

# Putting the Plant Metabolic Network (PMN) to work for you



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*curator*

PMN/TAIR

# Presentation plan

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- Introduction and content overview
- Search tools and tips
- Cross-species analyses
- OMICs data visualization
- Data and software downloads
- Creating new PMN content

# What is the PMN?

- PMN = The **P**lant **M**etabolic **N**etwork
  - Created in 2008



- Funded by the National Science Foundation

# What is the PMN?

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**PMN**  
Plant Metabolic Network

Search PlantCyc search

About PMN Search Tools Downloads Useful Sites Submit Data Help Feedback

### Introduction

The **Plant Metabolic Network (PMN)** is a collaborative project among databases and biochemists with a common goal to build a broad network of plant metabolic pathway databases. A central feature of the PMN is **PlantCyc**, a comprehensive plant biochemical pathway database, containing curated information from the literature and computational analyses about the genes, enzymes, compounds, reactions, and pathways involved in primary and secondary metabolism.

**AraCyc 6.0**  
5501 enzymes  
2690 compounds  
408 pathways

**PlantCyc 3.0**  
10964 enzymes  
2679 compounds  
714 pathways

### News

**New PMN releases - PoplarCyc debut!**

The latest PMN release includes:

- A new database: [PoplarCyc 1.0](#)
- A new search tool: [PMN BLAST](#)
- Two new releases:
  - [PlantCyc 3.0](#)
  - [AraCyc 6.0](#)

Please check our [release notes](#) to learn about our new data and visit our [content statistics](#) page to get an overview of our database contents.

**Additional exciting news ...**

### Item of the Month

**Isoprene Biosynthesis in Poplar**

Isoprene, a gaseous hydrocarbon, is emitted in substantial quantities by

species

way

pathways

metabolism

# What is in the PMN?

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- Databases contain detailed information about:
  - Pathways
  - Enzymes
  - Reactions
  - Compounds
  - Genes
  
- Data are entered and displayed using Pathway Tools software
  - Peter Karp, *et al*, SRI International
  
- Pathways are generated through:
  - Manual curation when a curator reads scientific literature
  - Computational predictions made by the Pathologic software

# What is in the PMN?

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- Databases created and maintained by the PMN
  - PlantCyc, AraCyc, PoplarCyc (new in October 2009!)
- Other plant databases accessible through 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
CapCyc	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

\*\* Significant numbers of genes from these databases have been integrated into PlantCyc

# What is in the PMN?

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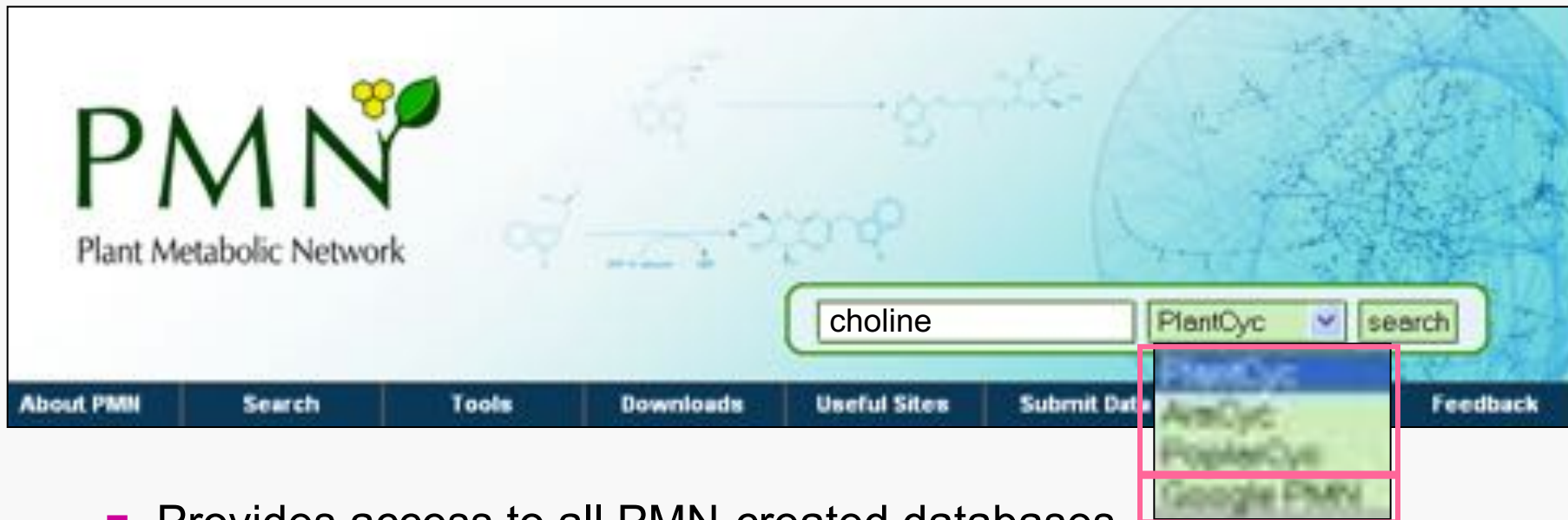
- Most recent release of PMN databases: October 15, 2009

Database contents	PlantCyc 3.0	AraCyc 6.0	PoplarCyc 1.0
<b>Base pathways*</b> (no superpathways)	<b>643</b>	<b>360</b>	<b>285</b>
<b>Experimentally-supported (EV-EXP)</b>	<b>585</b>	<b>299</b>	<b>25</b>
<b>Enzymes**</b> (monomers and complexes)	<b>10964</b>	<b>5501</b>	<b>3434</b>
<b>in reactions (EV-EXP) in pathways</b>	<b>1974</b>	<b>858</b>	<b>1</b>
<b>Reactions</b>	<b>2709</b>	<b>2323</b>	<b>1668</b>
<b>in pathways with enzymes (EV-EXP)</b>	<b>1614</b>	<b>829</b>	<b>2</b>
<b>Compounds</b>	<b>2679</b>	<b>2630</b>	<b>1363</b>
<b>Organisms</b>	<b>376</b>	<b>1</b>	<b>1***</b>
<b>Citations</b>	<b>4803</b>	<b>2691</b>	<b>903</b>

- How can I access all this information?

# Searching in PMN databases

## □ Quick search bar



- Provides access to all PMN-created databases
- Allows Google-based text-mining of summaries, comments, etc.
  - For example, search “plant defense”
- PMN searches:
  - Match partial words
  - Search across all fields (compound, enzyme, etc.)
  - Return a list of items grouped by data type



## Searching in PMN databases

The query `choline` matched the following

## Pathways

Pathway pages contain a pathway, of chromosomal genes, and of regulatory

- **choline biosynthesis I**
- **choline biosynthesis II**
- **choline biosynthesis III**
- phosphatidylcholine biosynthesis
- phosphatidylcholine biosynthesis
- phosphatidylcholine biosynthesis
- phosphatidylcholine biosynthesis
- superpathway of phosphatidylcholine biosynthesis
- superpathway of phosphatidylcholine biosynthesis

## Genes

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

- [choline monoxygenase](#)

### Proteins

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

- choline kinase fpol
- choline kinase fpol
- choline kinase fpol
- choline kinase fpol
- choline kinase fpol
- choline kinase fpol
- choline kinase fpol
- choline kinase fpol
- choline kinase fpol
- choline kinase fpol
- choline kinase fpol
- CHOLINE MONOOX
- choline monooxyge
- choline monooxyge
- choline monooxyge expressed
- choline-phosphate AT2G32260
- choline-phosphate AT4G15130
- choline-phosphate LOC\_Os02g07720.1
- cholinophosphate

### Compounds

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

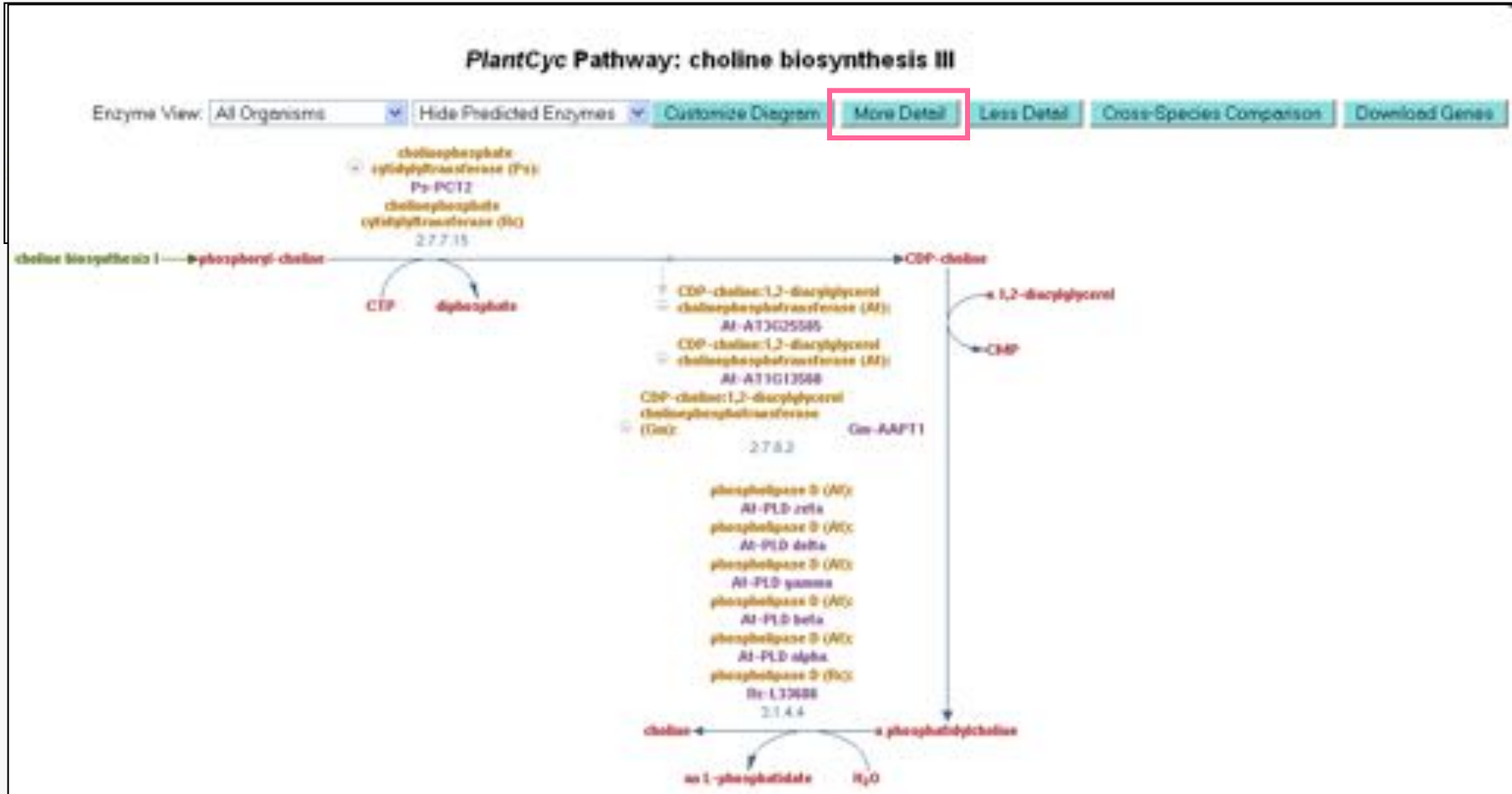
- 18:0-18:1-PC (1-18)
- 18:0-18:2-PC (1-18)
- 18:0-18:3-PC (1-18)
- 18:1-18:1-PC (1-18)
- 3-phosphocholine
- 18:1-18:2-PC (1-18)
- 18:1-18:3-PC (1-18)
- 18:2-18:1-PC (1-18)
- 18:2-18:2-PC (1-18)
- 3-phosphocholine
- 18:2-18:3-PC (1-18)
- 18:3-18:1-PC (1-18)
- 18:3-18:2-PC (1-18)
- 18:3-18:3-PC (1-18)
- **choline**
- **Q-sinagoylcholine**
- **Sn-3-glycerophosp**
- **a-1-acyl-2-lyso-gly**
- **a-1-alkyl-2-acetyl-a**
- **a-1-alkyl-sn-glycen**
- **a-1-lyso-2-acyl-sn-**
- **a-1-oryanyl-2-acyl-**
- **a-2-lyso-phosphatid**

### 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.

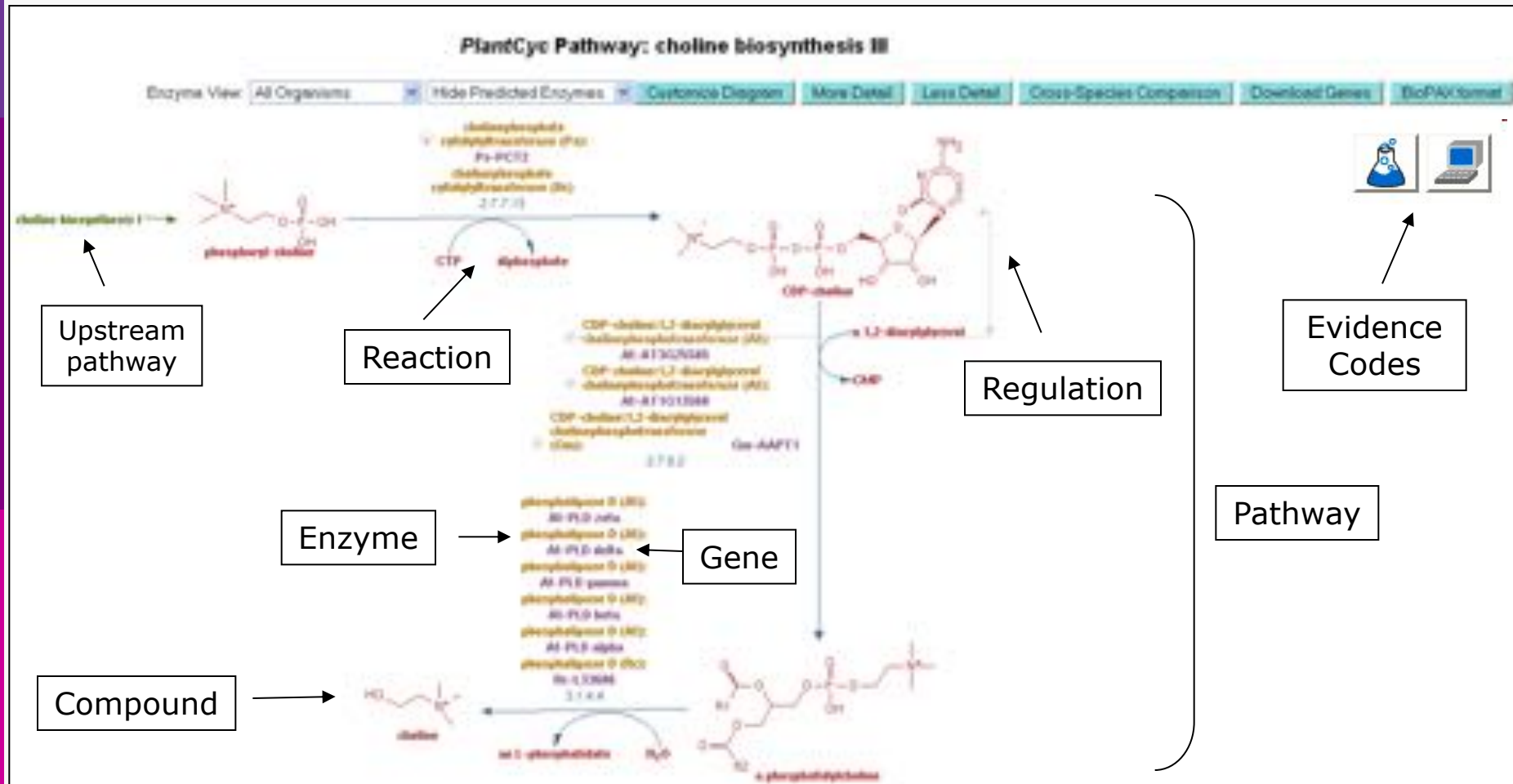
- $1\text{-O-sinapoyl-}\beta\text{-D-glucose} + \text{choline} = \text{O-sinapoylcholine} + \beta\text{-D-glucose}$
- $\text{choline} + \text{ATP} = \text{phosphorylcholine} + \text{ADP}$
- $\text{a 1,2-diacylglycerol} + \text{CDP-choline} = \text{a phosphatidylcholine} + \text{CMP}$
- $\text{a phosphatidylcholine} + \text{H}_2\text{O} = \text{a 1-acyl-2-lysophosphatidylcholine} + \text{a carboxylate}$
- $\text{a phosphatidylcholine} + \text{H}_2\text{O} = \text{an L-phosphatidate} + \text{choline}$
- $\text{phosphorylcholine} + \text{CTP} = \text{CDP-choline} + \text{diphosphate}$

# Getting information from PMN pathway pages



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

# Getting information from PMN pathway pages



# Getting information from PMN pathway pages

Superclasses [Biosynthesis -> Fatty Acids and Lipids Biosynthesis -> Choline Biosynthesis](#)

Species Data Available for [Arabidopsis thaliana cel.](#), [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 certain plants such as spinach, where this osmoprotectant 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 [ [McNeil01](#) ].

The choline biosynthetic pathway enables plants to decouple choline synthesis from lipid metabolism (Kennedy pathway - [triacylglycerol biosynthesis](#) ) and provides them with the metabolic flexibility to adapt to environmental conditions where large and variable amounts of choline are beneficial for survival [ [Ronten01](#) ].

**Pathway information:** The first step in choline biosynthesis is the direct decarboxylation of serine to ethanolamine [ [Ronten01](#) ], which is catalyzed by a serine decarboxylase unique to plants [ [Ronten03](#) ]. Ethanolamine is widely recognized as the entrance compound to choline biosynthesis.

## References

[Curator09](#): 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: 1) 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 3) the pathway is expected to exist in all plants."

[Datko88](#): 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 soybean and carrot." *Plant Physiol.* (1988), 88, 854-861.

[Hitz81](#): Hitz WD, Rhodes D, Hanson AD. (1981) "Radio-tracer evidence implicating phosphoryl and phosphatidyl bases as intermediates in betaine synthesis by water-stressed barley leaves." *Plant Physiol.* (1981), 68, 814-822.

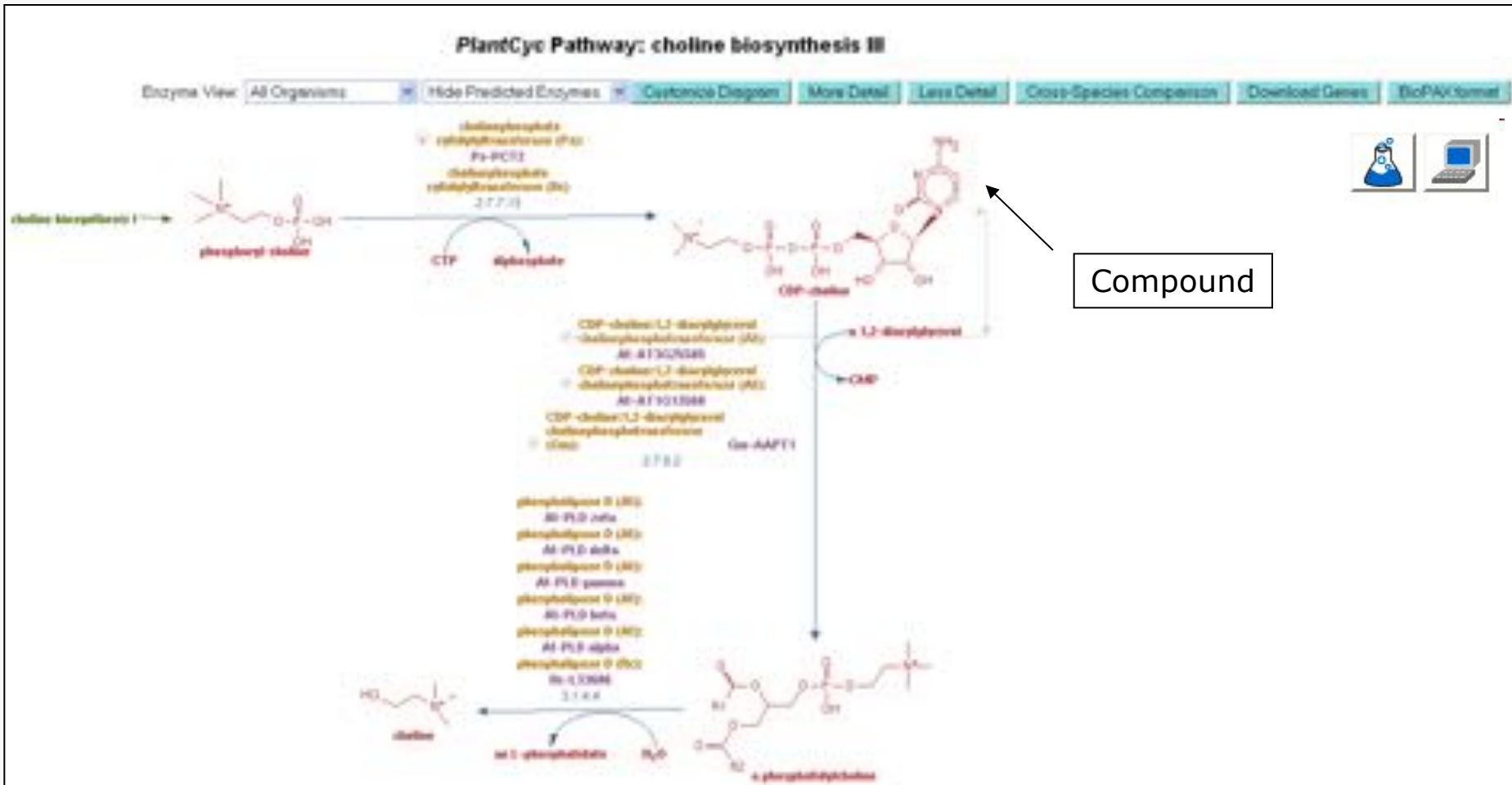
[Kinney93](#): Kinney AJ. (1993) "Phospholipid head groups." In: Moore, TS, Jr. (ed.) *Lipid metabolism in plants*. CRC Press Boca Raton Ann Arbor London Tokyo (1993), 259-264.

[Kirk99](#): Kirk Pagan, Xuemin Wang "Molecular and biochemical properties and physiological roles of plant phospholipase D." *Biochimica Biophysica Acta* (1999) 1439, 151-166.

[McNeil00](#): McNeil SD, Nuccio ML, Rhodes D, Shachar-Hill Y, Hanson AD (2000). "Radio-tracer and computer modeling evidence that phospho-base methylation is the main route of choline synthesis in tobacco." *Plant Physiol* 123(1):371-80. PMID: 10806254



## Getting information from PMN pathway pages



# PMN compound pages

Compound:  
CDP-choline

Synonyms: [cibcoline](#) , [cibcholine](#) , [cibfite](#) , [cylcholine](#) , [cytidine 5'-diphosphocholine](#) , [cytidine diphosphate choline](#)

Synonyms

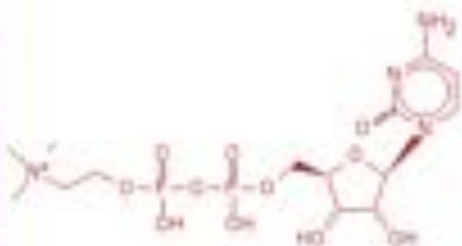
Superclasses: [a nucleic acid component](#) -> [a base derivative](#)  
[a nucleic acid component](#) -> [a pyrimidine-related compound](#)

Classification(s)

Empirical Formula:  $C_{14}H_{27}N_4O_{11}P_2$

Molecular Weight: 489.34 daltons

Molecular Weight / Formula



Smiles: C(=O)OP(=O)(=O)OP(=O)(=O)OCCN(=O)C1=CC=C(C=C1)OC(C(=O)O)N(C)C

Unification Links: [CAS:967-78-0](#)

Gibbs Energy of Formation (kcal/mol, estimated): -116.7

In Pathway Reactions as a Reactant:

[phospholipid biosynthesis:](#)

[a 1,2-diacylglycerol](#) + **CDP-choline** = [a phosphatidylcholine](#) + [CMP](#)

Appears as Reactant

[choline biosynthesis III:](#)

[a 1,2-diacylglycerol](#) + **CDP-choline** = [a phosphatidylcholine](#) + [CMP](#)

In Pathway Reactions as a Product:

[phospholipid biosynthesis:](#)

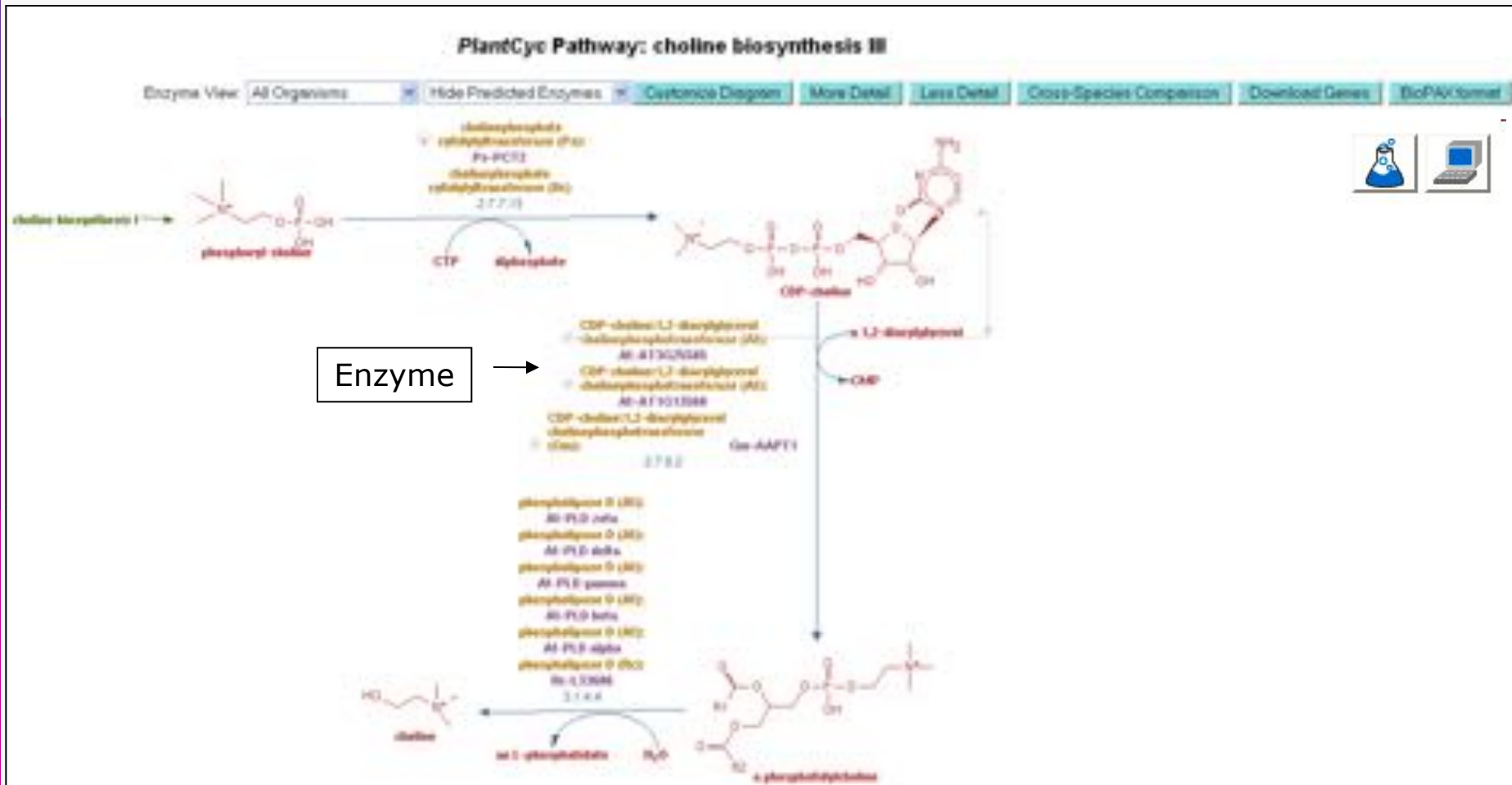
[phosphorylcholine](#) + [CTP](#) = **CDP-choline** + [diphosphate](#)

Appears as Product

[choline biosynthesis III:](#)

[phosphorylcholine](#) + [CTP](#) = **CDP-choline** + [diphosphate](#)

# Getting information from PMN pathway pages



# PMN enzyme pages

## *Arabidopsis* Enzyme: phosphatidyltransferase

Synonyms: aminolipidphosphotransferase

Gene: [AT1G13680](#)

Sequence Length: 1196 AAs

Unification Links: [Entrez: AAC61750](#)

Gene-Reaction Schematic: 



Multifunctional protein

\*

\*

Enzymatic reaction of: cholinephosphotransferase (phosphatidyltran

[1,3-diacylglycerol + CDP-choline <=> 1-phosphatidylcholine + CMP](#)

Enzymatic reaction of: ethanolaminephosphotransferase (phosphatidyltransferase)

[1,3-diacylglycerol + CDP-ethanolamine <=> sn-1'-phosphatidyl-ethanolamine + CMP](#)

Pathway Tools evidence ontology click on:  
<http://bioinformatics.wri.com/evidence-ontology/>

 **Experimental Evidence:**

Evidence code: EV-EXP-IDA-UNPURIFIED-PROTEIN  
Source: [Goad99](#)  
Definition: Direct assay of unpurified protein. Presence of a protein activity is indicated by an assay. However, the precise identity of the protein with that activity is not established by this experiment (protein has not been purified).

**References**

[Goad99](#): Goad JH, Dewey RE, (1999) "Characterization of aminolipidphosphotransferases from *Arabidopsis thaliana* and soybean." *Plant Physiol. Biochem.* (1999), 37(5), 485-497.

Home Help Contact [CMA/PMN LMR](#)  



# PMN enzyme pages

## *Arabidopsis* Enzyme: phosphatidyltransferase

Enzymatic reaction of: cholinephosphotransferase (phosphatidyltransferase)



$1,2\text{-diacylglycerol} + \text{CDP-choline} \rightleftharpoons \text{a phosphatidylcholine} + \text{CMP}$

The reaction direction shown, that is,  $A + B \rightleftharpoons C + D$  versus  $C + D \rightleftharpoons A + B$ , is in accordance with the Enzyme Commission system.

Reversibility of this reaction is unspecified.

In Pathways: [choline biosynthesis II](#), [phospholipid biosynthesis](#)

Pathway(s)

### Summary:

Two cDNA's from *Arabidopsis thaliana* (AtAAPT1, AtAAPT2) have been isolated from an *Arabidopsis* cDNA library using the AAPT cDNA from soybean as a heterologous hybridization probe. Both cDNA's encode aminoalcoholphosphotransferases involved in the nucleotide pathway of the biosynthesis of phosphatidylethanolamine (PE) and phosphatidylcholine (PC) as demonstrated by gene expression in yeast mutants lacking these enzyme activities. It has been demonstrated that both AtAAPT1 and AtAAPT2 convert CDP-ethanolamine and CDP-choline into the corresponding phosphatidylethanolamines although with slight differences regarding the substrate preference. AtAAPT2 showed a higher preference for CDP-choline over CDP-ethanolamine in comparison to AtAAPT1 and was also inhibited to a lesser degree by  $\text{Ca}^{2+}$  and Cytidine monophosphate (CMP) than AtAAPT1 [Goode99]. Both enzymes (AtAAPT1, AtAAPT2) were able to catalyze the reverse reaction supporting the proposal that diacylglycerol, involved as substrate in both PC and triacylglycerol biosynthesis [triacylglycerol biosynthesis], is in equilibrium with PC and maintains this equilibrium via the reversibility of the cholinephosphotransferase reaction [Slack85]. AtAAPT1 and AtAAPT2 seem to represent the only aminoalcoholphosphotransferases in *Arabidopsis* as concluded from the Southern blotting patterns. Both polypeptides contain seven membrane spanning regions as shown by their hydropathy files. This finding is in agreement with other AAPT's isolated so far and confirms their localization in membranes [Goode99].

Inhibitors (Allosteric): [CMP](#) [Goode99]

Inhibitors, Kinetic Parameters, etc.

Summary

Inhibitors (Unknown): [Ca<sup>2+</sup>](#) [Goode99]

Primary Physiological Regulators of Enzyme Activity: [CMP](#)

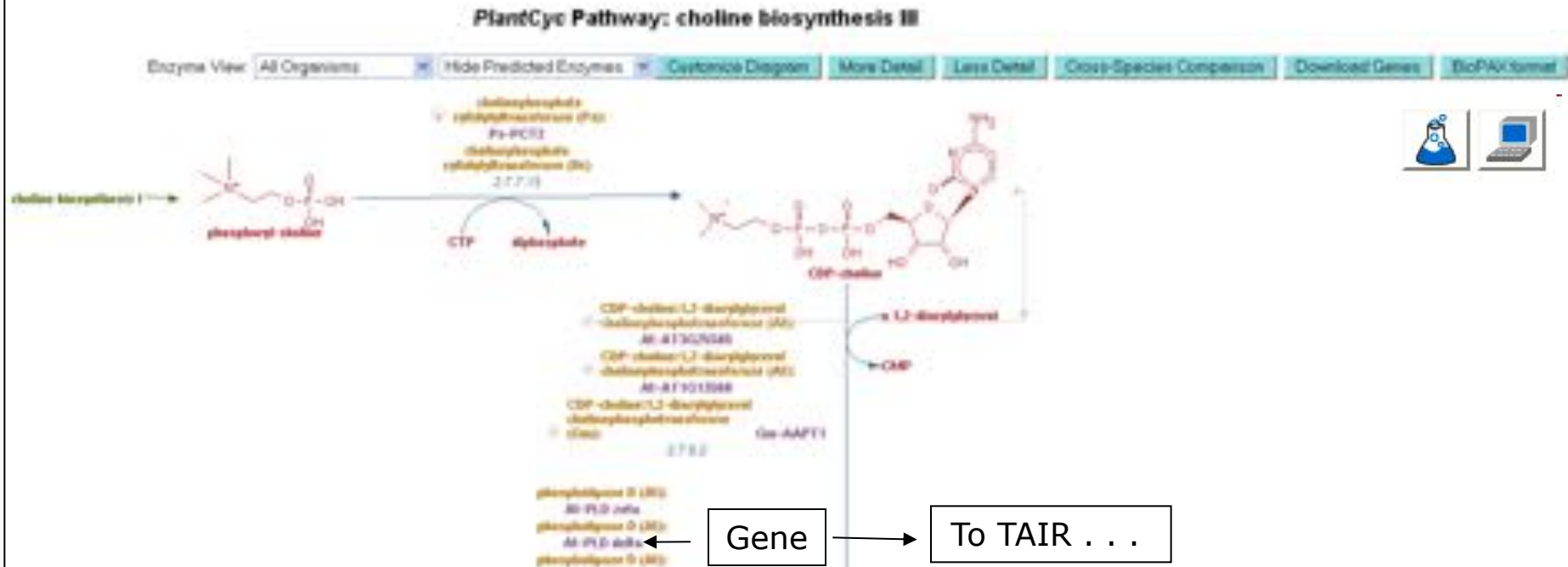
### References

Goode99. Goode JH, Dewar SE, (1999) "Characterization of aminoalcoholphosphotransferases from *Arabidopsis thaliana* and soybean." *Plant Physiol. Biochem.* (1999), 37(5), 445-457.

Slack85. Slack CR, Broughan PG, Brown JA, Gardner SE, (1985) "Some properties of cholinephosphotransferase from developing safflower cotyledons." *Biochim. Biophys. Acta* (1985), 833, 439-446.

References

## Getting information from PMN pathway pages



Locus: AT4G15790

Date last modified: 2018-08-01

11/11/2018 11:11:11 AM

Reprints available from <http://www.tandf.co.uk>

Carpenter, H. 1992. 67

Official name(s): ADENOSINE THALAMYL PHOSPHOTRANSFERASE D DELTA, ATP/DDELTA, F4814.10, F4814.100, P/DDELTA

**Description** Encodes a protein with phospholipase D activity involved in phospholipase metabolism. Mutants are affected in histamine peroxide mediated cell death.

# Getting information from PMN pathway pages

## □ Download a complete gene list

Gene ID	Gene name	Reaction ID	Reaction EC	Enzymatic activity	Evidence	Organism
JGI-710905	JGI-710905	R3N-5701	2.7.8.2	ethanolaminephosphotransferase	No Evidence Code	Populus trichocarpa
JGI-225724	JGI-225724	R3N-5701	2.7.8.2	ethanolaminephosphotransferase	No Evidence Code	Populus trichocarpa
AT3G25585	AT3G25585	R3N-5701	2.7.8.2	CSP-choline:1,2-diacylglycerol cholinephosphotransferase	EV-EXP	Arabidopsis thaliana col
AT3G25585	AT3G25585	R3N-5701	2.7.8.2	cholinephosphotransferase	EV-EXP	Arabidopsis thaliana col
AT1G13560	AT1G13560	R3N-5701	2.7.8.2	CSP-choline:1,2-diacylglycerol cholinephosphotransferase	EV-EXP	Arabidopsis thaliana col
AT1G13560	AT1G13560	R3N-5701	2.7.8.2	cholinephosphotransferase	EV-EXP	Arabidopsis thaliana col
AT1G13560	AT1G13560	R3N-5701	2.7.8.2	cholinephosphotransferase	EV-EXP	Arabidopsis thaliana col
WIP.6494.1.S1_AT	BQ146449	R3N-5701	2.7.8.2	aminoalcoholphosphotransferase	EV-COMP	Medicago truncatula
WIP.32591.1.S1_AT	AM696770	R3N-5701	2.7.8.2	aminoalcoholphosphotransferase	EV-COMP	Medicago truncatula
WIP.1715.1.S1_AT	AW774344	R3N-5701	2.7.8.2	aminoalcoholphosphotransferase	EV-COMP	Medicago truncatula
G-6304	LAFT1	R3N-5701	2.7.8.2	CSP-choline:1,2-diacylglycerol cholinephosphotransferase	EV-EXP	Glycine max
JGI-819577	JGI-819577	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-180605	JGI-180605	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-755219	JGI-755219	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-550827	JGI-550827	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-415367	JGI-415367	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-550891	JGI-550891	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-763496	JGI-763496	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-417354	JGI-417354	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-833366	JGI-833366	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-240457	JGI-240457	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-730956	JGI-730956	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-578949	JGI-578949	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-817396	JGI-817396	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-593768	JGI-593768	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-810176	JGI-810176	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-781949	JGI-781949	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-811801	JGI-811801	PHOSCHOL-R3N	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
AT3G16785	FLD eta	PHOSCHOL-R3N	3.1.4.4	phospholipase D	EV-EXP	Arabidopsis thaliana col
AT4G03790	FLD delta	PHOSCHOL-R3N	3.1.4.4	phospholipase D	EV-EXP	Arabidopsis thaliana col
AT4G11850	FLD gamma	PHOSCHOL-R3N	3.1.4.4	phospholipase D	EV-EXP	Arabidopsis thaliana col
AT3G41030	FLD beta	PHOSCHOL-R3N	3.1.4.4	phospholipase D	EV-EXP	Arabidopsis thaliana col
AT3G15730	FLD alpha	PHOSCHOL-R3N	3.1.4.4	phospholipase D	EV-EXP	Arabidopsis thaliana col
AT5G25370	AT5G25370	PHOSCHOL-R3N	3.1.4.4	phospholipase D	EV-COMP	Arabidopsis thaliana col
AT4G11840	AT4G11840	PHOSCHOL-R3N	3.1.4.4	phospholipase D	EV-COMP	Arabidopsis thaliana col
AT4G11830	AT4G11830	PHOSCHOL-R3N	3.1.4.4	phospholipase D	EV-COMP	Arabidopsis thaliana col
AT4G00240	AT4G00240	PHOSCHOL-R3N	3.1.4.4	phospholipase D	EV-COMP	Arabidopsis thaliana col

# Getting information from PMN pathway pages

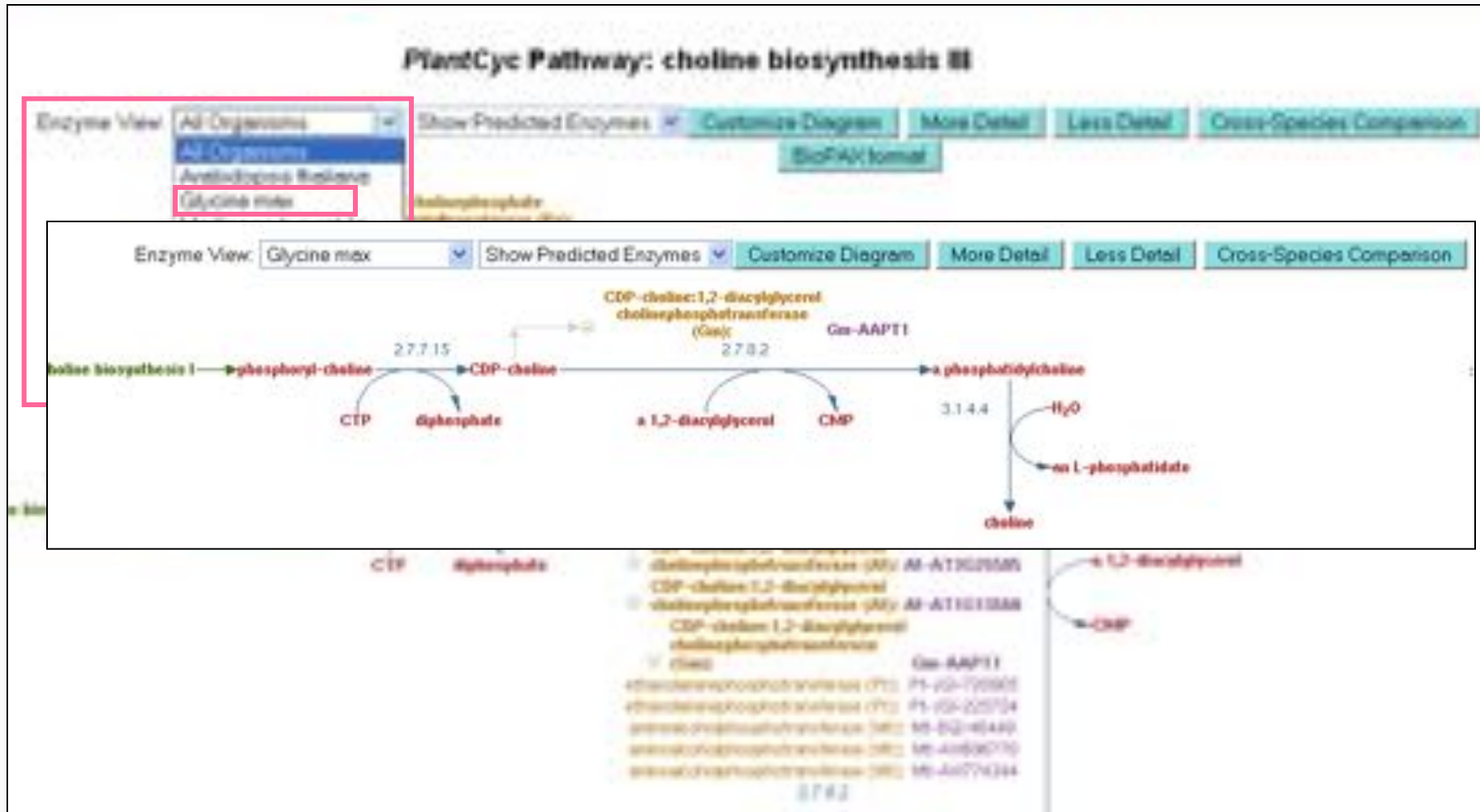
## □ Download the pathway in BioPAX format

```
- <rdf:RDF xml:base="http://www.pilotcyc.org/1555/ARA/pathway-biopax/objects=PWY-3561">
-   <owl:Ontology rdf:about="">
-     <owl:imports rdf:resource="http://www.biopax.org/release/biopax-level2.owl"/>
-     <rdf:type rdf:type="owl:Class">
-       <rdf:type rdf:type="owl:Class">
-         This BioPAX Level 2 output for <organism Arabidopsis%3Dthaliana%3Dcol, pathway choline%3Dbiosynthesis%3DIII was automatically generated from URL http://www.pilotcyc.org/1555/ARA/pathway-biopax/objects=PWY-3561 on 18-Oct-2009 18:06:51. Note that all IDs are auto-generated, and are valid in the scope of this file only. If the data is regenerated at some later time, or data for another pathway is generated from this same site, there are no guarantees that the same IDs will refer to the same objects. To retrieve a file containing a complete list of pathways for this organism in BioPAX format, please visit http://biocyc.org/download-flatfiles.shtml
-       </rdf:type>
-     </owl:Class>
-   </owl:Ontology>
-   <bp:catalysis rdf:ID="catalysis637">
-     <bp:CONTROLLED>
-       <bp:biochemicalReaction rdf:ID="biochemicalReaction584">
-         <bp:EC-NUMBER rdf:datatype="http://www.w3.org/2001/XMLSchema#string">2.7.7.15</bp:EC-NUMBER>
-       <bp:LEFT>
-         <bp:physicalEntityParticipant rdf:ID="phys-ent-participant613">
-           <bp:PHYSICAL-ENTITY>
-             <bp:smallMolecule rdf:ID="smallMolecule608">
-               <bp:MOLECULAR-WEIGHT>184.152</bp:MOLECULAR-WEIGHT>
-               <bp:NAME rdf:datatype="http://www.w3.org/2001/XMLSchema#string">phosphoryl-choline</bp:NAME>
-             <bp:STRUCTURE>
-               <bp:chemicalStructure rdf:ID="chemicalStructure612">
-                 <bp:STRUCTURE-FORMAT rdf:datatype="http://www.w3.org/2001/XMLSchema#string">CML</bp:STRUCTURE-FORMAT>
-               <bp:STRUCTURE-DATA rdf:datatype="http://www.w3.org/2001/XMLSchema#string">
-                 <mol> <molecule id="PHOSPHORYL-CHOLINE" title="phosphoryl-choline" dictRef="dictPHOSPHORYL-CHOLINE"> <atomArray> <atom
- id="PHOSPHORYL-CHOLINE-atom1" elementType="N" x2="28208.0" y2="-10708.0" formalCharge="1"/> <atom id="PHOSPHORYL-CHOLINE-atom2"
- elementType="C" x2="36954.0" y2="-5625.0"/> <atom id="PHOSPHORYL-CHOLINE-atom3" elementType="C" x2="19213.0" y2="-5583.0"/> <atom
- id="PHOSPHORYL-CHOLINE-atom4" elementType="C" x2="28208.0" y2="-21250.0"/> <atom id="PHOSPHORYL-CHOLINE-atom5" elementType="C"
- x2="18750.0" y2="-16125.0"/> <atom id="PHOSPHORYL-CHOLINE-atom6" elementType="C" x2="43460.0" y2="-9356.0"/> <atom id="PHOSPHORYL-
- CHOLINE-atom7" elementType="O" x2="49944.0" y2="-5587.0"/> <atom id="PHOSPHORYL-CHOLINE-atom8" elementType="P" x2="53417.0"
- y2="-5583.0"/> <atom id="PHOSPHORYL-CHOLINE-atom9" elementType="O" x2="64917.0" y2="-5583.0"/> </atom id="PHOSPHORYL-CHOLINE-
```



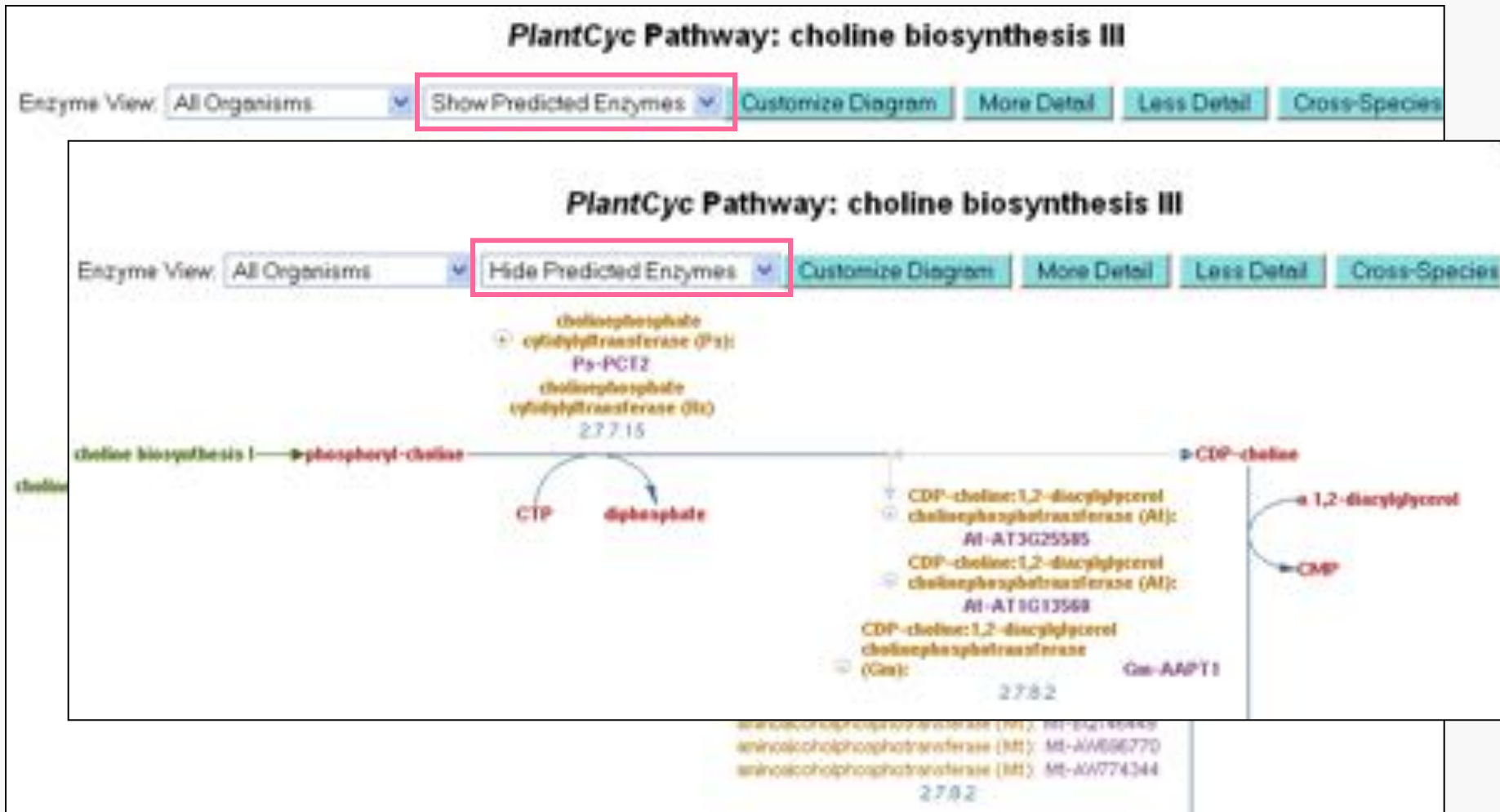
## Getting information from PMN pathway pages

- Set organism viewing preferences on PlantCyc pages



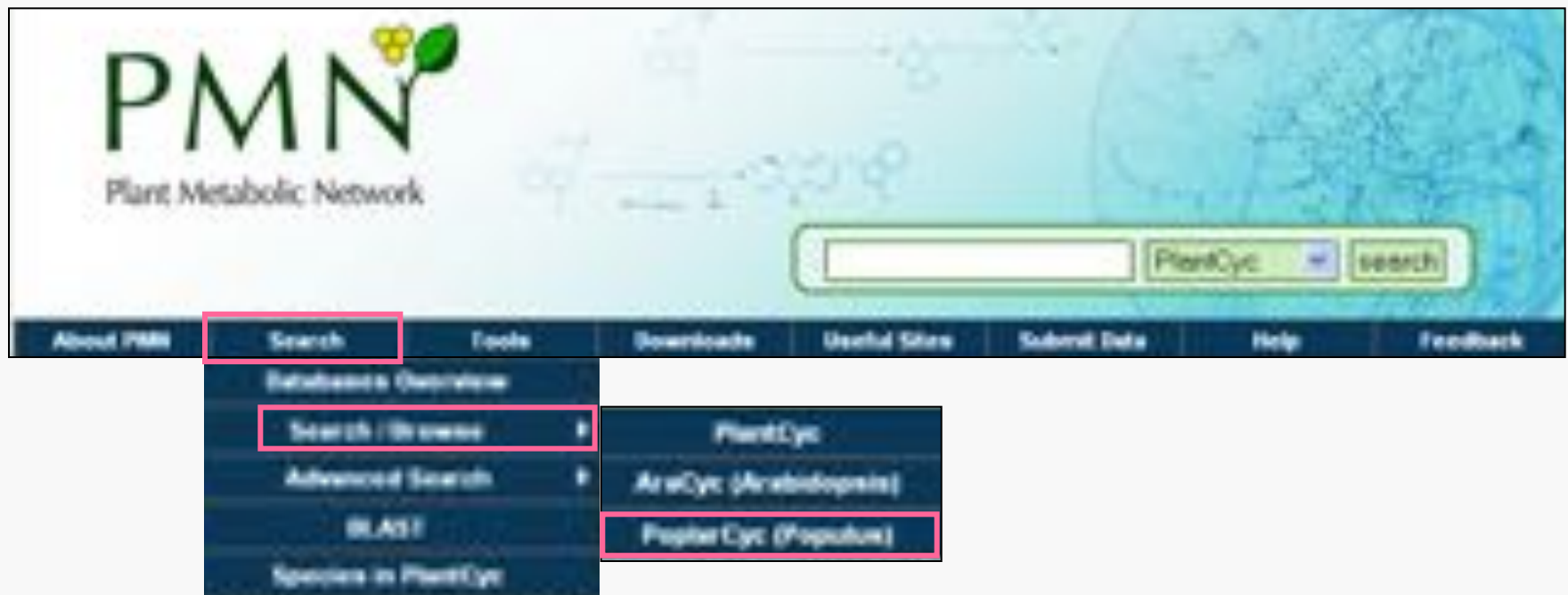
## Getting information from PMN pathway pages

- View predicted or experimentally supported enzymes



# Searching in PMN databases

- Search page
  - Provides more selective searches
  - Allows browsing



# Searching in PMN databases

**Pathway Tools Query Page**

This form provides several different mechanisms for querying Pathway Tools databases.

**Select a database:**  3 available

**Query**

- ☐ All (by name or EC)
- ☐ Protein (by name or EC)
- ☐ Pathway (by name)
- ☐ Reaction (by name or EC)
- ☐ Compound (by name)
- ☐ Gene (by name)
- ☐ Path (by name)

**Browse**

- ☐ Pathways
- ☐ EC Hierarchy
- ☐ Compounds
- ☐ Gene Ontology
- ☐ MultiFun Gene Taxonomy

**Expand All** **Collapse All**


**Pathways**

- ☐ [Biosynthesis](#)
- ☐ [Degradation/Utilization/Assimilation](#)
  - ☐ [Alcohols Degradation](#)
  - ☐ [Aldehyde Degradation](#)
  - ☐ [Amines and Polyamines Degradation](#)
  - ☐ [Amino Acids Degradation](#)
  - ☐ [Aromatic Compounds Degradation](#)
  - ☐ [C1 Compounds Utilization and Assimilation](#)
  - ☐ [Carbohydrates Degradation](#)
  - ☐ [Carboxylates Degradation](#)
  - ☐ [Cofactors, Prosthetic Groups, Electron Carriers Degradation](#)
  - ☐ [Degradation/Utilization/Assimilation - Other](#)
  - ☐ [Fatty Acid and Lipids Degradation](#)
  - ☐ [Hormones Degradation](#)
  - ☐ [Inorganic Nutrients Metabolism](#)
  - ☐ [Nucleosides and Nucleotides Degradation and Recycling](#)
  - ☐ [Secondary Metabolites Degradation](#)
- ☐ [Detoxification](#)
- ☐ [Generation of precursor metabolites and energy](#)
- ☐ [Superpathways](#)



# Advanced searching in PMN databases

- Advanced search page
  - Allows the construction of very complex queries



**1. Enter your query here:**

In database PlantCyc search for Compounds (2679 instances) add a condition

insert a new search component here

**2. Select fields to include in the query output:**

**Column 1**  
☒ Sort based on this column add a column

NAME

**3. Select query output format:**

☒ HTML ☐ Tab Delimited Text (columns are separated by tabs)

**4. Submit Query** **Reset Query**

# Advanced searching in PMN databases

- Find all of the 30-carbon compounds that appear as products in reactions
  - Construct query

1. Enter your query here:

In database  search for

Where

# Advanced searching in PMN databases

- Find all of the 30-carbon compounds that appear as products in reactions
  - Construct query

1. Enter your query here:

In database  search for

Where  contains the substring

Where  contains the substring

“Appears as product in reaction” is not in the list

# Advanced searching in PMN databases

- Find all of the 30-carbon compounds that appear in reactions as products

In database	PlantCyc	search for	Compounds (2679 instances)	remove condition
Where	Chemical-Formula	contains the substring	C30	
and	the number of objects of	Appears-In-Right-Side-Of	is greater than	0
add a condition				

- Select desired data outputs

## 2. Select fields to include in the query output:

<b>Column 1</b> <input checked="" type="radio"/> Sort based on this column NAME	<b>Column 2</b> <input checked="" type="checkbox"/> <input type="radio"/> Sort based on this column Chemical-Formula	add a column
---	--	--------------

<b>Column 1</b> <input checked="" type="radio"/> Sort based on this column NAME	<b>Column 2</b> <input checked="" type="checkbox"/> <input type="radio"/> Sort based on this column Chemical-Formula	<b>Column 3</b> <input checked="" type="checkbox"/> <input type="radio"/> Sort based on this column Appears-In-Right-Side-Of	<b>Column 4</b> <input checked="" type="checkbox"/> <input type="radio"/> Sort based on this column Molecular-Weight	<b>Column 5</b> <input checked="" type="checkbox"/> <input type="radio"/> Sort based on this column Names
---	--	--	--	---

# Advanced searching in PMN databases

## Advanced Query Results

Your query in BioVelo is `sort (((x1^?NAME, x1^?CHEMICAL-FORMULA, x1^?APPEARS-IN-RIGHT-SIDE-OF, x1^?MOLECULAR-WEIGHT, x1^?NAMES) : x1<-PLANT^Compounds, ("C30" instringei x1^CHEMICAL-FORMULA) & ((#x1^APPEARS-IN-RIGHT-SIDE-OF) > 0)).1)`

This query resulted in a single table of 53 rows.

Column 1 for (x1 ^? NAME)	Column 2 for (x1 ^? CHEMICAL-FORMULA)	Column 3 for (x1 ^? APPEARS-IN-RIGHT-SIDE-OF)	Column 4 for (x1 ^? MOLECULAR-WEIGHT)	Column 5 for (x1 ^? NAMES)
<a href="#">α-amyrin</a>	<a href="#">C30H50O1</a>	<a href="#">(S)-2,3-epoxysqualene = α-amyrin</a>	<a href="#">426.724</a>	<a href="#">α-amyrin, viminalol, alpha-Amyrenol</a>
<a href="#">β-amyrin</a>	<a href="#">C30H50O1</a>	<a href="#">(S)-2,3-epoxysqualene = β-amyrin</a>	<a href="#">426.724</a>	<a href="#">β-amyrin, β-amyrenol</a>
<a href="#">(E)-cinnamoyl-CoA</a>	<a href="#">C30H42N7O17P3S1</a>	<a href="#">trans-cinnamate + coenzyme A = (E)-cinnamoyl-CoA + H<sub>2</sub>O</a>	<a href="#">897.68</a>	<a href="#">(E)-cinnamoyl-CoA</a>
<a href="#">(S)-2,3-epoxysqualene</a>	<a href="#">C30H50O1</a>	<a href="#">squalene + NADPH + O<sub>2</sub> = (S)-2,3-epoxysqualene + NADP<sup>+</sup> + H<sub>2</sub>O, O<sub>2</sub> + a reduced acceptor + squalene = (S)-2,3-epoxysqualene + H<sub>2</sub>O + an acceptor</a>	<a href="#">426.724</a>	<a href="#">(S)-2,3-epoxysqualene, squalene 2,3-epoxide, squalene 2,3-oxide, (S)-squalene-2,3-epoxide, 2,3-EDSQ, 2,3-epoxisqualene, oxidosqualene, 2,3-oxidosqualene</a>
<a href="#">24-ethylidenelophanol</a>	<a href="#">C30H50O1</a>	<a href="#">24-methylenelophanol + S-adenosyl-L-methionine = 24-ethylidenelophanol + S-adenosyl-L-homocysteine</a>	<a href="#">426.724</a>	<a href="#">24-ethylidenelophanol, (7Z)-24-ethylidenelophanol, citrostadienol</a>
<a href="#">4,4-dimethyl-14α-formyl-5α-cholesta-8,24-dien-3β-ol</a>	<a href="#">C30H48O2</a>	<a href="#">4,4-dimethyl-14α-hydroxymethyl-5α-cholesta-8,24-dien-3β-ol + NADPH + O<sub>2</sub> = 4,4-dimethyl-14α-formyl-5α-cholesta-8,24-dien-3β-ol + NADP<sup>+</sup> + 2 H<sub>2</sub>O</a>	<a href="#">440.708</a>	<a href="#">4,4-dimethyl-14α-formyl-5α-cholesta-8,24-dien-3β-ol</a>
<a href="#">4,4-dimethyl-14α-hydroxymethyl-5α-cholesta-8,24-dien-3β-ol</a>	<a href="#">C30H50O2</a>	<a href="#">lanosterol + NADPH + O<sub>2</sub> = 4,4-dimethyl-14α-hydroxymethyl-5α-cholesta-8,24-dien-3β-ol + NADP<sup>+</sup> + H<sub>2</sub>O</a>	<a href="#">442.724</a>	<a href="#">4,4-dimethyl-14α-hydroxymethyl-5α-cholesta-8,24-dien-3β-ol</a>
<a href="#">4-(1-methyl-2-pyrrolidinyl)-3-oxobutanoyl-CoA</a>	<a href="#">C30H49NBO18P3S1</a>	<a href="#">1-methylpyrrolidine-2-acetyl-CoA + acetyl-CoA = 4-(1-methyl-2-pyrrolidinyl)-3-oxobutanoyl-CoA + coenzyme A</a>	<a href="#">934.741</a>	<a href="#">4-(1-methyl-2-pyrrolidinyl)-3-oxobutanoyl-CoA, N-methylpyrrolidineacetoacetyl-CoA</a>
<a href="#">4-coumaroyl-CoA</a>	<a href="#">C30H42N7O18P3S1</a>	<a href="#">coenzyme A + 4-coumarate + ATP = 4-coumaroyl-CoA + diphosphate + AMP</a>	<a href="#">913.629</a>	<a href="#">4-coumaroyl-CoA, p-coumaroyl-CoA, 4-coumaroyl-CoA, coumaroyl-CoA, p-coumaroyl-CoA</a>

# Advanced searching in PMN databases

---

- Other queries?
  - Identify all of the “glycosyltransferase” enzymes associated with more than two reactions in AraCyc
    - List their:
      - name
      - subcellular localization
      - molecular weight
      - inhibitors, activators, etc.
  - Find all of the biochemical pathways in PoplarCyc that have more than 5 reactions and where at least one of those reactions lacks enzymes
    - List their:
      - name
      - reactions
      - citations and evidence codes
  - These searches can be used to span more than one PMN database
- What if I only have a gene or protein sequence?



# PMN BLAST 2.2.8

Please note that this is a beta version of the PMN BLAST 2.2.8.

Blast

BLAST Species: [Arabidopsis thaliana col](#)

Database Summary:

When recombinantly expressed in *E. coli*, this enzyme was shown to have ACS activity [ [Yamagami03](#) ].

Gene: [ACS11](#)

Sequence Length: 1825/3 AAs

Unification Links: [Phytozome Plant Orthologs AT4G08040.1](#)

Upload Gene-Reaction Schematic: 

Raw, FASTA  
☒ [FASTA](#)

Advanced BLAST  
[expand](#)

Results Ref

Output Title:

E-mail address:

Return Results:

Result Format:

Please be patient

Selecting an

## PlantCyc Enzyme: 1-aminocyclopropane-1-carboxylate synthase



### Enzymatic reaction of: 1-aminocyclopropane-1-carboxylate synthase



[S-adenosyl-L-methionine](#)  $\rightleftharpoons$  [S-methyl-5'-thioadenosine](#) + [1-aminocyclopropane-1-carboxylate](#)

The reaction direction shown, that is,  $A + B \rightleftharpoons C + D$  versus  $C + D \rightleftharpoons A + B$ , is in accordance with the Enzyme Commission system.

Reversibility of this reaction is unspecified.

In Pathways: [ethylene biosynthesis from methionine](#)

Citations: [ [Yamagami03](#) ]

Score E  
(bits) Value

<a href="#">921</a>	0.0
<a href="#">652</a>	0.0
<a href="#">652</a>	0.0
<a href="#">652</a>	0.0
<a href="#">635</a>	0.0
<a href="#">633</a>	0.0
<a href="#">632</a>	0.0
<a href="#">631</a>	0.0
<a href="#">631</a>	0.0
<a href="#">614</a>	e-176
<a href="#">613</a>	e-176
<a href="#">613</a>	e-176
<a href="#">538</a>	e-154
<a href="#">526</a>	e-150
<a href="#">526</a>	e-150
<a href="#">524</a>	e-149
<a href="#">520</a>	e-148
<a href="#">513</a>	e-146
<a href="#">503</a>	e-143
<a href="#">501</a>	e-143
<a href="#">500</a>	e-142
<a href="#">498</a>	e-142
<a href="#">486</a>	e-138
<a href="#">414</a>	e-116
<a href="#">392</a>	e-110
<a href="#">392</a>	e-110

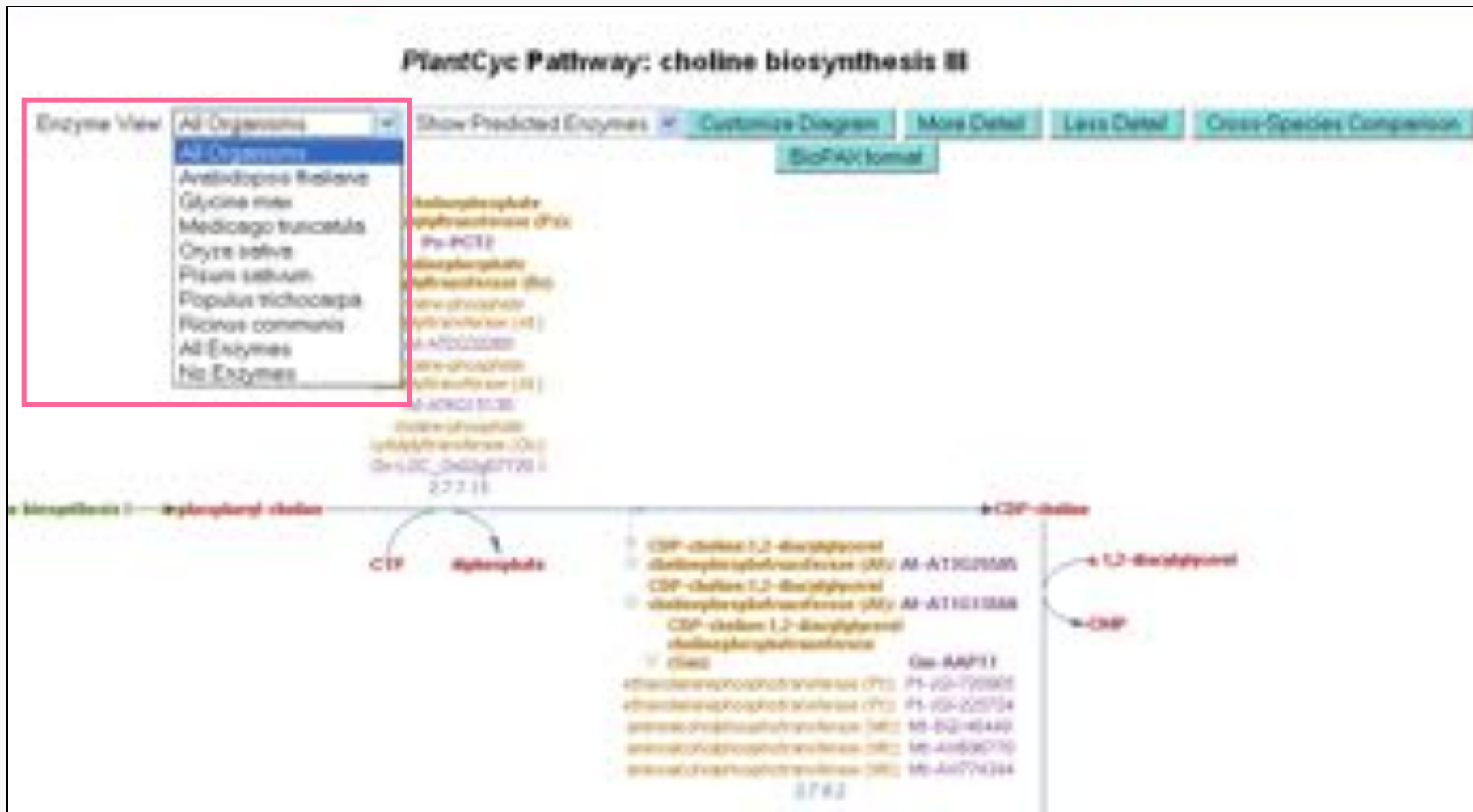
Run BLAST

reset

[Q8GYO](#) | PlantCyc: [AT5G51690-WONKER](#) | aromatic-amino-acid ...  
[Q570P9](#) | PlantCyc: [AT5G51690-WONKER](#) | aromatic-amino-acid ...

# Comparing across species

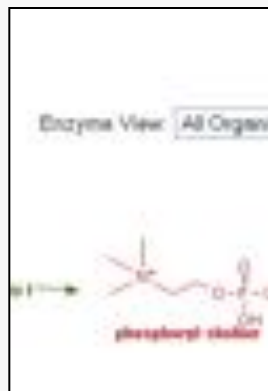
- Use species selection tool on pathway pages





## Compa

■ Us



Organism	Evidence Glyph	Enzymes and Genes for choline biosynthesis III	
<a href="#">AcaCyc.col</a>		<a href="#">EC#2.7.7.15</a>	choline-phosphate cytidylyltransferase: <a href="#">AT4G15130</a> choline-phosphate cytidylyltransferase: <a href="#">AT2G32280</a>
		<a href="#">EC#2.7.8.2</a>	phosphatidyltransferase: <a href="#">AT3G25995</a> phosphatidyltransferase: <a href="#">AT1G13980</a>
		<a href="#">EC#3.1.4.4</a>	phospholipase D: <a href="#">AT1G52570</a> phospholipase D: <a href="#">AT1G55180</a> phospholipase D: <a href="#">AT3G05630</a> phospholipase D: <a href="#">AT4G00240</a> phospholipase D: <a href="#">AT4G11830</a> phospholipase D: <a href="#">AT4G11840</a> phospholipase D: <a href="#">AT5G25370</a> phospholipase D: <a href="#">PLD.alpha</a> phospholipase D: <a href="#">PLD.beta</a> phospholipase D: <a href="#">PLD.gamma</a> phospholipase D: <a href="#">PLD.delta</a> phospholipase D: <a href="#">PLD.zeta</a>
<a href="#">P.trichocarpa</a>		<a href="#">EC#2.7.7.15</a>	None
		<a href="#">EC#2.7.8.2</a>	diacylglycerol cholinephosphotransferase: <a href="#">JGI-225724</a> diacylglycerol cholinephosphotransferase: <a href="#">JGI-720905</a>
		<a href="#">EC#3.1.4.4</a>	phospholipase D: <a href="#">JGI-811801</a> phospholipase D: <a href="#">JGI-781949</a> phospholipase D: <a href="#">JGI-810175</a> phospholipase D: <a href="#">JGI-593768</a> phospholipase D: <a href="#">JGI-827395</a> phospholipase D: <a href="#">JGI-578949</a> phospholipase D: <a href="#">JGI-730956</a> phospholipase D: <a href="#">JGI-240457</a> phospholipase D: <a href="#">JGI-833366</a> phospholipase D: <a href="#">JGI-417354</a> phospholipase D: <a href="#">JGI-763496</a> phospholipase D: <a href="#">JGI-558891</a> phospholipase D: <a href="#">JGI-415367</a> phospholipase D: <a href="#">JGI-550827</a> phospholipase D: <a href="#">JGI-756219</a> phospholipase D: <a href="#">JGI-180605</a> phospholipase D: <a href="#">JGI-829577</a>

[Download Genes](#)

[BioPAFormat](#)

# Comparing across species

## ■ Use general Comparative Analyses tools

### Comparative Analysis and Statistics

This page allows you to compute statistics for a single Pathway/Genome Database, and to compute comparisons across multiple Pathway/Genome Databases for the set of organisms listed below. Note that computing summary statistics for the organism databases you have chosen may take several minutes. For faster operation, install Pathway Tools on your own computer! [Click here](#) for details.

[Click here](#) to go to the Webinar page, where you can watch the Comparative and Omics Tools in BioCyc instructional videos.

Note: In addition to reflecting differences in biology of different organisms, these statistics will reflect differences in the levels of curation, data availability, and completeness of the PGDBs for these organisms.

Select which set(s) of comparative-analysis tables you wish to generate:

- ☐ **Reactions:** breakdowns by type of substrate, by EC Number, by number of isozymes, etc.
- ☐ **Pathways:** breakdown by pathway class, information on pathway holes.
- ☐ **Compounds:** small molecules that act as substrates, enzyme activators/inhibitors/cofactors.
- ☐ **Proteins:** breakdown of protein complexes by type and number of subunits, number of enzymes, number of enzymes with activators/inhibitors/cofactors, multifunctional enzymes.
- ☐ **Orthologs:** proteins shared among organisms or unique to an organism.
- ☐ **Transporters:** proteins that facilitate the movement of compounds across cell membranes.
- ☐ **Transcription Units:** number of genes per transcription unit, number of operons per pathway.

Select one or more organism databases:

☐ *Arabidopsis thaliana* col ☐ PlantCyc ☐ *Populus trichocarpa*

# Comparing across species

Pathway Class	Pathway Class: Biosynthesis - Amines and Polyamines Biosynthesis	AraCyc col	P. trichocarpa
Biosynthesis	glycine betaine biosynthesis III (plants)	X	X
- Amines and Polyamines Biosynthesis	putrescine biosynthesis by agmatinase	X	
- Amino acids Biosynthesis	putrescine biosynthesis II		X
- Aminoacyl-tRNA Charging	putrescine biosynthesis IV	X	
- Aromatic Compounds Biosynthesis	putrescine biosynthesis via N-carbamoylputrescine	X	X
- Carbohydrates Biosynthesis	spermidine biosynthesis	X	X
- Cell structures Biosynthesis	spermine biosynthesis	X	X
- Cofactors, Prosthetic Groups, Electron Co	UDP-N-acetyl-D-glucosamine biosynthesis	X	X
- Fatty Acids and Lipids Biosynthesis	urate biosynthesis	X	
- Hormones Biosynthesis			
- Metabolic Regulators Biosynthesis			
- Nucleosides and Nucleot			
- Other Biosynthesis			
- Polysaccharides			
- Secondary Metabolism			
- Secondary Metabolites B			
- Siderophore Biosynthesis			
- Siderophore Biosynthesis			
Degradation/Utilization/Aas			
- Alcohols Degradation			
- Aldehyde Degradation			
- Amines and Polyamines			

Pathway Holes	AraCyc col	P. trichocarpa
Number of Pathway Holes	435	545
Pathway Holes as a percentage of total reactions in pathways	29%	45%
Pathways with No Holes	100	93
Pathways with 1 Hole	80	76
Pathways with 2 Holes	45	43
Pathways with 3 Holes	13	22
Pathways with 4 Holes	12	14
Pathways with 5 Holes	7	9
Pathways with > 5 Holes	20	28
Total Pathways with Holes	178	192





# Comparing across species

## Overview of the AraCyc Metabolic Map

This diagram provides a schematic of all pathways of AraCyc metabolism in the aracyc database. Nodes represent metabolites, with shape indicating class of metabolite (see key to right). Lines represent reactions. Move the mouse over a metabolite icon to navigate to the metabolite page or a related pathway page.

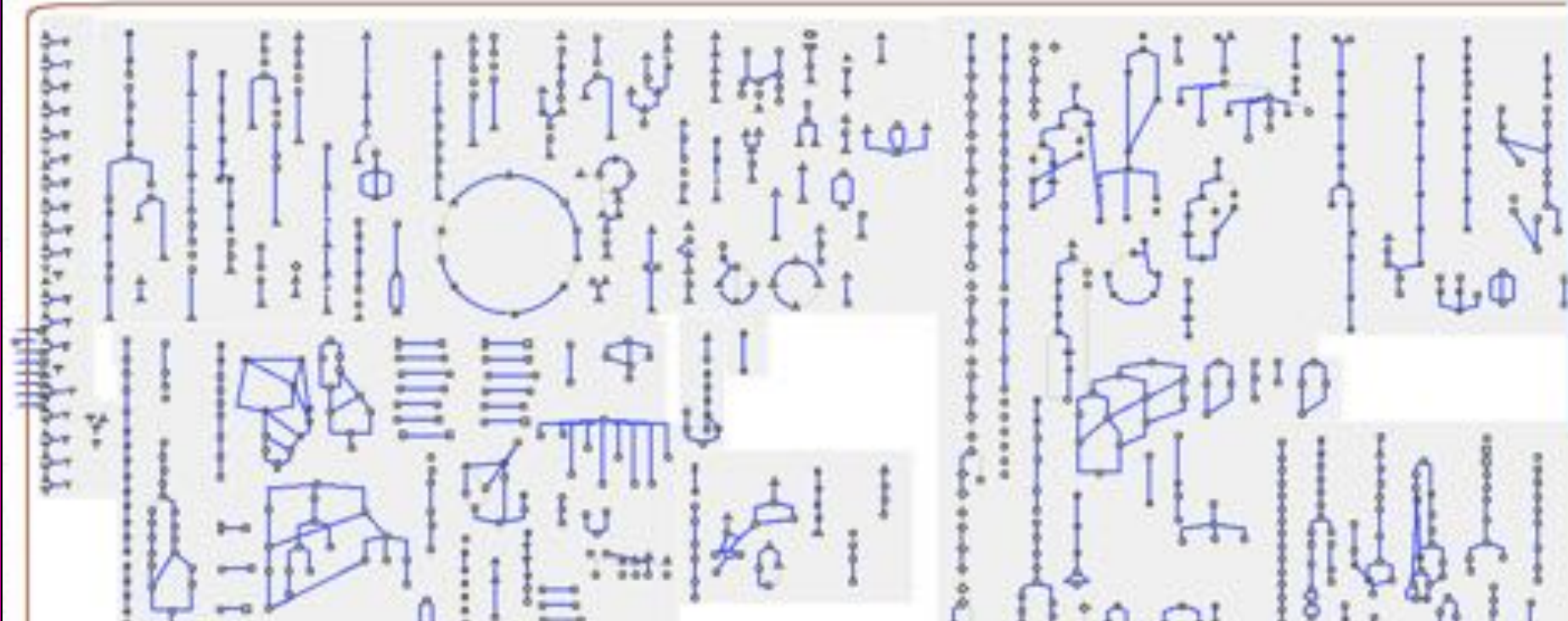
- [Instructions](#)
- [Pathway Tools query page](#)
- [Omics Viewer: Paint omics data onto this diagram](#)
- [Species Comparison: Highlight reactions shared with other organisms](#)

Select one or more organisms:

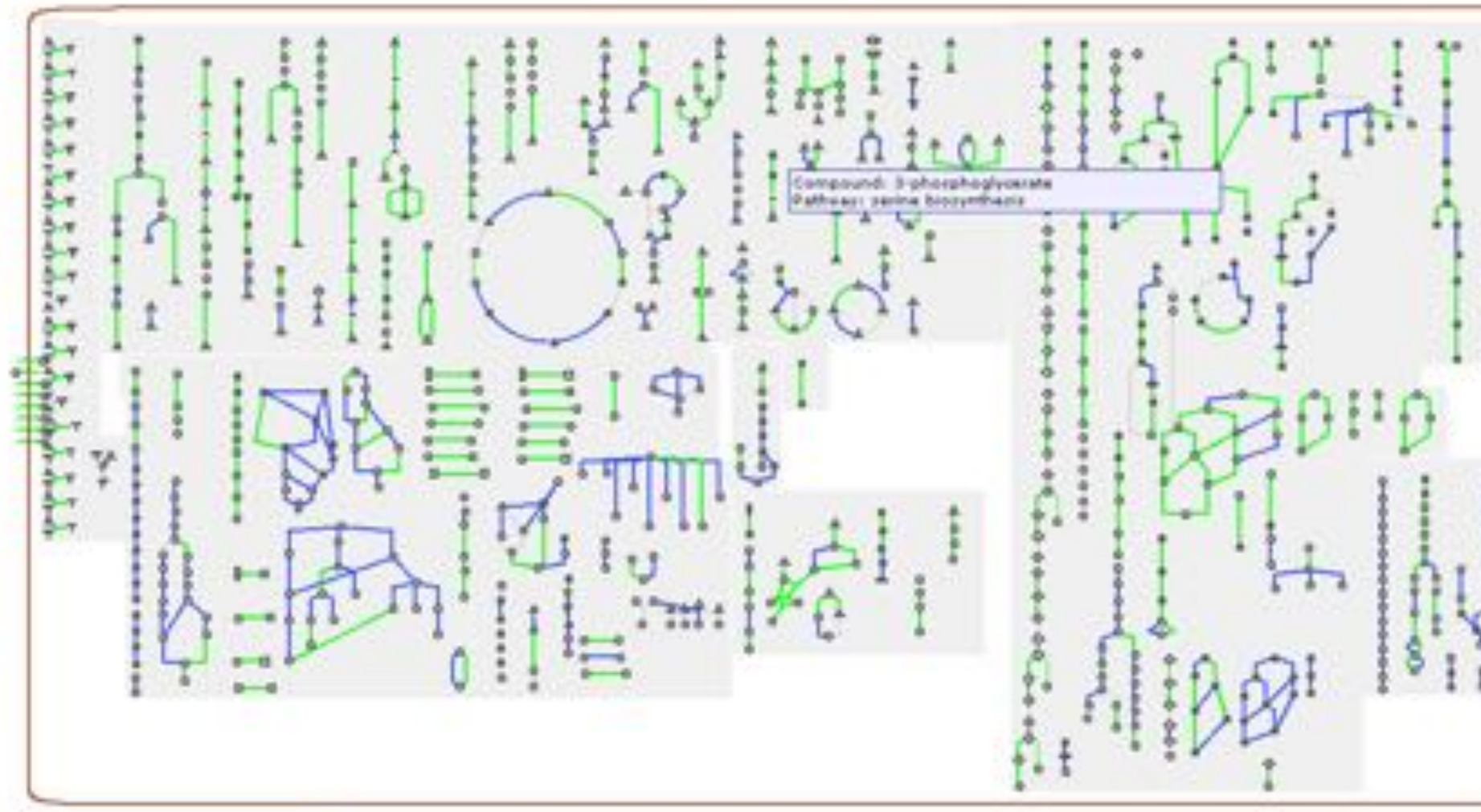
☐ PlantCyc ☒ Populus trichocarpa

Submit

Clear All



## Comparing across species



# Visualizing OMICs data

---

- Overlay “pre-cleaned” data sets on a metabolic map
  - ▣ Gene transcription data
  - ▣ Proteomic data
  - ▣ Metabolomic data

# Visualizing OMICs data

---

- ❑ Case study: Analyzing an Arabidopsis mutant with “no phenotype”
  - Basic phenotypic analyses do not reveal any differences:
    - ❑ growth
    - ❑ development
    - ❑ response to hormones
    - ❑ etc.
  - Perform a microarray analysis
    - ❑ Measure transcript levels in wild-type and mutant plants
  - Clean and process data
    - ❑ Remove genes expressed below background levels
    - ❑ Measure fold-increase or decrease in mutant vs. wild-type
    - ❑ Discard statistically insignificant data
  - **Do these transcript differences highlight possible metabolic perturbations?**



# Visualizing OMICs data



File Edit Format View Help

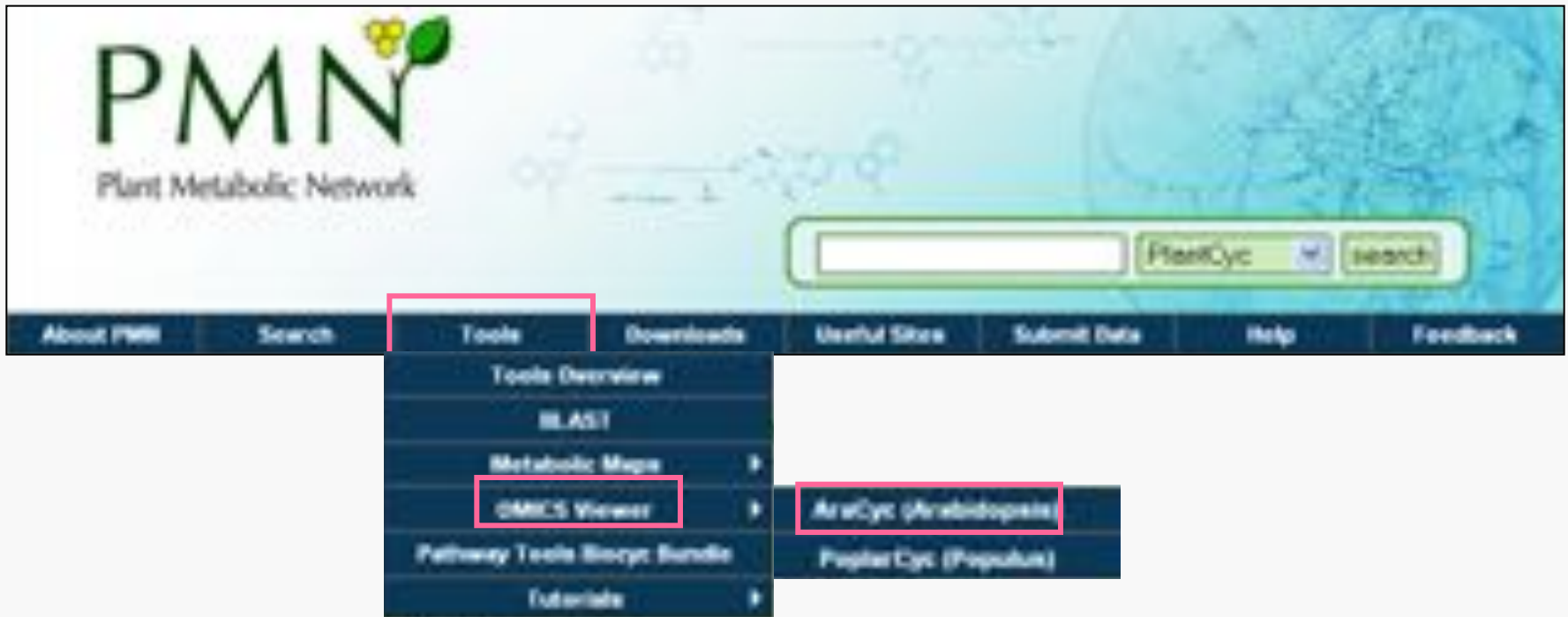
PMW\_workshop\_part\_2\_data\_file.txt - Notepad

> All genes with significantly altered expression levels in csm1-1 mutants relative to wild type

gene	change in expression in csm1-1 mutant relative to wild type
AT2G08510	1
AT3G08510	7
AT2G03960	-3
AT3G02100	2
AT3G031800	3
AT2G02040	1
AT3G052570	-2
AT2G02170	-5
AT2G05180	-2
AT3G05180	-6
AT2G078090	1
AT3G078090	7
AT2G07110	7
AT2G02260	-4
AT2G42030	-5
AT3G06870	10
AT3G04870	1
AT3G05630	-8
AT3G05630	-2
AT3G020230	6
AT3G020230	1
AT3G020230	11
AT3G04440	6
AT3G021730	-6
AT3G026785	-1
AT3G04220	4
AT3G04220	2
AT3G025585	-5
AT3G025585	-1
AT3G025585	-5

# Visualizing OMICs data

- Upload data in the OMICs viewer



# Visualizing OMICs data

- Upload data in the OMICs viewer

**Pathway Tools Omics Viewers**

Select a dataset: Arabidopsis thaliana col

File containing experimental data (NOT a URL): Browse...

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

If displaying relative data values, use

☒ a single data column  
☐ the ratio of two data columns

☒ 0-centered scale (e.g. log scale)  
☐ 1-centered scale (negative values will be discarded)

Data values use a: Gene names and/or identifiers

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

Data column (numerator in ratios): 1

If using two columns, denominator data column:

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.

# Visualizing OMICs data

- Set display parameters in the OMICs viewer

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 either paint data values on the genomic map, or 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 one of these alternative displays, choose the corresponding option below and specify the threshold if appropriate. Note that if both the cellular and genome overviews are specified, the genome overview will appear in a new browser window (you must have popups enabled for this site or this will not work).

- ☒ Paint data on cellular overview chart (default)
- ☐ Paint data on genome overview chart
- ☒ Generate a table of individual pathways exceeding threshold:

**Submit**

Note that this request will take several minutes to complete (possibly longer for large datasets). For faster operation, install Pathway Tools on your own computer! [Click here](#) for details.

# Visualizing OMICs data

Navigate to...

Pathway: [trans-lycopene biosynthesis](#)

Superpathway: [superpathway of carotenoid biosynthesis](#)

Compound: [geranylgeranyl diphosphate](#)

2 geranylgeranyl diphosphate

## *Arabidopsis thaliana* col Pathway: trans-lycopene biosynthesis

[Customize Diagram](#)

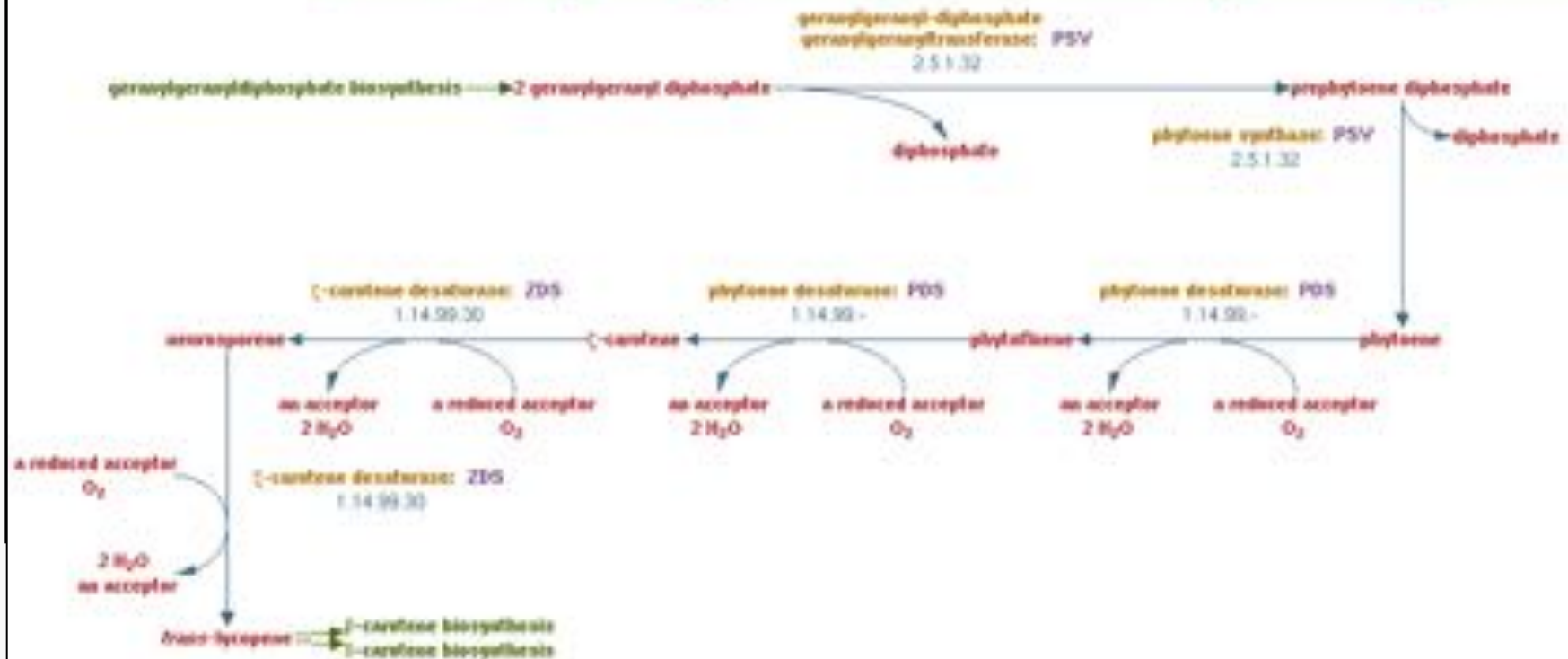
[More Detail](#)

[Less Detail](#)

[Cross-Species Comparison](#)

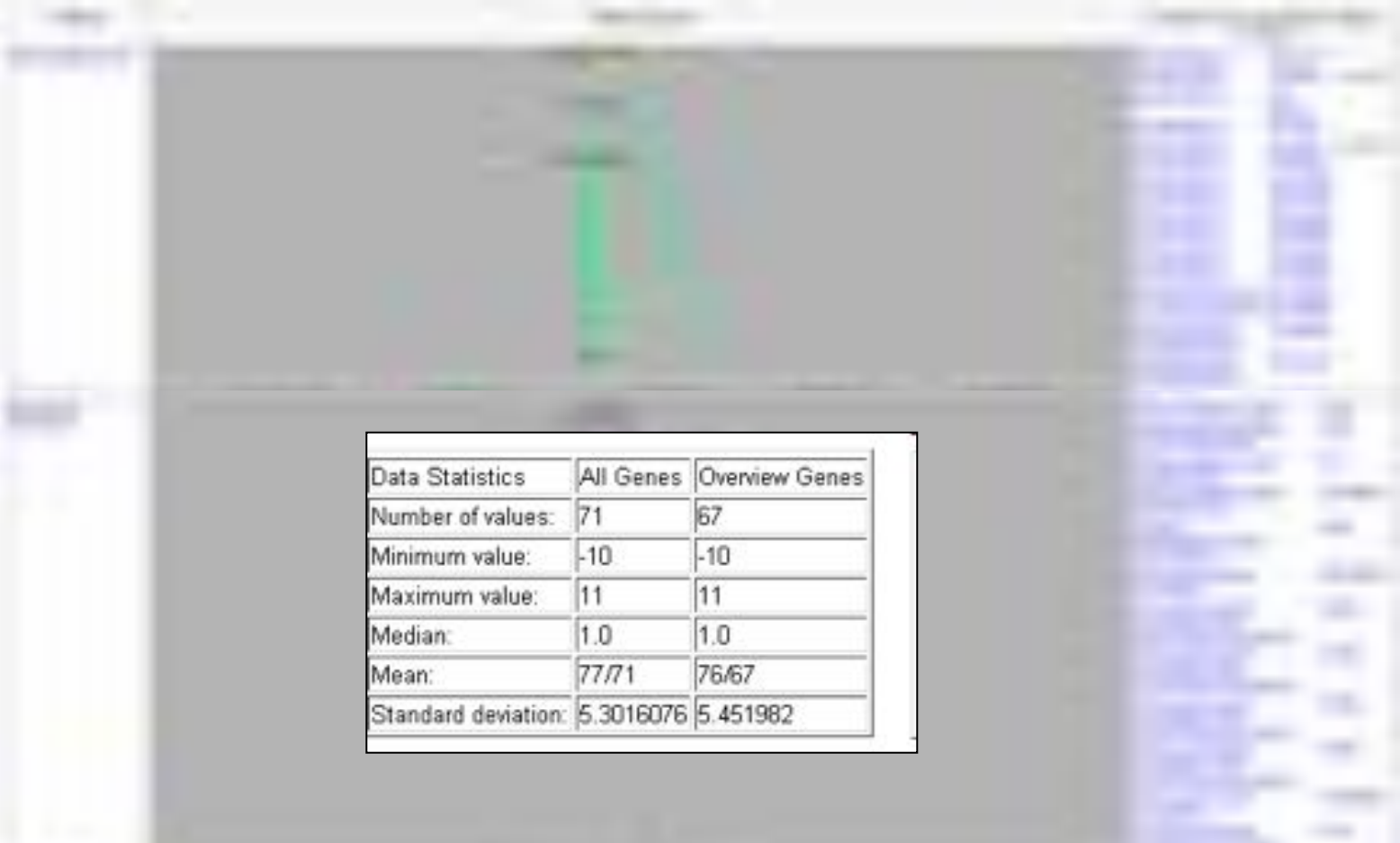
[Download Genes](#)

[BioPAX format](#)





## Visu



Data Statistics	All Genes	Overview Genes
Number of values:	71	67
Minimum value:	-10	-10
Maximum value:	11	11
Median:	1.0	1.0
Mean:	77/71	76/67
Standard deviation:	5.3016076	5.451982

- The mutant with “no phenotype” has
  - decreased levels of transcripts related to phospholipid biosynthesis
  - elevated levels of transcripts related to carotenoid biosynthesis
- Future targeted experiments can be planned!

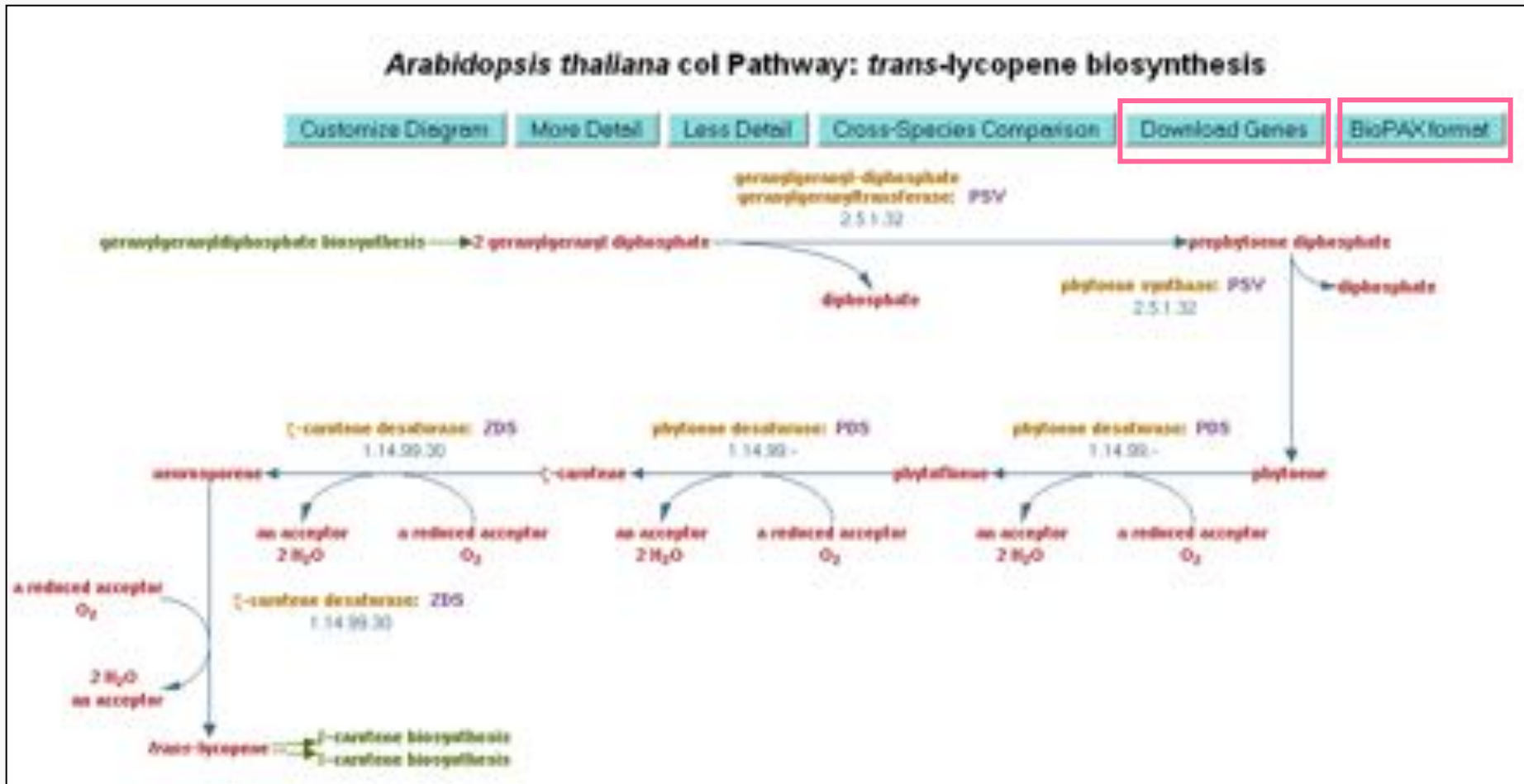
# Visualizing OMICs data

---

- Many applications
- View changes in transcript, protein, or metabolite levels related to:
  - Mutant phenotype
  - Biotic stresses
  - Abiotic stresses
  - Natural variation
  - Developmental stage
  - Tissue type
- Display static measurements or changes over time
  - Animation feature is available

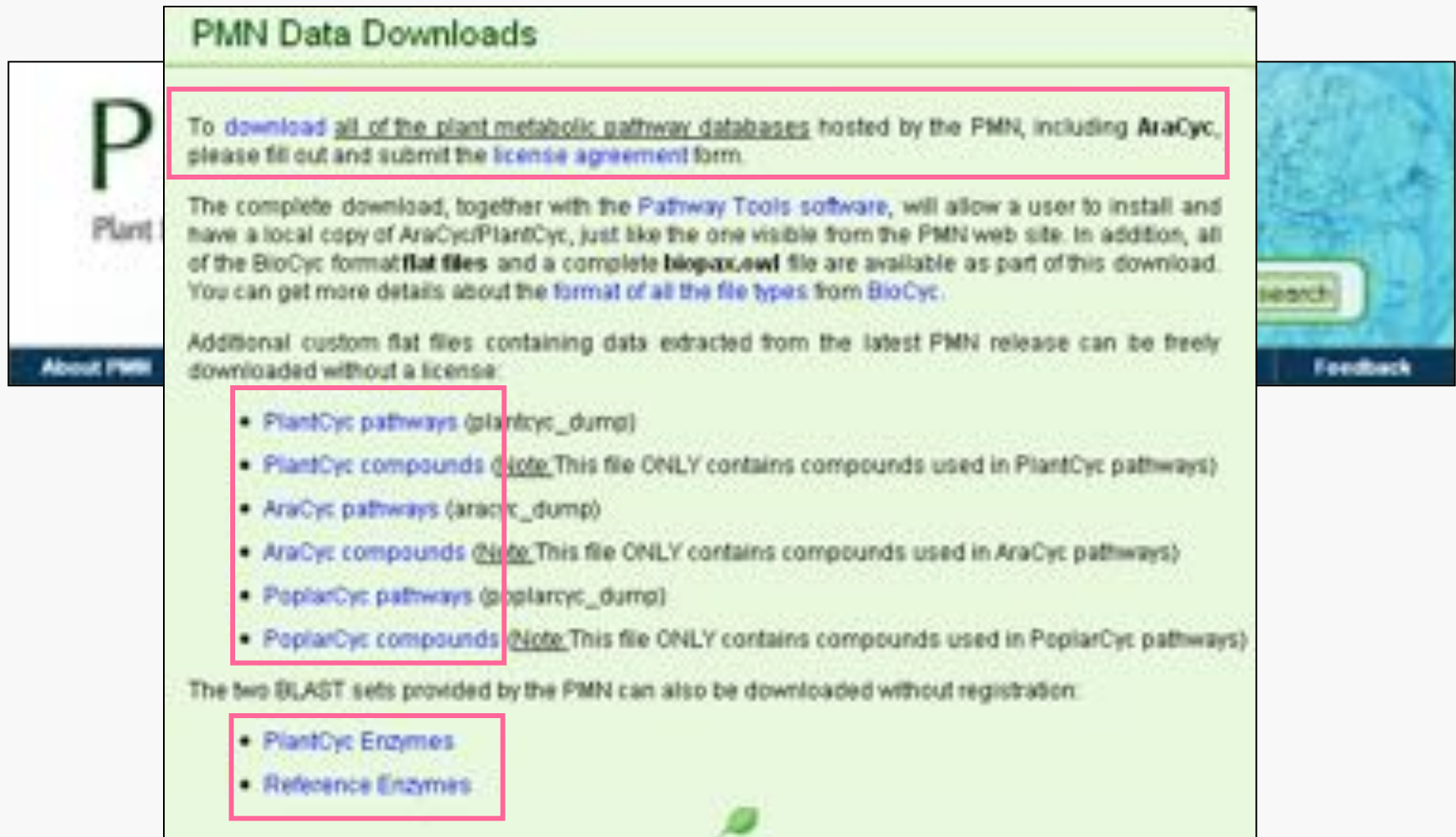
## Data and software downloads

- Get pathway data sets from pathway pages



# Data and software downloads

- Obtain large data sets



The image is a screenshot of the 'PMN Data Downloads' page. The page has a light green header with the title 'PMN Data Downloads'. Below the header, there is a pink-bordered box containing text about downloading plant metabolic pathway databases and the need to submit a license agreement form. The main content area is white and contains several paragraphs and a bulleted list. A second pink-bordered box highlights a list of six data sets: PlantCyc pathways, PlantCyc compounds, AraCyc pathways, AraCyc compounds, PoplarCyc pathways, and PoplarCyc compounds. A third pink-bordered box at the bottom highlights two BLAST sets: PlantCyc Enzymes and Reference Enzymes. The page also features a search bar and a feedback link on the right side.

## PMN Data Downloads

To [download all of the plant metabolic pathway databases](#) hosted by the PMN, including AraCyc, please fill out and submit the [license agreement form](#).

The complete download, together with the [Pathway Tools software](#), will allow a user to install and have a local copy of AraCyc/PlantCyc, just like the one visible from the PMN web site. In addition, all of the BioCyc format [flat files](#) and a complete [biogpx.xml](#) file are available as part of this download. You can get more details about the [format of all the file types](#) from BioCyc.

Additional custom flat files containing data extracted from the latest PMN release can be freely downloaded without a license:

- [PlantCyc pathways \(plantcyc\\_dump\)](#)
- [PlantCyc compounds](#) ([Note](#) This file ONLY contains compounds used in PlantCyc pathways)
- [AraCyc pathways \(aracyc\\_dump\)](#)
- [AraCyc compounds](#) ([Note](#) This file ONLY contains compounds used in AraCyc pathways)
- [PoplarCyc pathways \(poplarcyc\\_dump\)](#)
- [PoplarCyc compounds](#) ([Note](#) This file ONLY contains compounds used in PoplarCyc pathways)

The two BLAST sets provided by the PMN can also be downloaded without registration:

- [PlantCyc Enzymes](#)
- [Reference Enzymes](#)

# Data and software downloads

PMN: Complete Database Download

Welcome to PMN and AraCyc users!

Approximately one business day after you agree to the terms of the license and submit the completed form, a staff member will review your request and email you download instructions.  
If you have any questions please email: [curator@plantcyc.org](mailto:curator@plantcyc.org)

Title

Name \*

Email \*

Repeat your email

Institution \*

Department

<input checked="" type="checkbox"/> biopax	<input type="checkbox"/> genes	<input type="checkbox"/> proteins	<input type="checkbox"/> species
<input type="checkbox"/> classes	<input type="checkbox"/> overview-graph	<input type="checkbox"/> profligandplives	<input type="checkbox"/> terminators
<input checked="" type="checkbox"/> compounds	<input type="checkbox"/> pathways	<input type="checkbox"/> pubo	<input type="checkbox"/> transporters
<input type="checkbox"/> dualindoles	<input type="checkbox"/> pathways	<input type="checkbox"/> reactions	<input type="checkbox"/> transcripts
<input type="checkbox"/> enzymes	<input type="checkbox"/> promoters	<input type="checkbox"/> reactions-dmj	
<input type="checkbox"/> enzymes	<input type="checkbox"/> protoplus	<input type="checkbox"/> regulation	
<input type="checkbox"/> genes	<input type="checkbox"/> protein-features	<input type="checkbox"/> regions	

 Database  
002 of 16  
13,873 kb

- Data formats include:
  - ocelot, Biopax (OWL), SBML, .dat



# Data and software downloads

- Install a local copy of the Pathway Tools software



**How to Obtain Downloads**

The software and databases are available through different license agreements; please choose the license that is best suited to your needs:

	Complete License	Data File License
<b>Materials Provided</b>	1. Software/Database Bundle 2. Data Files	Data files only
<b>Licensing Speed</b>	Online license reviewed by SRI, usually within one business day	Quick online licensing
<b>License Terms</b>	Free to academics for research purposes; fee for commercial use	Free to all
<b>Obtain License</b>	<a href="#">click here</a>	<a href="#">click here</a>



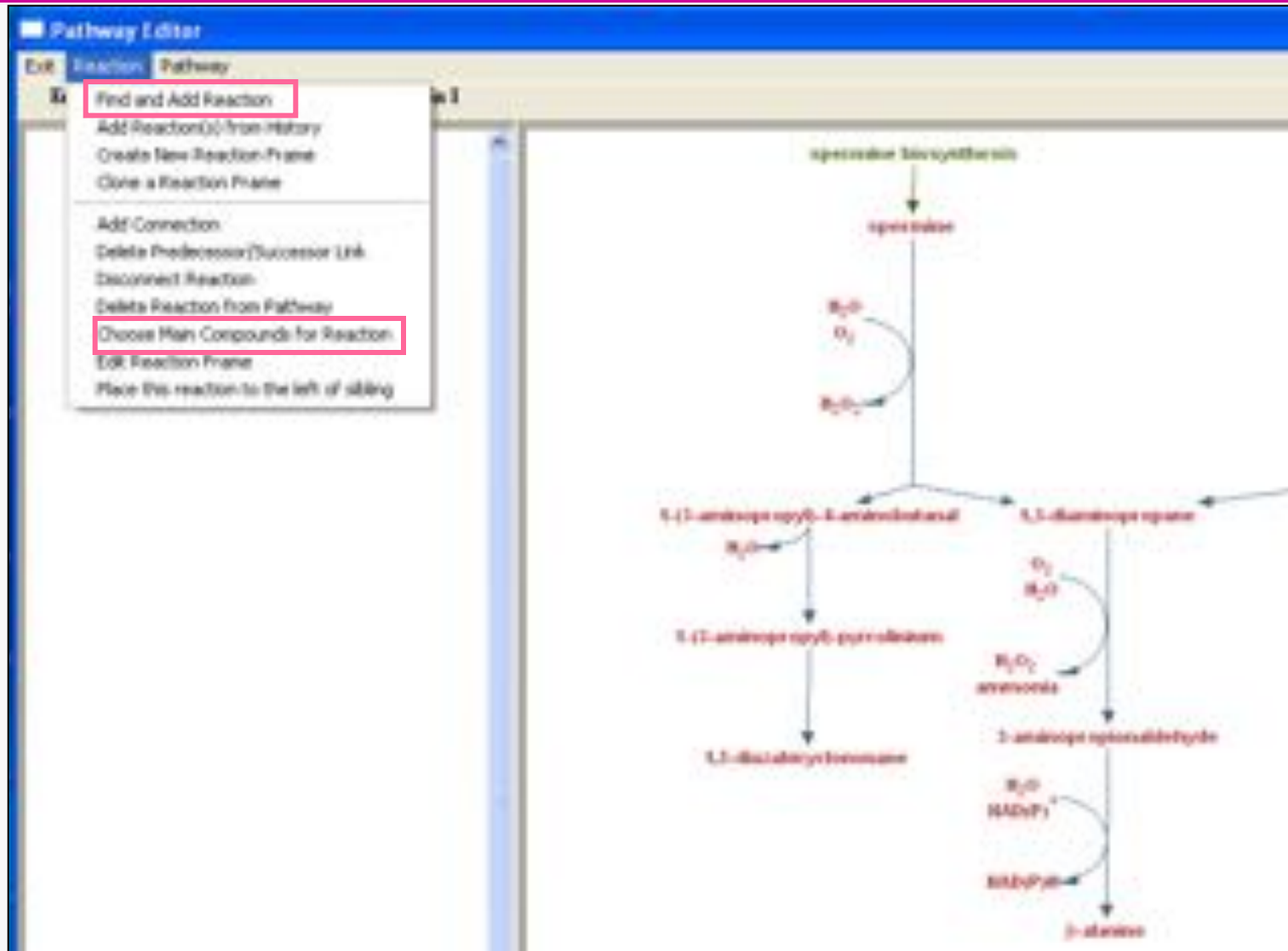
# Data and software downloads

- Desktop version offers additional features

The screenshot shows the Pathway Tools version 12.5 desktop application. The title bar reads "Pathway Tools version 12.5". The menu bar includes "File", "Overview", "Pathway", "Reaction", "Protein", "RNA", "Gene", "Compound", "Chromosome", "Tools", and "Help". The main window title is "Populus trichocarpa". Below the title bar, there are buttons for "Home", "Back", "Forward", "History", "New", "Recent", "Clone", and "Save DB". The main content area displays the species name *Populus trichocarpa* in a large, stylized font, with "version: 1.0" below it. There are two buttons: "Generate Pathway Evidence Report" and "Generate Pathway Histo Report". Below these buttons is a table with the following data:

<u>Replicon</u>	<u>Total Genes</u>	<u>Protein Genes</u>	<u>RNA Genes</u>	<u>Pseudogenes</u>	<u>Size (bp)</u>
Chromosome 1	271	271	0	0	
Chromosome 2	237	237	0	0	
Chromosome 3	149	149	0	0	
Chromosome 4	114	114	0	0	
Chromosome 5	156	156	0	0	
Chromosome 6	175	175	0	0	

# Data and software downloads



# Data and software downloads

- Trace metabolites through metabolic pathways

The screenshot shows a software interface for metabolic tracing. The main window has a menu bar with 'File', 'Overview', 'Pathway', 'Reaction', 'Protein', 'RNA', 'Gene', 'Compound', 'Oversonse', 'Tools', and 'Help'. The 'Overview' menu is open, showing options like 'Omics Viewer: Overlay Experimental Data from', 'Clear All Highlighting', 'Show Cellular Overview' (CTRL+O), 'Show Key', 'Show/Hide Transport Links', 'Highlight', 'Metabolite Tracing' (highlighted with a red box), 'Print as Poster', 'Update...', 'Show Complete Regulatory Overview' (CTRL+R), 'Highlight Genes', 'Redisplay Highlighted Genes Only', 'Zoom Regulatory Overview', 'Preferences for Regulatory Overview', 'Show Regulatory Key Code', 'Save Current Regulatory Overview to File', 'Load Regulatory Overview from File', 'Show Genome Overview' (CTRL+G), and 'Highlight Genes by Substring'. A 'Metabolite Tracing Controls' dialog box is open, showing 'Exit', 'Restart', 'View', and 'Help' buttons. The dialog has a 'Starting Metabolite: L-glutamate' field, a 'Trace Direction: Forward' dropdown (highlighted with a red box), and a 'Number of levels to expand at a time' field with a value of 1 (highlighted with a red box). The background shows a complex metabolic pathway diagram with various metabolites and reactions.

# Data and software downloads

- Trace metabolites through metabolic pathways

**Metabolic Tracing Controls**  
File Replot View Help

Starting Metabolite: L-glutamate  
Trace Direction: Forward  
Number of levels to expand at a time: 1

☒ Show not-followed branches?

Show traced connections between pathways:  
For all compounds on chosen path

**Key to node and edge colors:**  
L-glutamate  
Reactions and compounds in chosen path  
Reactions and compounds in candidate paths  
Reactions and compounds not followed

Candidate end metabolites and those that can be further expanded:  
alpha-ketoglutarate

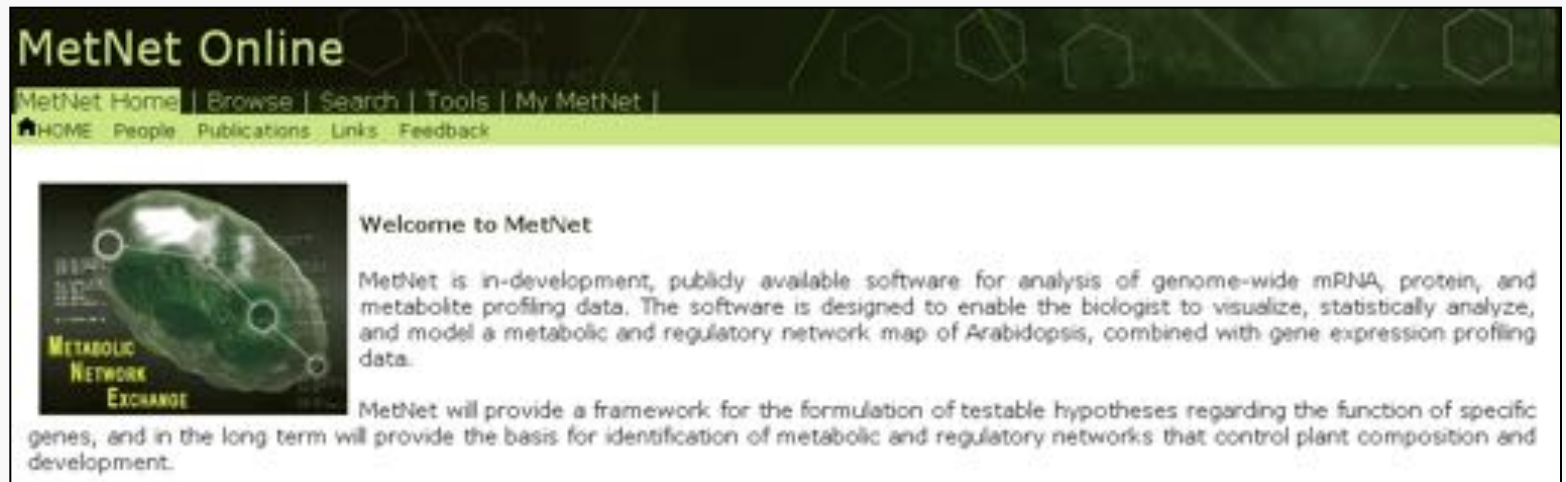
EC# 2.6.1.42 [L-alanine + alpha-ketoglutarate → L-glutamate + 2-oxo-3-methylvalerate]  
Enzymes: catalytic, branched-chain amino acid aminotransferase/branched-chain amino acid transaminase, branched-chain amino acid aminotransferase, branched-chain amino acid aminotransferase, branched-chain amino acid transaminase  
Pathway: valine biosynthesis

1,4-bisphosphonate  
N-acetyl-L-glutamate  
N-acetyl-L-cysteine  
α,1,10-methylene tetrahydrofolate  
α-bisphosphonate  
α-tetrahydrofolate polyglutamate  
an H2O-formyl tetrahydrofolate  
glutamate (H2O & Lys)  
glycine  
indole-3-acetyl glutamate



## Data and software downloads

- Coming soon . . . create and work with “groups” of objects
  - ▣ For some AraCyc pathways and other plant metabolic pathways, you can create and work with groups of objects NOW at:
  - ▣ MetNetDB: <http://metnet3.vrac.iastate.edu/index.php>



**MetNet Online**

MetNet Home | Browse | Search | Tools | My MetNet |  
HOME People Publications Links Feedback

**Metabolic Network Exchange**

**Welcome to MetNet**

MetNet is in-development, publicly available software for analysis of genome-wide mRNA, protein, and metabolite profiling data. The software is designed to enable the biologist to visualize, statistically analyze, and model a metabolic and regulatory network map of Arabidopsis, combined with gene expression profiling data.


MetNet will provide a framework for the formulation of testable hypotheses regarding the function of specific genes, and in the long term will provide the basis for identification of metabolic and regulatory networks that control plant composition and development.

# Creating new PMN content

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- Manual curation
  - ▣ Entering experimental data
- Computational prediction

Ac



PlantCycsearch

[About PMN](#)[Search](#)[Tools](#)[Downloads](#)[Useful Sites](#)[Submit Data](#)[Help](#)[Feedback](#)

### Contact Us

- [Contact Info](#)
- [Feedback Form](#)
- [Submit Data](#)

## Data Submission

[Data Submission](#)[Feedback Form](#)

Please help us expand the content of the PMN databases, including AraCyc and PlantCyc!

- We welcome any and all **new** data submissions related to plant biochemical pathways.
- You can also **correct** an existing pathway
  - Not sure what types of information to include?  
Try using one of our [data submission / correction forms](#) below.
- Or, just use our [Feedback Form](#) or **send an e-mail** to [curator@plantcyc.org](mailto:curator@plantcyc.org) and append your data as an attachment

### Data submission / correction forms

\*\*\*\* You do not need to fill in all the columns. (See our [tutorial](#) for help)

We will be happy to accept whatever information you can easily provide ...

[Compound form](#)

[Enzyme / Reaction form](#)

[Pathway form](#)

About PMN	Search	Tools	Downloads	Useful Sites	Submit Data	Help	Feedback
Project Overview							
Documentation							
Presentations							
Statistics							
Release Notes							
Contact Info							
News							
PMN Staff							
Collaborators							
<b>Contributors</b>							
Editorial Board							

## PMN Contributors

PMN contributors from around the world have added to or helped to improve the content of AraCyc, PlantCyc, and the other PlantCyc-derived databases that are part of the PMN.

In addition to the active contributions from the PMN [editorial board](#) and PMN [collaborators](#), the following individuals have contributed significantly in improving the content of PlantCyc, AraCyc, and the other PlantCyc-derived databases that are part of the PMN:

- Some contributors have [contacted](#) us with suggestions and revisions.
- Some have generously responded to appeals for help from the curators.
- Some have attended curatorial jamborees.

### General Assistance

- E.J. Bollen - Wageningen, The Netherlands
- Mark Pooleman - Oxford Brookes University, UK
- Bryan Raymont - Universidad de Chile, Chile

### Contributors to Pathways of Primary and Secondary Metabolism

#### Primary Metabolism

##### Amino and Polyamines

- John J. Jansz - Virginia Tech, USA

##### Amino Acids

- Vijay Joshi - Cornell University, USA

##### Carbohydrates

- Christophe D'Hulst - Unité de Glycobiologie Structurale et Fonctionnelle, France

##### Cofactors, Prosthetic Groups, and Electron Carriers

- Inad Aggar - Michigan State University, USA
- J. Clark Lagarias - University of California, Davis, USA
- Rob Last - Michigan State University, USA
- Carlos Menck - Universidade de São Paulo, Brazil
- David Oliver - Iowa State University, USA
- Stéphane Ravieret - Institut de Recherches en Technologies et Sciences pour le Vivant, France

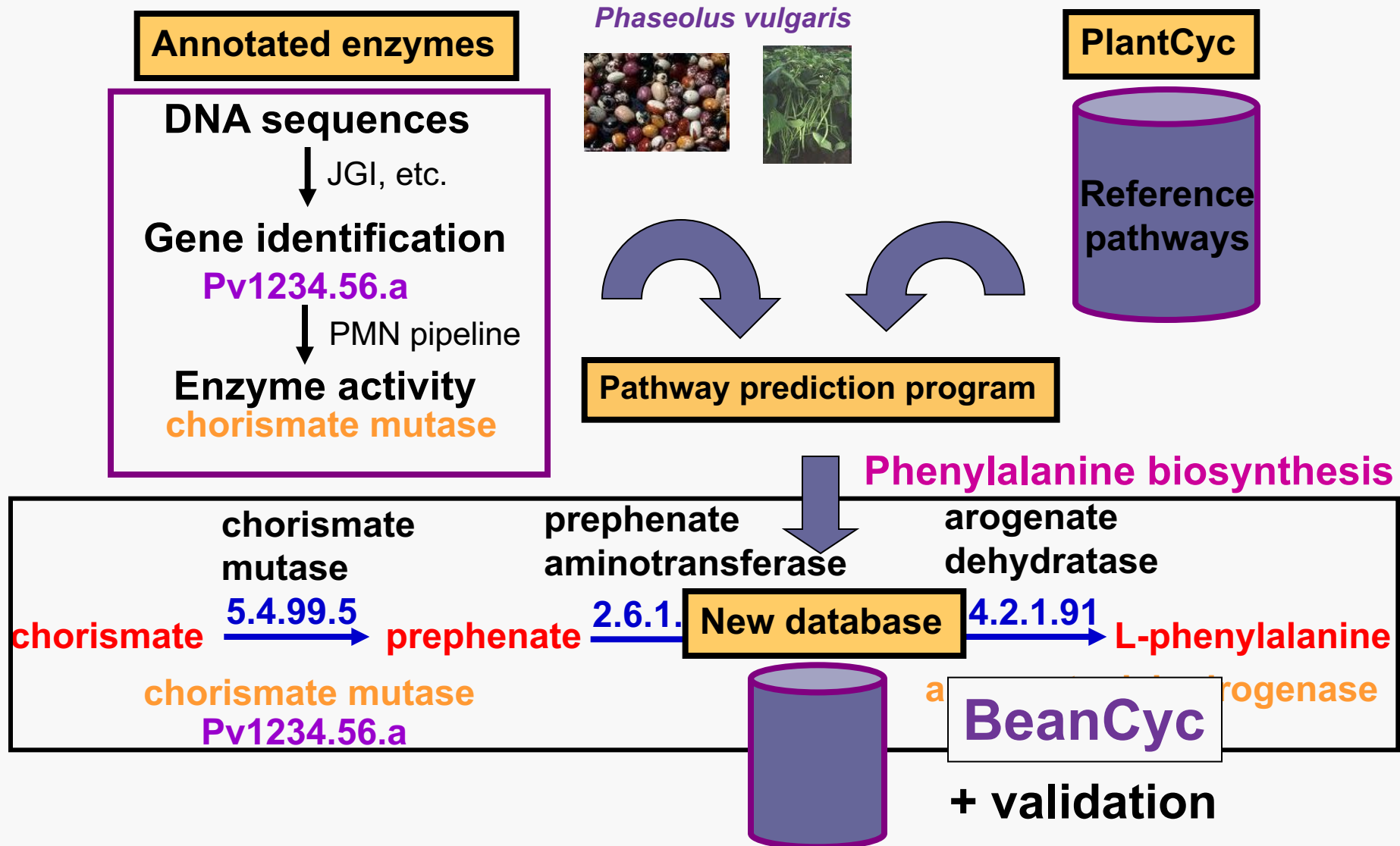
# Creation of new PMN databases

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- New sets of DNA sequences become available
  - ▣ Genomes are sequenced
  - ▣ Large EST data sets are created
    - Unigene builds are generated
- PMN pipeline predicts enzyme functions
  - ▣ Performed using computer algorithms based on sequence similarity
- Set of predicted enzymes is used to predict metabolic pathways
  - ▣ The pathway program (Pathologic) uses:
    - Enzyme functional annotations
    - A reference set of pathways (e.g. PlantCyc)
- Curators validate predicted pathways in the new database
  - ▣ Curators remove incorrect information and add additional data



# Creation of new PMN databases



# Creation of new PMN databases

---

- BeanCyc will be added to the PMN databases
- BeanCyc enzymes will be added to PlantCyc

# How can you put the PMN to work for you?

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- ❑ Learn background information about particular metabolic pathways
- ❑ Create customized metabolic data sets
- ❑ Compare metabolism across plant species
- ❑ Analyze experimental OMICs data in a metabolic context
- ❑ Manipulate and study data offline
- ❑ Create new metabolic pathway databases

# We are here to help: [www.plantcyc.org](http://www.plantcyc.org)

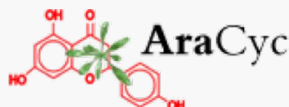
---

- Please use our data
- Please use our tools
- Please help us to improve our databases!
- Please contact us if we can be of any help!
  - Stay around for the help session from 8-9 PM
  - Visit the PMN poster - #322
  - Make an appointment to meet with me during the conference
    - Sign-up on sheet in the back of the room
    - Send an e-mail



[curator@plantcyc.org](mailto:curator@plantcyc.org)

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



# We are here to help: [www.plantcyc.org](http://www.plantcyc.org)

The screenshot shows the Plant Metabolic Network (PMN) website. The header features the PMN logo with a plant icon and the text "Plant Metabolic Network". Below the logo is a search bar with the text "PlantCyc" and a "search" button. A navigation bar contains links: "About PMN", "Search", "Tools", "Downloads", "Useful Sites", "Submit Data", "Help", and "Feedback". A sidebar on the left lists various sections: "Project Overview", "Documentation", "Presentations" (highlighted with a red box), "Statistics", "Release Notes", "Contact Info", "News", "PMN Staff", "Collaborators", "Contributors", and "Editorial Board". The main content area is titled "Summer 2009 Presentations" and contains a list of resources, with "TAIR ICAR Workshop Resource Guide" highlighted by a red box. Below this, there is a section titled "Part II: Hands-on exercises and individual help (presenters and participants)" which includes a list of resources, with "TAIR ICAR Workshop Practice Questions", "TAIR workshop - part 2 - data file (Microarray / OMICs viewer data file for Question #1)", and "TAIR ICAR Workshop Practice Questions with Answers" highlighted by a red box.

**PMN**  
Plant Metabolic Network

Search PlantCyc search

About PMN Search Tools Downloads Useful Sites Submit Data Help Feedback

Project Overview  
Documentation  
**Presentations**  
Statistics  
Release Notes  
Contact Info  
News  
PMN Staff  
Collaborators  
Contributors  
Editorial Board

**Summer 2009 Presentations**

- **TAIR ICAR Workshop Resource Guide**

**Part II: Hands-on exercises and individual help**  
(presenters and participants)

- TAIR ICAR Workshop Practice Questions
- TAIR workshop - part 2 - data file  
(Microarray / OMICs viewer data file for Question #1)
- TAIR ICAR Workshop Practice Questions with Answers

# PMN Acknowledgements

---

Peifen Zhang (*Director*)

Sue Rhee (*PI*)

Eva Huala (*Co-PI*)

## Current Curators:

- A. S. Karthikeyan (*curator*)

## Recent Past Contributors:

- Christophe Tissier (*curator*)
- Hartmut Foerster (*curator*)

## Collaborators:

- Peter Karp (SRI)
- Ron Caspi (SRI)
- SRI Tech Team
- Lukas Mueller (SGN)
- Anuradha Pujar (SGN)
- Gramene and MedicCyc

## Tech Team Members:

- Bob Muller (*Manager*)
- Larry Ploetz (*Sys. Administrator*)
- Raymond Chetty
- Anjo Chi
- Vanessa Kirkup
- Cynthia Lee
- Tom Meyer
- Shanker Singh
- Chris Wilks



CARNEGIE  
INSTITUTION FOR  
SCIENCE



# We are here to help: [www.plantcyc.org](http://www.plantcyc.org)

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- Please use our data
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[curator@plantcyc.org](mailto:curator@plantcyc.org)

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



# What is in the PMN?

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- Databases focus on “small” molecule metabolism
  - “Small”
    - No strict standards
    - Generally exclude macromolecules that are built using templates
  - “Large” molecules **Not In** the PMN:
    - chromosomes, proteins (as substrates), mRNA transcripts
      - but the building blocks of macromolecules are included
        - nucleotides and amino acids are in the PMN
  - “Large” molecules **In** the PMN:
    - cellulose
    - rubber
    - homogalacturonan / pectin