# CARNEGIE SCIENCE

Department of Plant Biology















### Putting the PMN (and TAIR) to work for you:

# Tips and Techniques for Accessing Data for Plant Biology Research

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### **Overview**

- Introduction to the PMN
- Accessing data in the PMN
- Case study: Putting the PMN and TAIR to work for you

### Welcome to the PMN

- The Plant Metabolic Network (PMN) maintains a set of metabolic pathway databases for Arabidopsis and other plants (AraCyc, PlantCyc, etc.)
- www.plantcyc.org



- Curators and programmers at the PMN:
  - Collect and store metabolic pathway information
  - Provide tools to analyze data
  - Work to generate new metabolic pathway databases for crops and other important plants

### **PMN** databases

- Current PMN databases: PlantCyc, AraCyc, PoplarCyc
  - Coming soon: databases for wine grape, maize, cassava, Selaginella, and more . . .
- Other plant databases accessible from the PMN:

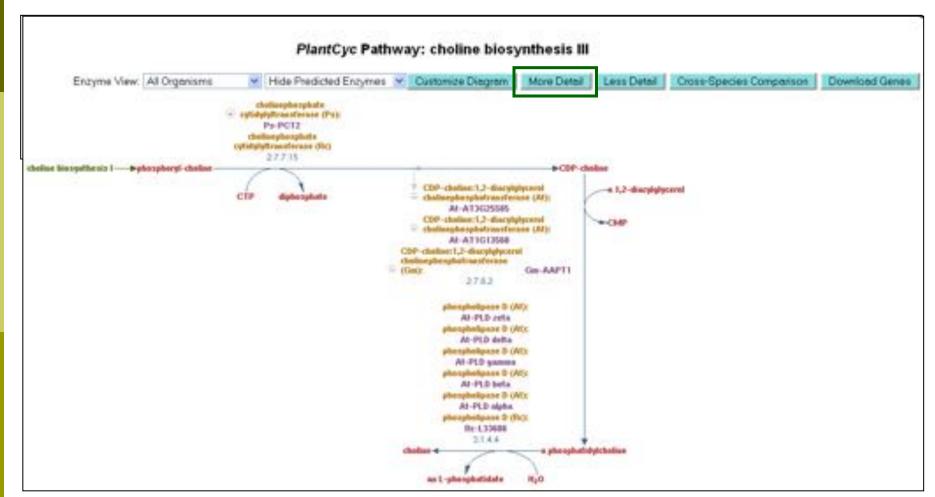
PGDB	Plant	Source	Status
RiceCyc **	Rice	Gramene	some curation
SorghumCyc	Sorghum	Gramene	no curation
MedicCyc **	Medicago	Noble Foundation	some curation
LycoCyc **	Tomato	Sol Genomics Network	some curation
PotatoCyc	Potato	Sol Genomics Network	no curation
СарСус	Pepper	Sol Genomics Network	no curation
NicotianaCyc	Tobacco	Sol Genomics Network	no curation
PetuniaCyc	Petunia	Sol Genomics Network	no curation
CoffeaCyc	Coffee	Sol Genomics Network	no curation

<sup>\*\*</sup> Significant numbers of genes from these databases have been integrated into PlantCyc

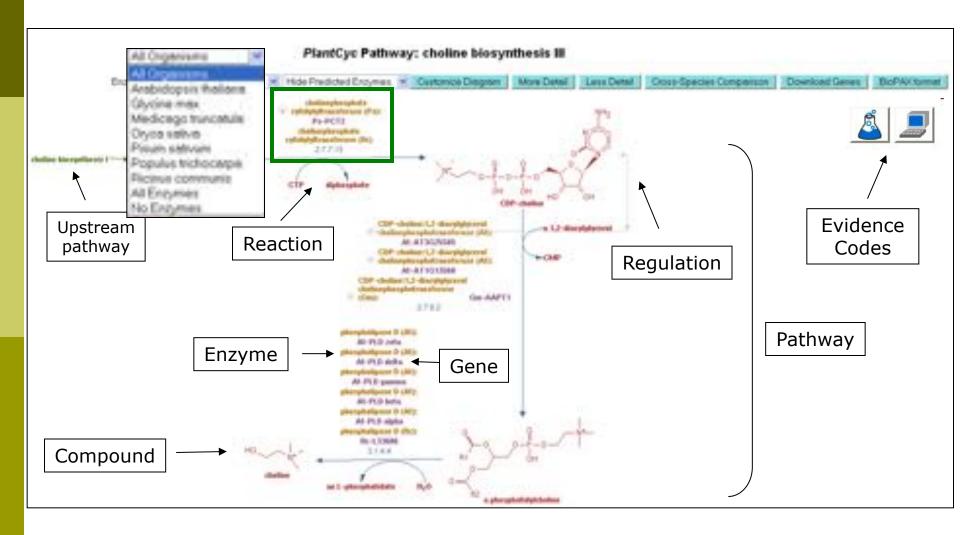
### **PMN** database content statistics

	PlantCyc 4.0
Pathways	685
Enzymes	11058
Reactions	2929
Compounds	2966
Organisms	343

#### Species (A - D) (back to top) Ables grands (yellow fir, white fir, silver fir, lowland fir, grand fir). Aper poeudoplatanus Adono sestivale. Adonio annua (pheasants-eye, blood-drops) Ajuga reptans. Albigia julibrissini Alectoria Alliaceae (onion family). Allium pepe Allium salvum Allium Suberosum Alor arbonescent Amanita muscana Acomi maud Amorpha fluticosa Anabaena variabiliti Anchose officinalis Anreodue ácutangulue Antiminum majus (snapdragon) Apium graveowns Aquitegia vulgaria. Anabidopore lyvalla (furalle rockcress) Arabidopsis thaliana, Col (thate cress, mouse-ear cress) Arabidojos tharlana, Lar (thate oress, mouse-ear cress): Arachie rupogaea Arteminia annua (sweet Annie): Aschovas syriaca Altopa periadonna (deadly mgMshadk) Arena sative (outbraked out) Berbera beamana Serberis stolonitory Berberts Wilsoniae



- Better . . . but what about compound structures?
  - Keep clicking on "More Detail" sometimes several times



Superclasses Biosynthesis -> Fatty Acids and Lipids Biosynthesis -> Choline Biosynthesis

Species Data Available for Avabidossis thaliana col., Glycine max., Medicago truncatula., Oryza sativa Japonica Group., Pisum sativum., Populus trichocarpa., Ricinus communis

#### Summary:

General information: Choline is a fundamental metabolite in plants because of its contribution to the synthesis of the membrane phospholipid phosphatidylcholine, which accounts for 40 to 60% of lipids in non-plastid plant membranes [ Mou02 ]. Choline is also a precursor for the formation of glycine betaine ( glycine betaine biosynthesis ) in cettain plants such as spinach, where this componentant is accumulated and confers also tolerance to salinity, drought, and other environmental stresses. In addition choline has been recognized as an essential nutrient for humans [ McNeiD1 ]

The chaline biosynthetic pathway enables plants to decouple chaline synthesis from lipid metabolism (Kennedy pathway - triacyfglycerol biosynthesis ) and provides them with the metabolic flexibility to adapt to environmental conditions where large and variable amounts of choline are beneficial for survival [ Rontein01 ]

Pathway information. The first step in choline biosynthesis is the direct decarboxylation of serine to ethanolamine [ Romain01 ], which is catalyzed by a serine decarboxylase unique to plants | Rontein03 | Ethanolamine is widely recognized as the entrance compound to choline biosynthesis

#### References

Curater(9): Curator (2009): "Following the initial computational build of PoplarCyc in 2009, pathways were validated by PMN curators based on a preliminary literature search. For pathways that lacked direct experimental support, curators considered a number of factors to judge the validity of the predicted pathways including. To critical compound(s) in the pathway are found in a Populus species; 2) a Populus trichocarpa gene is predicted to catalyze a critical or unique reaction of the pathway, or 39 the pathway is expected to exist in all plants."

Datke88: Datko AH, Mudd SH. (1988) "Enzymes of phosphatidylcholine synthesis in Lemna, soybean, and carrot," Plant Physiol. (1988), 88, 1338-1348.

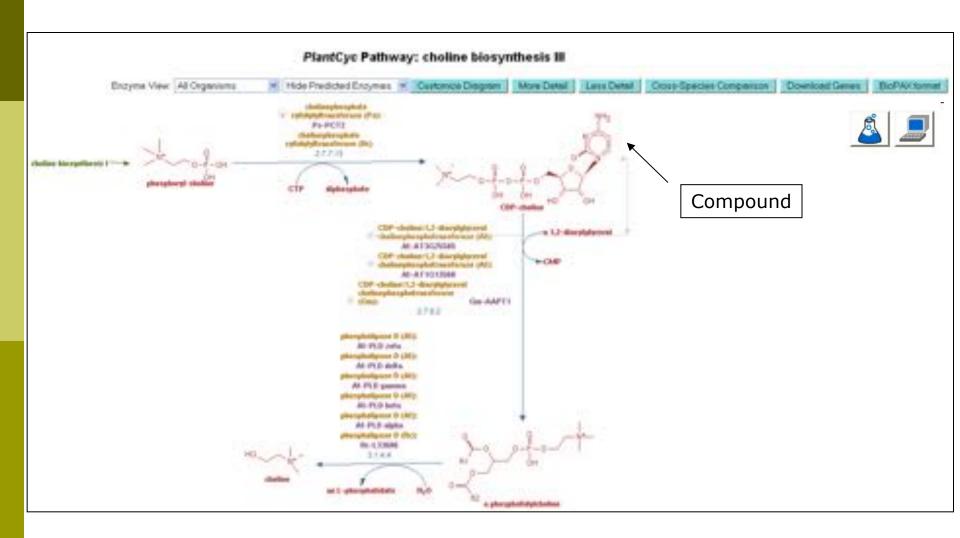
Datko88a: Datko AH, Mudd SH, (1988) "Phosphatidylcholine synthesis. Differing patterns in solybean and carrot." Plant Physiol. (1988), 88, 854-861.

Hitz81: Hitz WD, Rhodes D, Hanson AD, (1981) "Radiotracer evidence implicating phosphory) and phosphatidy! bases as intermediates in betaine synthesis by waterstressed barley leaves." Plant Physiol. (1981), 68, 814-822.

Kinney93: Kinney AJ. (1993) "Phospholipid head groups." In: Moore, TS Jr. (ed.) Lipid metabolism in plants. CRC Press Boca Raton Ann Arbor London Tokyo (1993). 259-284

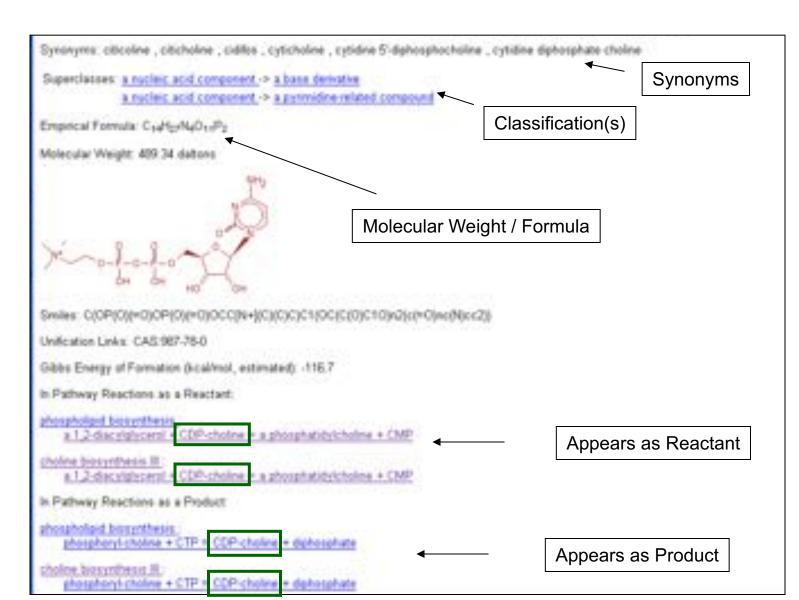
Kirk99: Kirk Pappan, Xuemin Wang "Molecular and biochemical properties and physiological roles of plant phospholigase 0." Biochimica Biophysica Acta (1999) 1439. 151-166

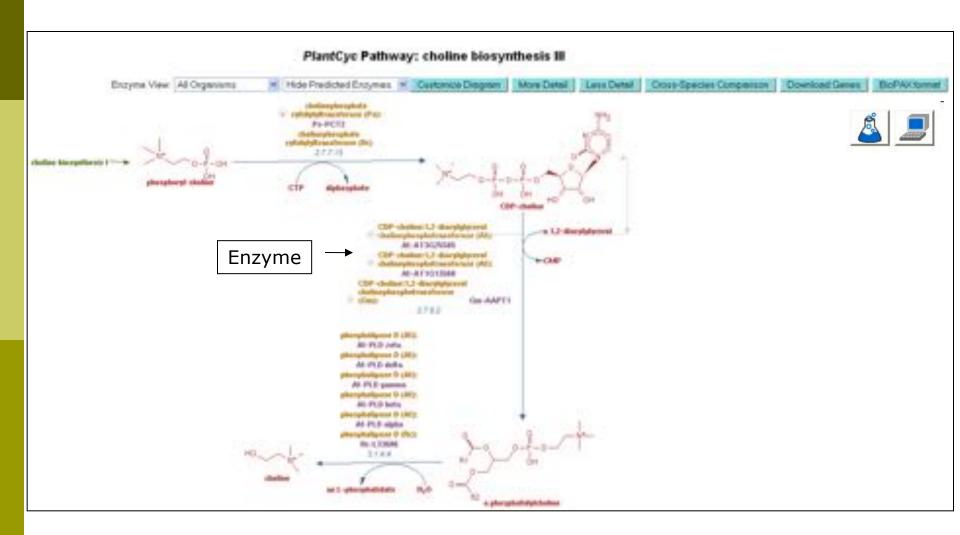
McNeill00: McNeil SD, Nuccio ML, Rhodes D, Shachar-Hill Y, Hanson AD (2000). "Radiotracer and computer modeling evidence that phospho-base methylation is the main route of choline synthesis in tobacco." Plant Physiol 123(1):371-80. PMD: 10806254



### **PMN** compound pages

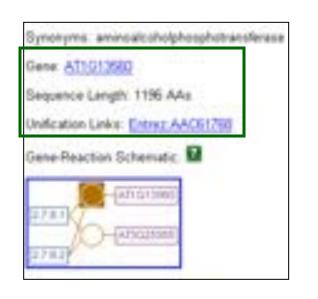
## Compound: CDP-choline





### **PMN** enzyme pages

#### Arabidopsis Enzyme: phosphatidyltransferase



Enzymatic reaction of: cholinephosphotransferase (phosphatidyltran



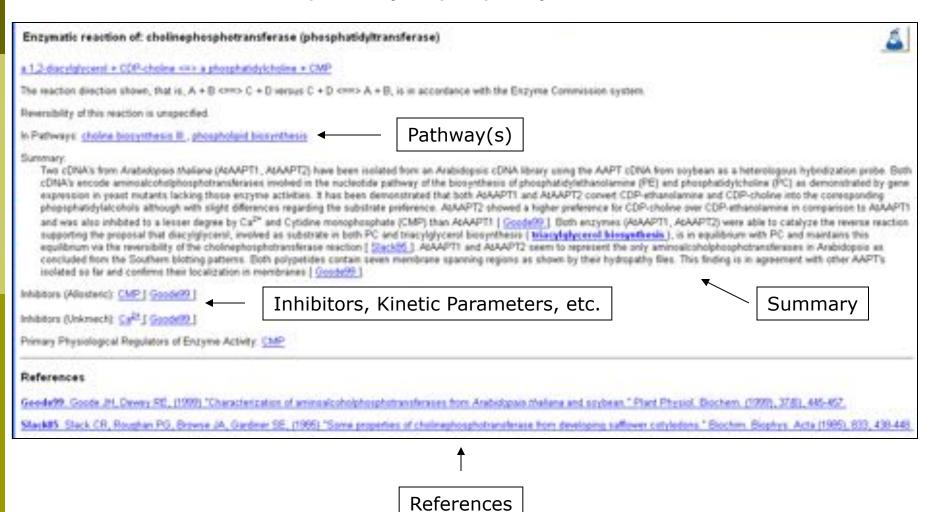
Enzymatic reaction of: ethanolaminephosphotransferase (phosphatidyltransferase)

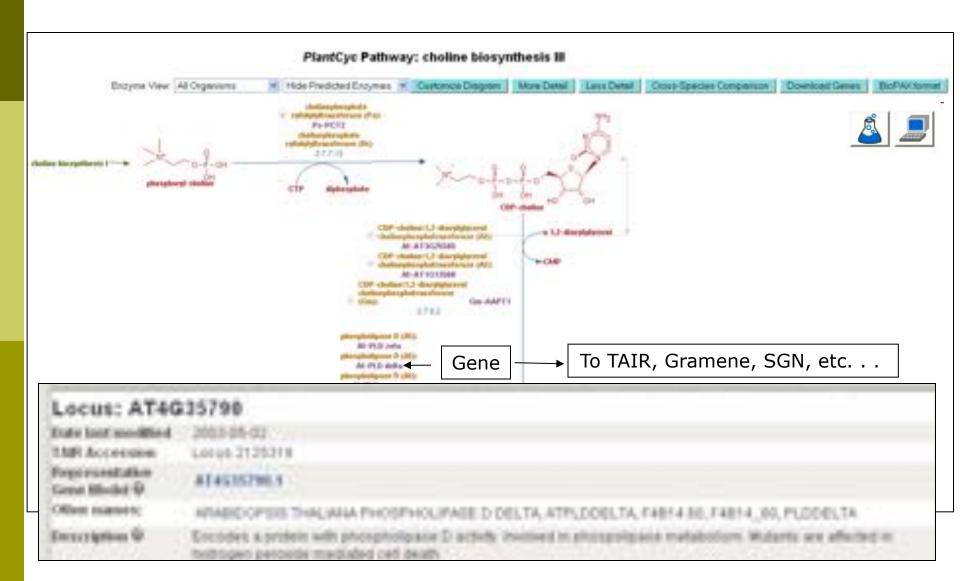
x 1,2-discylglycerot + COP-ethanolamine <=> an L-1-phosphatidyl-ethanolamine + CMP



### **PMN** enzyme pages

#### Arabidopsis Enzyme: phosphatidyltransferase





### **Searching in the PMN databases**

PMN quick search bar



### **Searching in PMN databases**

The guery choline matched the fo

#### Pathways.

Pathway pages co pathway, of chrom genes, and of regu

- choline biosynthesis !
- choline bipsynthesis II
- choline biosynthesis III
- shosphatidylcholine biosy
- phosphatidylcheline biosy
- ghosphatidylcholine biosy
- phosphatidylchelline biosy
- superpathway of phosphat
- superpathway of choline b

Gene pages contain: Genes depiction of its operor product information is corresponding protein

choline managaygenase

#### Proteins

Protein pages contain: Detailed comments and citations: subunit structure; cofactors. activators, and inhibitors (for enzymes), depiction of regular (for transcription factors).

- choline kinase (pol-
- cheline kinase (pp)
- cheline kinase (pol-
- cheline kinase (pol-
- cheline kinase (pol-
- cheline kinase (pol-
- cheline kinase (pol
- cheline kinase (polcheline kinase (pol-
- cheline kinase (pol-
- choline kinase (poli
- cheline kinase (poli
- CHOLINE MONOOS
- cheline monogxyge
- cheline monogypp
- choline monooxyp expressed
- cheline-phosphate AT2G32260
- choline-phosphate AT4G15130
- choline phosphate. LOC 0s02s07720.1
- cholinephosphate

#### Compounds

Compound pages contain: compound structural information, and links to all reactions and pathways in which the compound participates

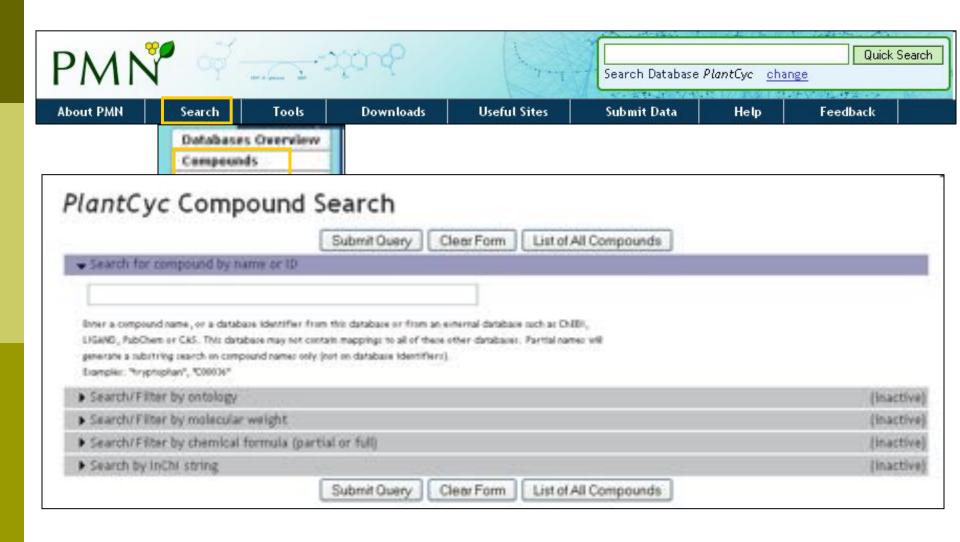
- 16:0-18:1-PC /7-16
- 16:0-18:2-PC /7-16
- 16/0-18:3-PC /7-16 18.1-18:1-PC /3-18
- 3-phosphocholine
- 18.1-18:2-PC /7-1/
- 18:1-18:3-PC://1-18
- 18:2-18:1-PC /1-18
- 18:2-18:2-PC //I-18 3-phosphocholine
- 18.2-18:3-PC /1-18
- 18.3-18.1-PC /1-18
- 18.3-18:2-PC /1-18 18:3-18:3-PC /1-18
- choline
- O-sinapoylcholine
- Sn-3-glycerophosphocholine a 1-acyl-2-lyso-glycerophosphocholine
- a 1-alkyl-2-acetyl-an-plycero-3-phosphocheline
- a 1-alkyl-so-glycero-3-phosphocheline
- a 1-lyso-2-acyl-an-plycero-3-phosphocholine
- a 1-organyl-2-acyl-so-glycero-3-phosphocholine
- a 2-lysophosphatidylcheline

#### Reactions

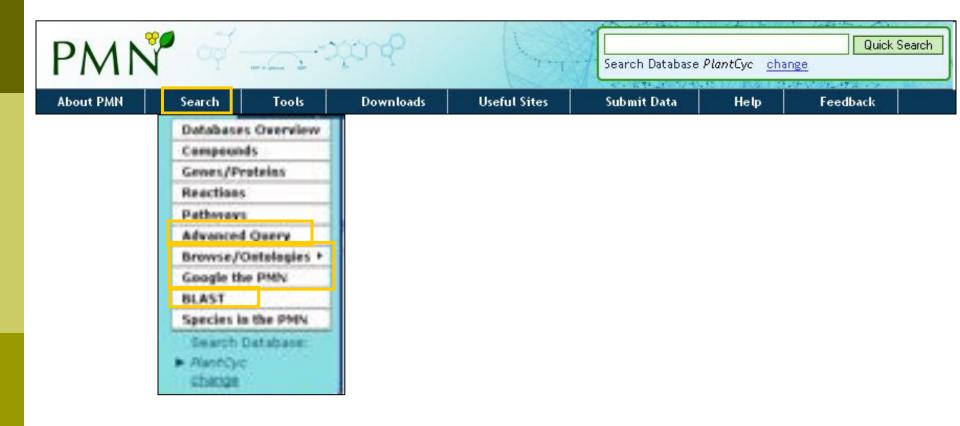
Reaction pages contain: reaction equation with chemical structures, links to all enzymes that catalyze the reaction, and all pathways in which the reaction participates.

- 1-O-sinapovi-B-D-glucose + chelline = O-sinapovicholine + B-D-glucose
- choline + ATP = phosphoryl-choline + ADP
- a 1.2-diacylglycerol + CDP-choline = a phosphatidylcholine + CMP
- a phosphatidylcheline + H<sub>2</sub>O = a 1-acyl-2-lyspglycerophosphocholine + a carboxylate
- a phosphatidylcheline + HyO = an L-phosphatidate + choline
- phosphoryl-choline + CTP = CDP-choline + diphosphate

### Specific search pages



### **Additional search options**

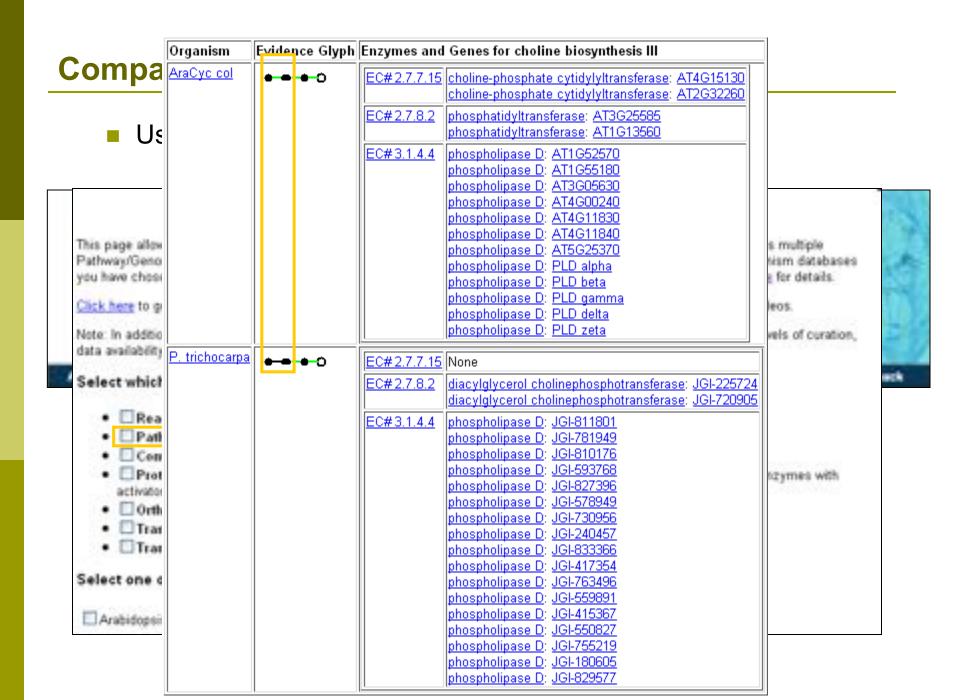




- PlantCyc, AraCyc, PoplarCyc Enzymes:
  - include enzymes with available sequence information from each database
- Reference Enzymes:
  - includes enzymes with experimental support from both plant and non-plant species

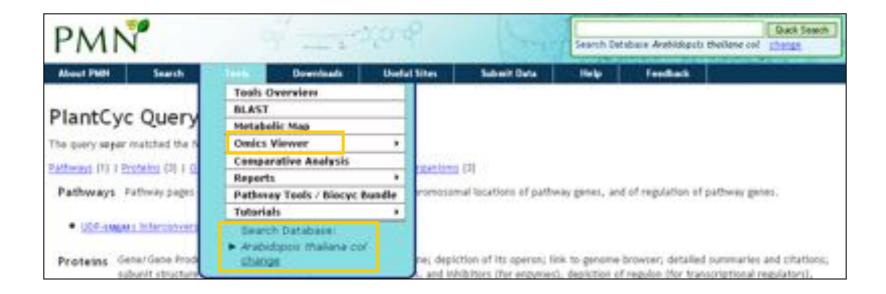
### Finding enzymes through BLAST





### Visualizing OMICs data

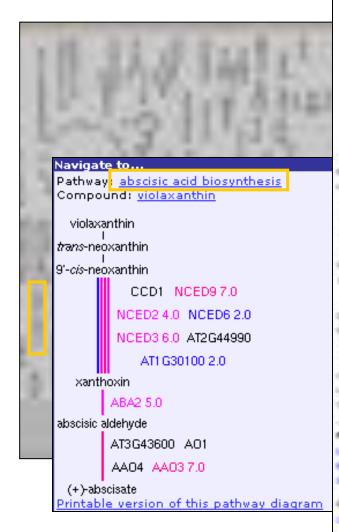
- Overlay "pre-cleaned" quantitative data sets on a metabolic map
  - Gene transcription data
  - Proteomic data
  - Metabolomic data
- Only available for single-species databases, not PlantCyc
- Demonstrations available from 3:30 5:30 PM!



### Visualizing OMICs data



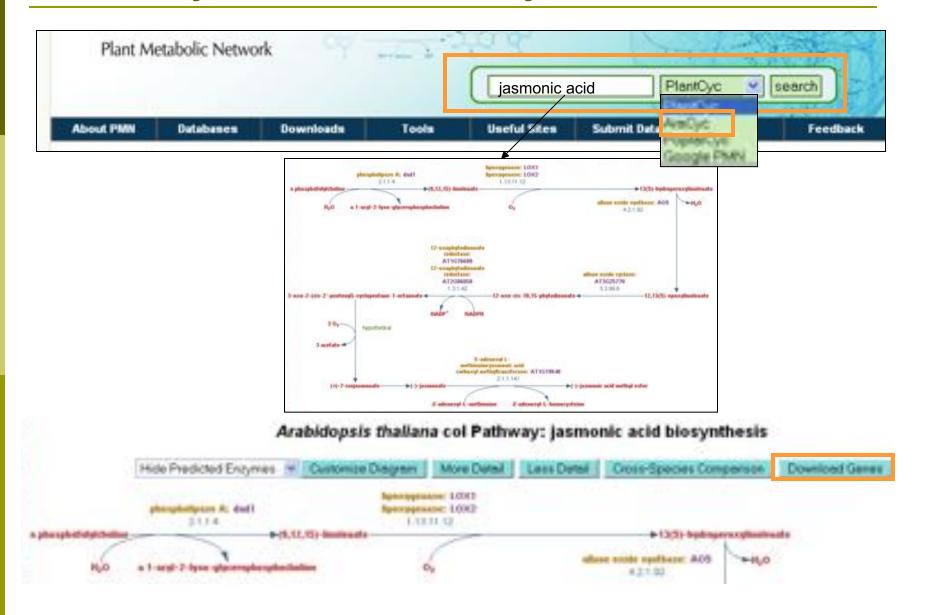
### Visualizing OMICs dat



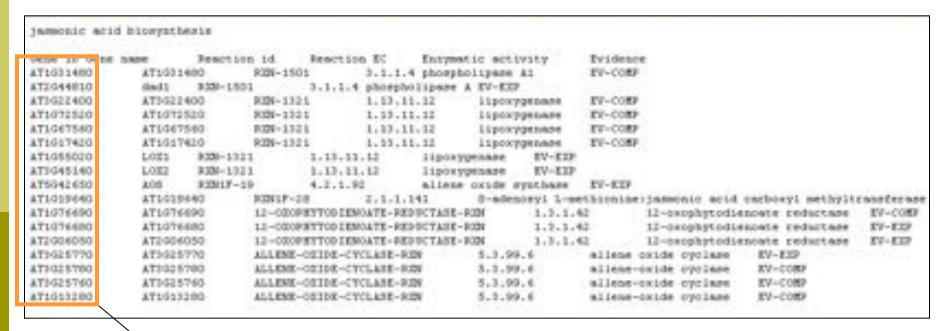
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Animation feature is available!

- You are studying jasmonic acid biosynthesis in your favorite plant
- You want to identify potential orthologs for all of the Arabidopsis enzymes associated with the pathway





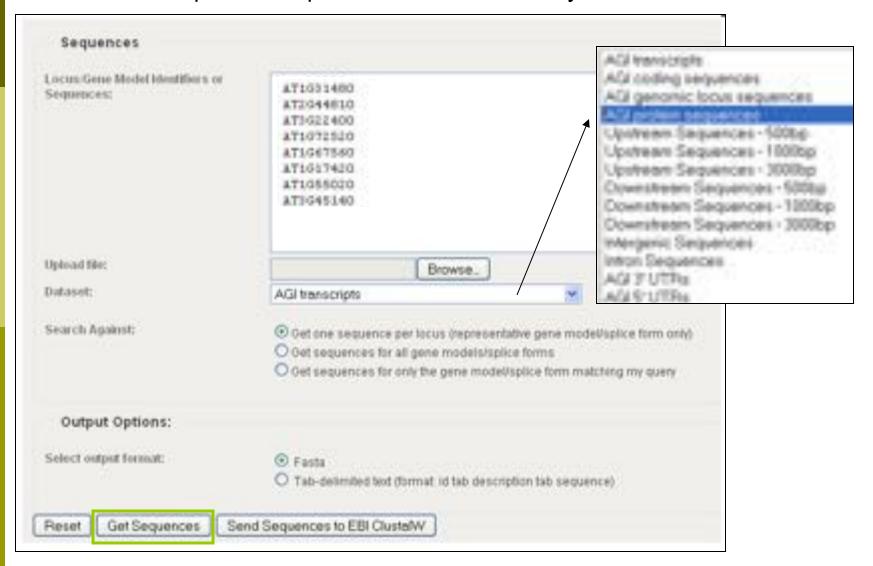


Take this gene list to TAIR to get sequences

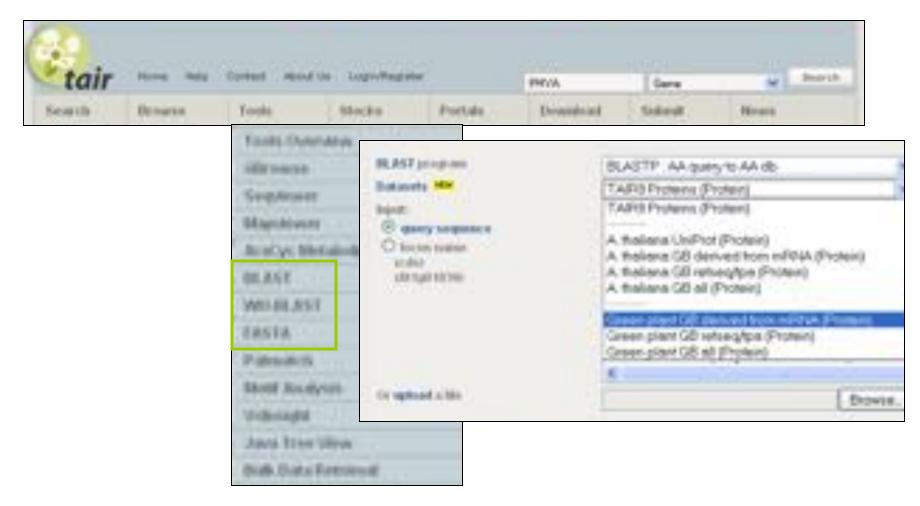
Obtain protein sequences for all of the enzymes



Obtain protein sequences for all of the enzymes



Blast enzymes against all Genbank Plant proteins in TAIR



Or use UniProt, Genbank, your species-specific database, etc.

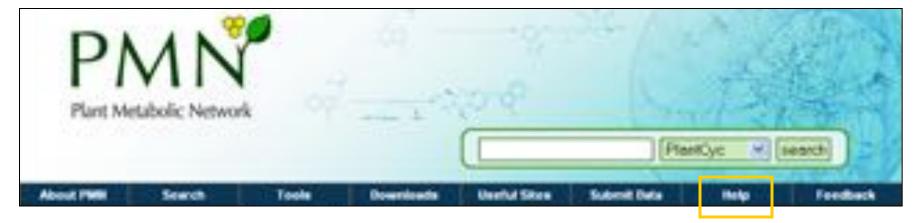
### Putting the PMN and TAIR to work for you

- Use the PMN to learn more about metabolic pathways
- Use TAIR to find detailed information for specific genes / proteins
- Use TAIR and the PMN to enhance your plant biology research

If you're having trouble getting any information you want . . .

# We are here to help!











# We appreciate YOUR help!





# PMN and TAIR Acknowledgements

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Peifen Zhang (Director-PMN)

#### **Current Curators:**

- -Tanya Berardini (lead curator)
- Philippe Lamesch (*lead curator*)
- Donghui Li (curator)
- Dave Swarbreck (former lead curator)
- Debbie Alexander (curator)
- A. S. Karthikeyan (curator)
- Marga Garcia (curator)
- Leonore Reiser

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- Ron Caspi (SRI)
- Suzanne Paley (SRI)
- SRI Tech Team
- Lukas Mueller (SGN)
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- Larry Ploetz (Sys. Administrator)
- Anjo Chi
- Raymond Chetty
- Cynthia Lee
- Shanker Singh
- Chris Wilks

#### PMN project post-doc

- Lee Chae





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