental information of enzymes and pathways for over 400 plant species

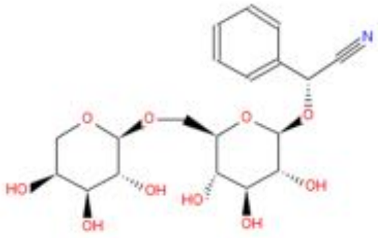
# PlantCyc



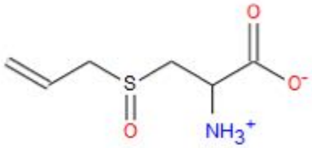
Morphine
(*Papaver somniferum*)



Taxol
(*Taxus brevifolia*)



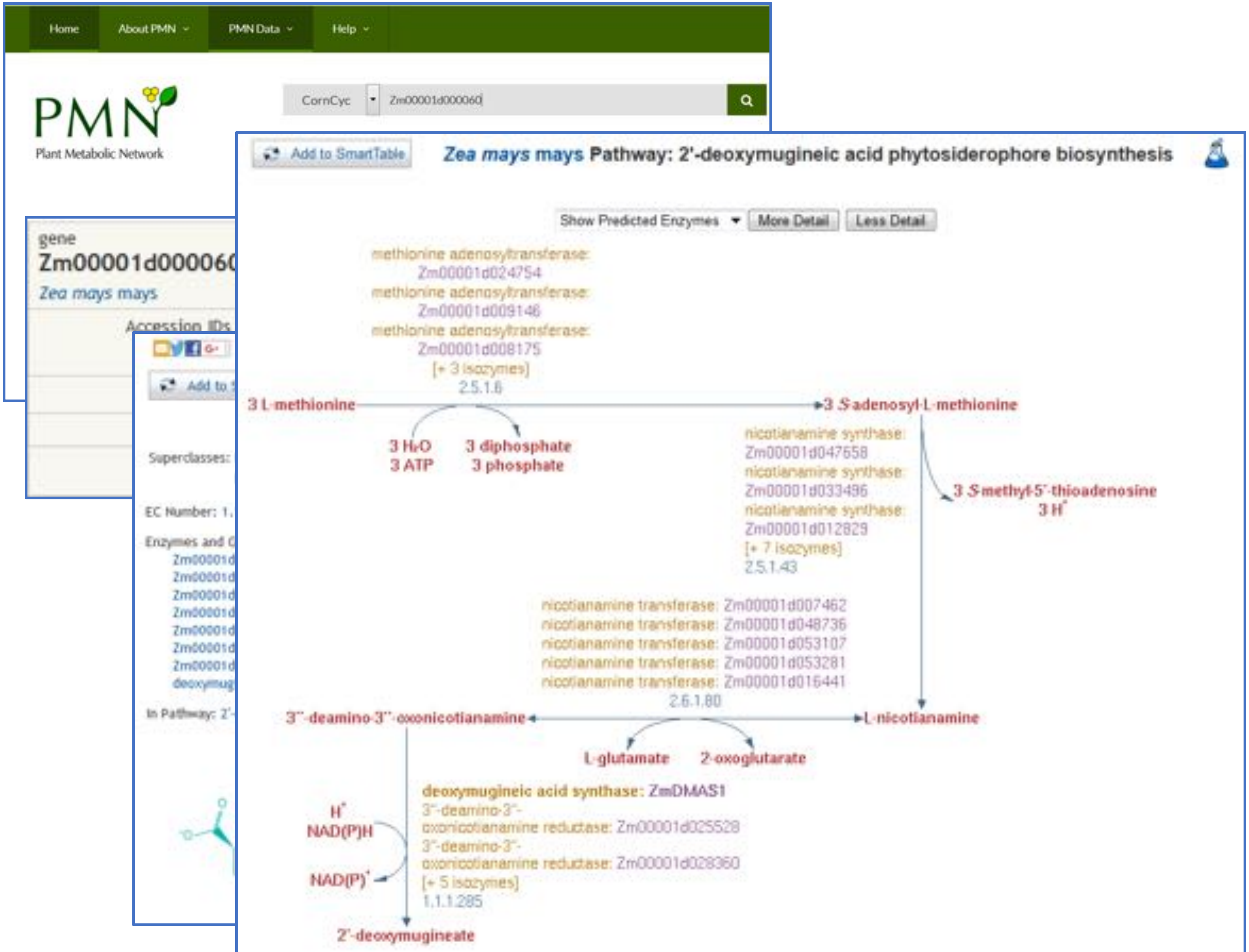
Vicianin
(*Vicia sativa*)



Alliin
(*Allium sativum*)

# PMN use case-1: my gene

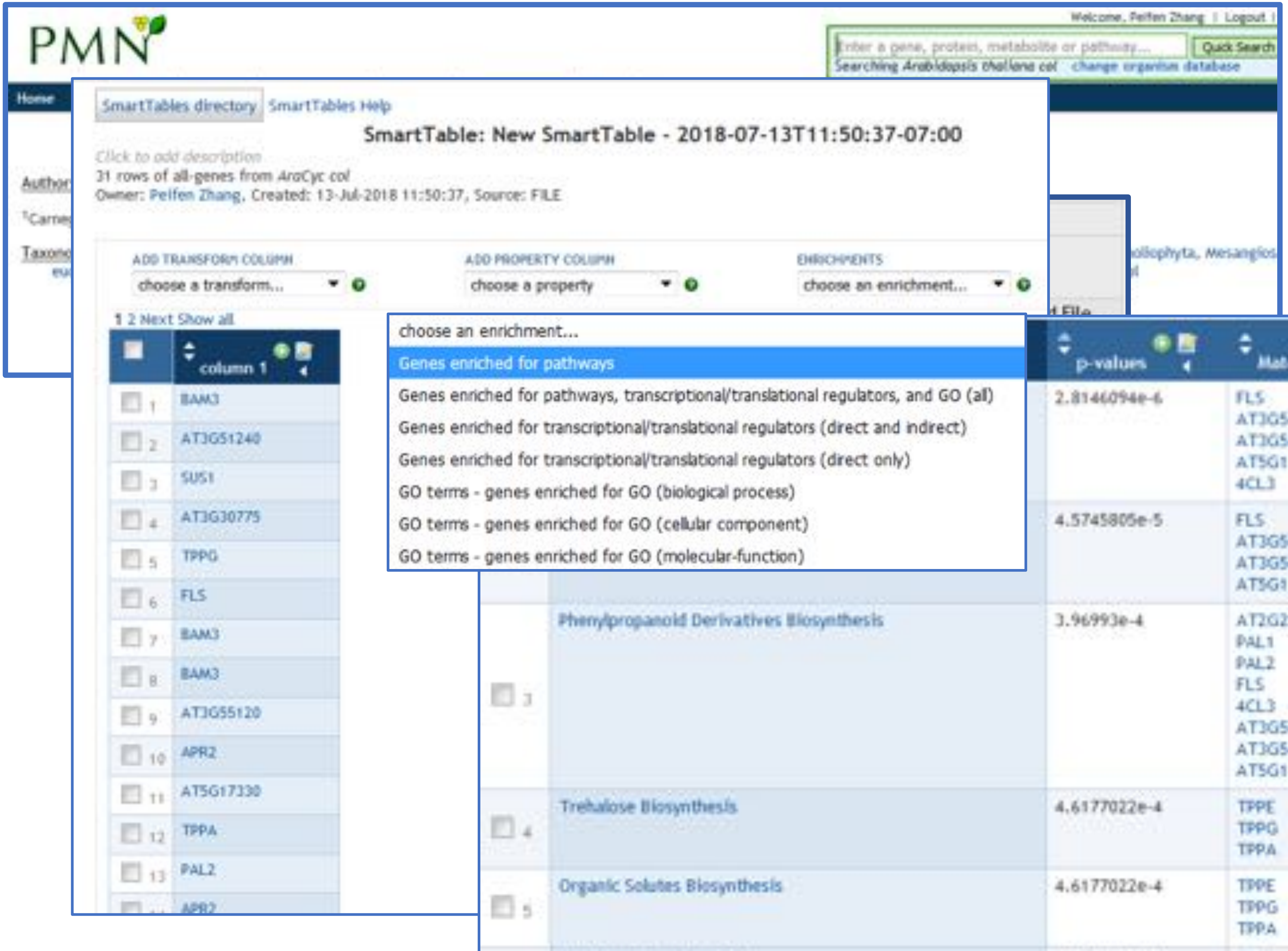
- Search for the gene
  - find reaction
    - find other genes annotated to the same reaction
  - find pathway
    - find upstream and downstream genes



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

gene
Zm00001d00006
*Zea mays mays*
Accession IDs

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



SmartTable: New SmartTable - 2018-07-13T11:50:37-07:00

Click to add description

31 rows of all-genes from AraCyc col

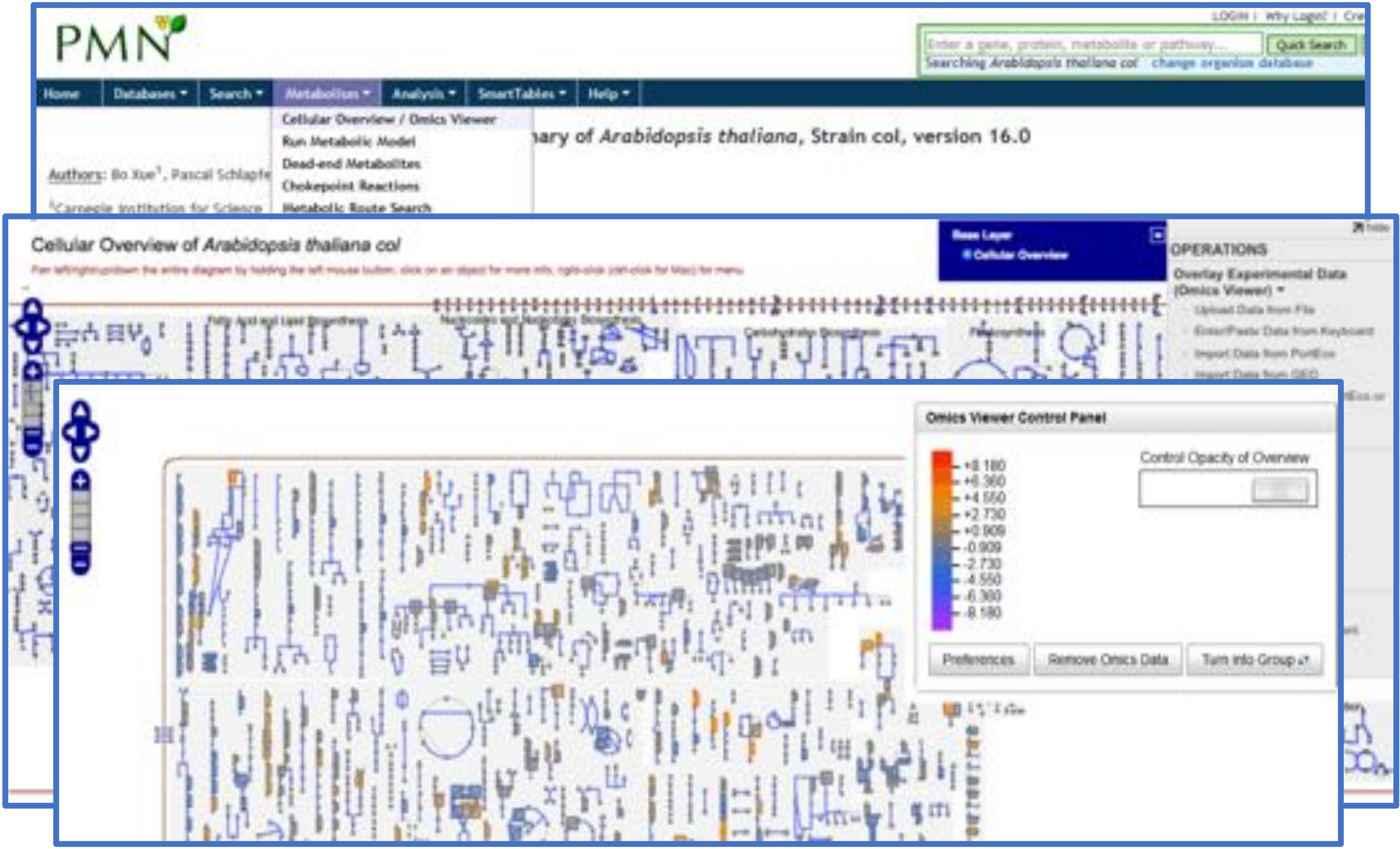
Owner: Peifen Zhang, Created: 13-Jul-2018 11:50:37, Source: FILE

| | column 1 |
|---|---|
| ☐ 1 | BAM3 |
| ☐ 2 | AT3G51240 |
| ☐ 3 | SUS1 |
| ☐ 4 | AT3G30775 |
| ☐ 5 | TPPG |
| ☐ 6 | FLS |
| ☐ 7 | BAM3 |
| ☐ 8 | BAM3 |
| ☐ 9 | AT3G55120 |
| ☐ 10 | APR2 |
| ☐ 11 | AT5G17330 |
| ☐ 12 | TPPA |
| ☐ 13 | PAL2 |
| ☐ | APR2 |

choose an enrichment...
- 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)

| | | p-values | Mat |
|---|---|---|---|
| | | 2.8146094e-6 | FLS<br>AT3G5<br>AT3G5<br>AT5G1<br>4CL3 |
| | | 4.5745805e-5 | FLS<br>AT3G5<br>AT3G5<br>AT5G1 |
| ☐ 3 | Phenylpropanoid Derivatives Biosynthesis | 3.96993e-4 | AT2G2<br>PAL1<br>PAL2<br>FLS<br>4CL3<br>AT3G5<br>AT3G5<br>AT5G1 |
| ☐ 4 | Trehalose Biosynthesis | 4.6177022e-4 | TPPE<br>TPPG<br>TPPA |
| ☐ 5 | Organic Solutes Biosynthesis | 4.6177022e-4 | TPPE<br>TPPG<br>TPPA |

# Overlay omics data on pathways



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

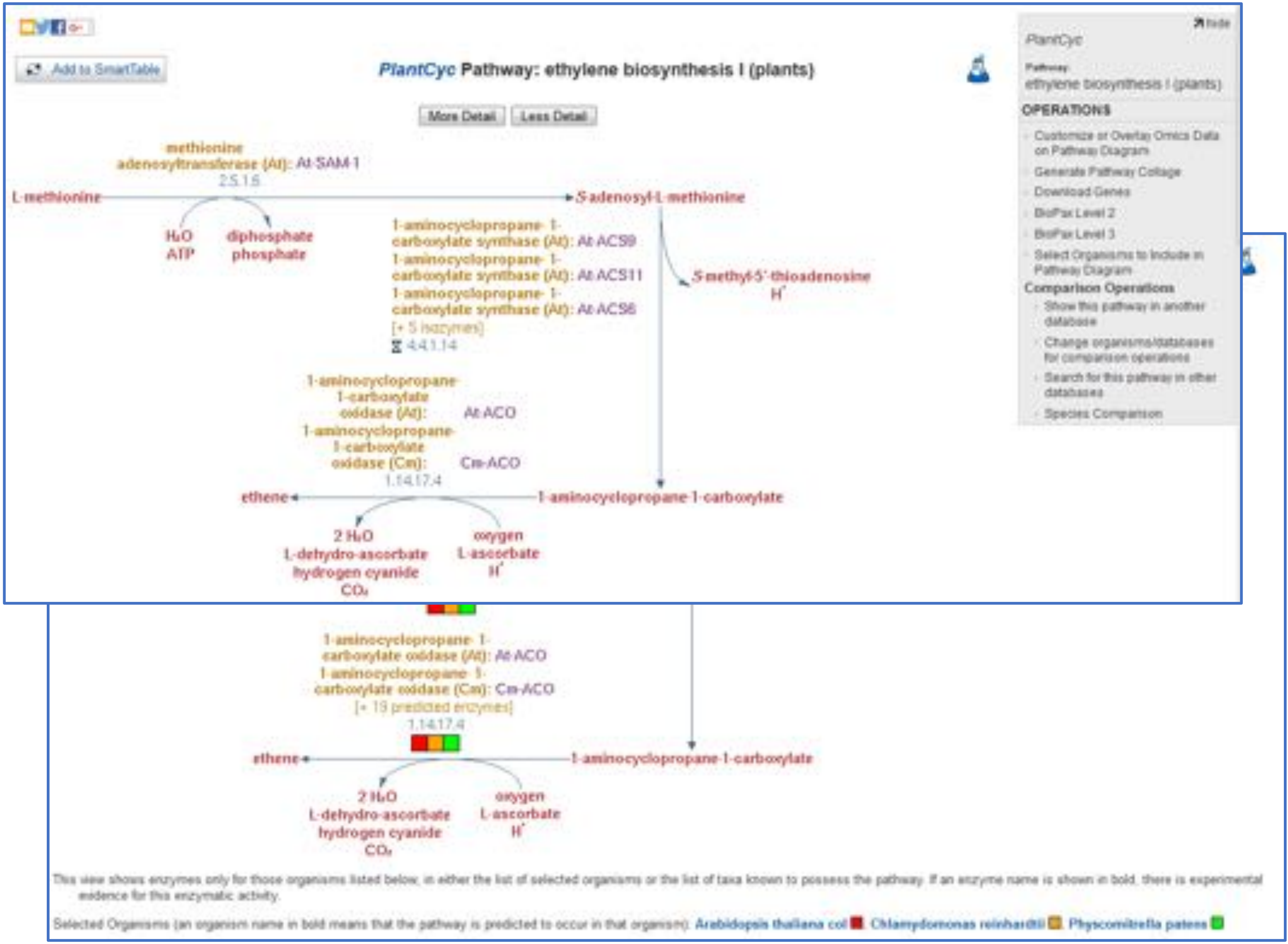
Authors: Bo Xue[1], Pascal Schlapfe

[1]Carnegie Institution for Science

Cellular Overview of *Arabidopsis thaliana col*

Pan 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

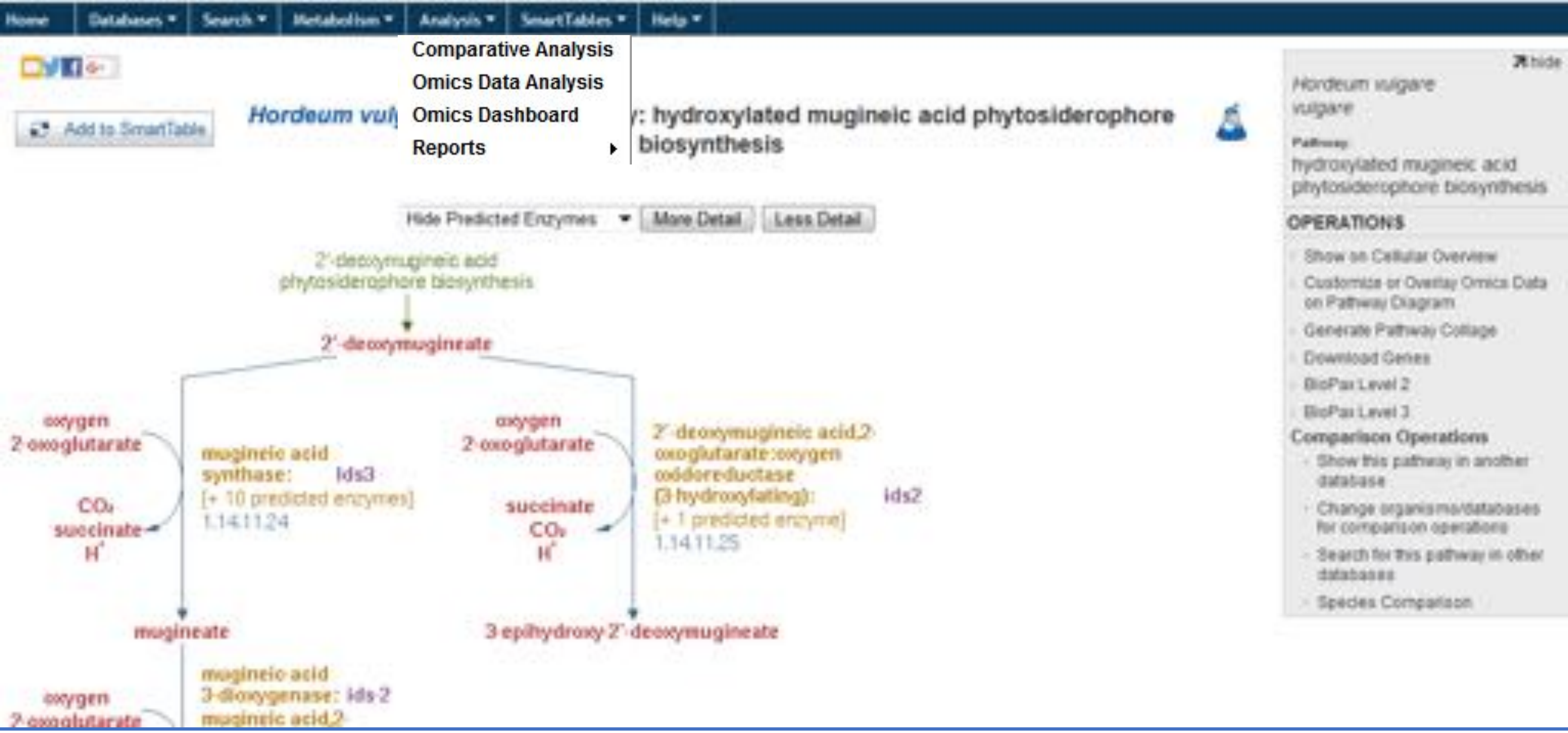
# Virtual data integration in PlantCyc

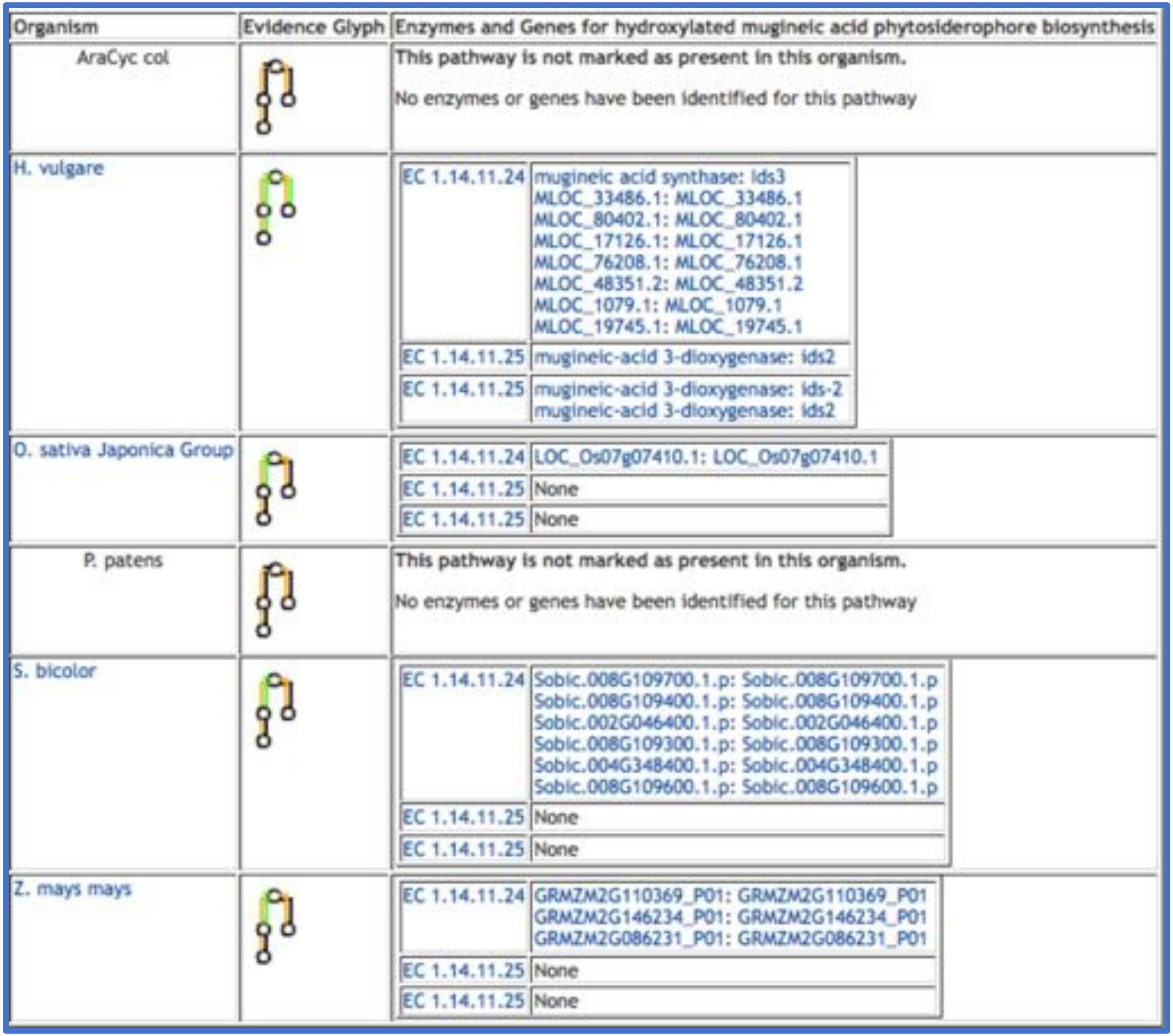


This view shows enzymes only for those organisms listed below, in either the list of selected organisms or the list of taxa known to possess the pathway. If an enzyme name is shown in bold, there is experimental evidence for this enzymatic activity.

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





| Organism | Evidence Glyph | Enzymes and Genes for hydroxylated mugineic acid phytosiderophore biosynthesis | |
|---|---|---|---|
| AraCyc col | | This pathway is not marked as present in this organism.<br>No enzymes or genes have been identified for this pathway | |
| H. vulgare | | EC 1.14.11.24 | mugineic acid synthase: ids3<br>MLOC_33486.1: MLOC_33486.1<br>MLOC_80402.1: MLOC_80402.1<br>MLOC_17126.1: MLOC_17126.1<br>MLOC_76208.1: MLOC_76208.1<br>MLOC_48351.2: MLOC_48351.2<br>MLOC_1079.1: MLOC_1079.1<br>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<br>mugineic-acid 3-dioxygenase: ids2 |
| O. sativa Japonica Group | | 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.<br>No enzymes or genes have been identified for this pathway | |
| S. bicolor | | EC 1.14.11.24 | Sobic.008G109700.1.p: Sobic.008G109700.1.p<br>Sobic.008G109400.1.p: Sobic.008G109400.1.p<br>Sobic.002G046400.1.p: Sobic.002G046400.1.p<br>Sobic.008G109300.1.p: Sobic.008G109300.1.p<br>Sobic.004G348400.1.p: Sobic.004G348400.1.p<br>Sobic.008G109600.1.p: Sobic.008G109600.1.p |
| | | EC 1.14.11.25 | None |
| | | EC 1.14.11.25 | None |
| Z. mays mays | | EC 1.14.11.24 | GRMZM2G110369_P01: GRMZM2G110369_P01<br>GRMZM2G146234_P01: GRMZM2G146234_P01<br>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 Schläpfer (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)

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