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

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curator

PMN/TAIR

Presentation plan

- 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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pathways

metabolism

What is in the PMN?

- 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?

- 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?

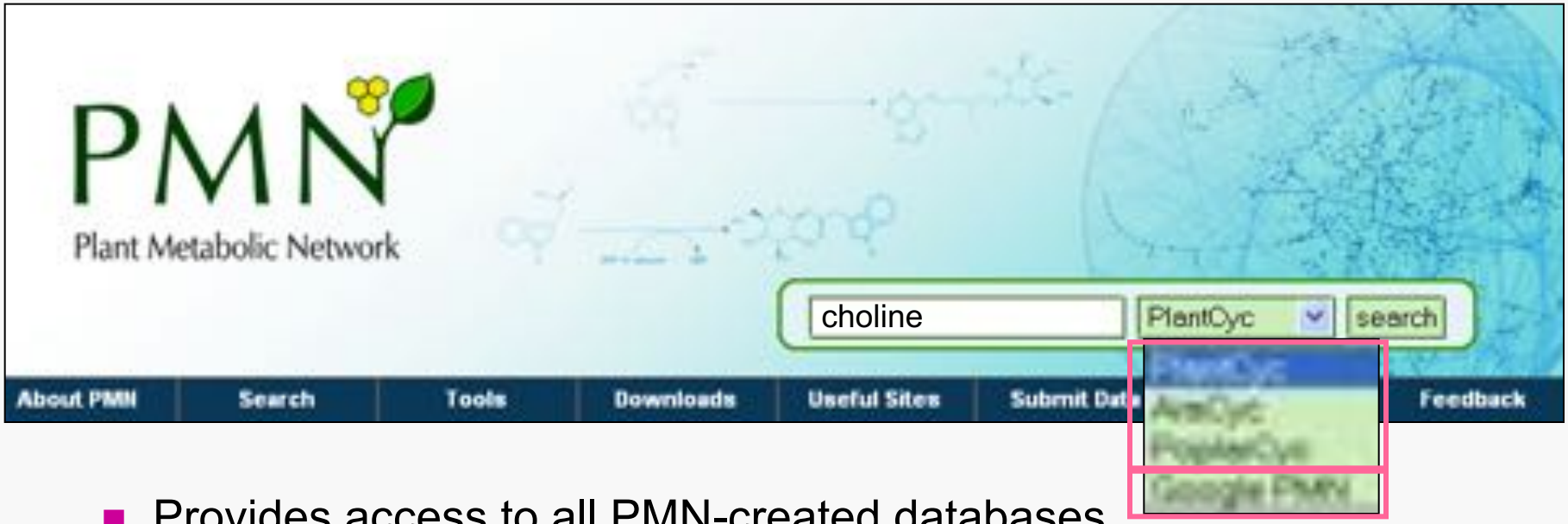
- Most recent release of PMN databases: October 15, 2009

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

- How can I access all this information?

Searching in PMN databases

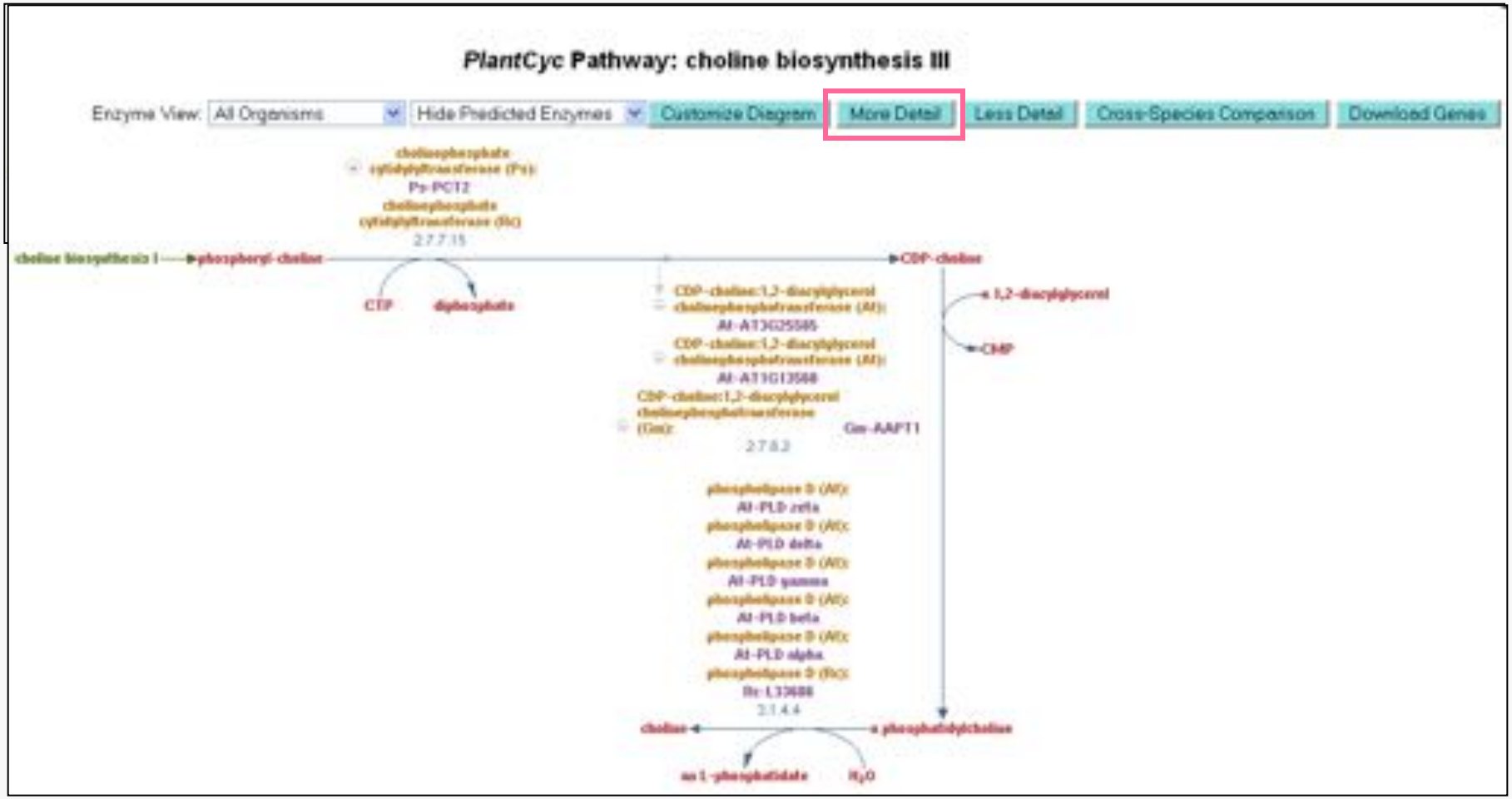
- Quick search bar



  - Provides access to <u>all PMN-created</u> 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

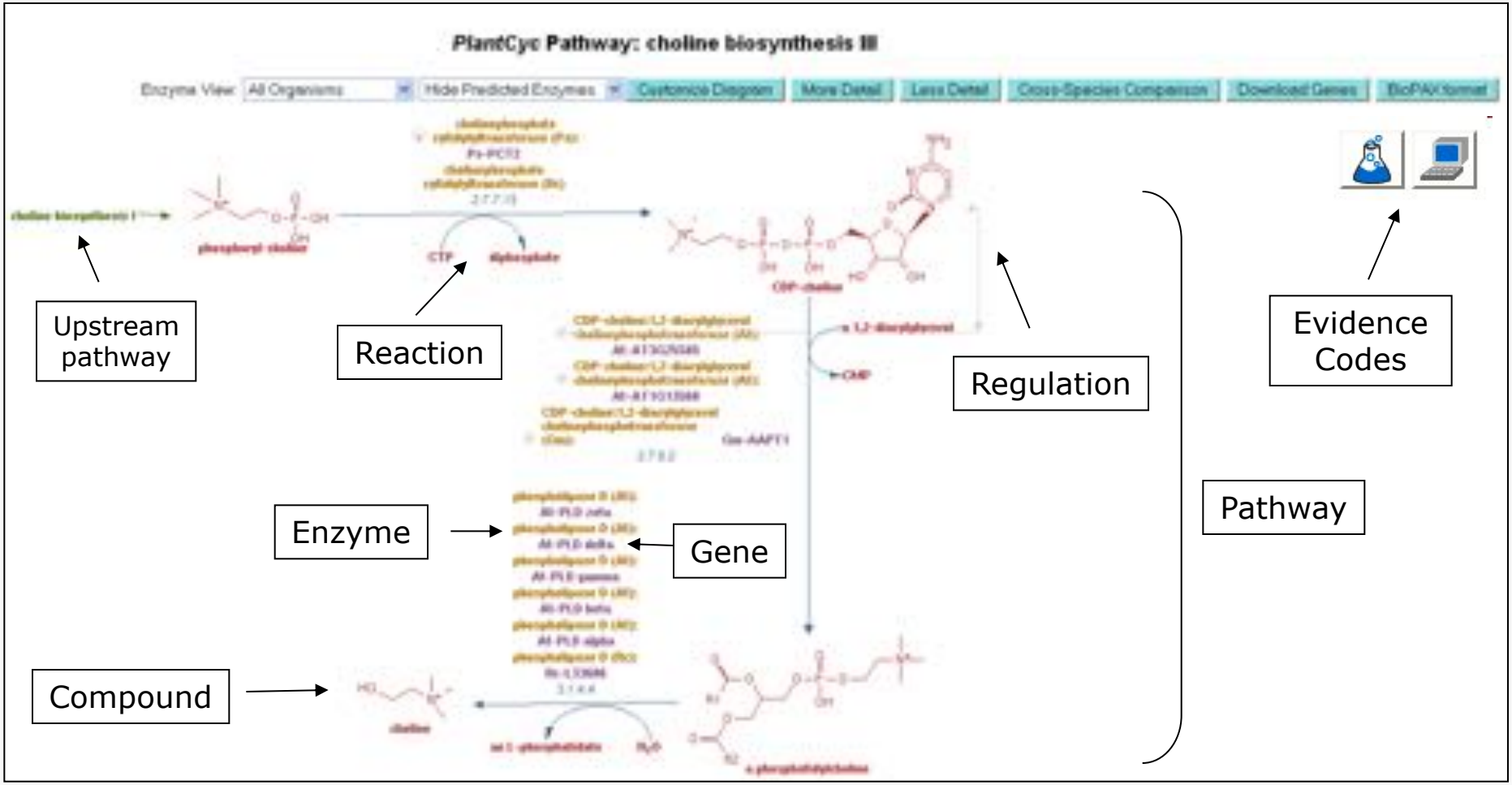
Searching in PMN databases

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 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 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.

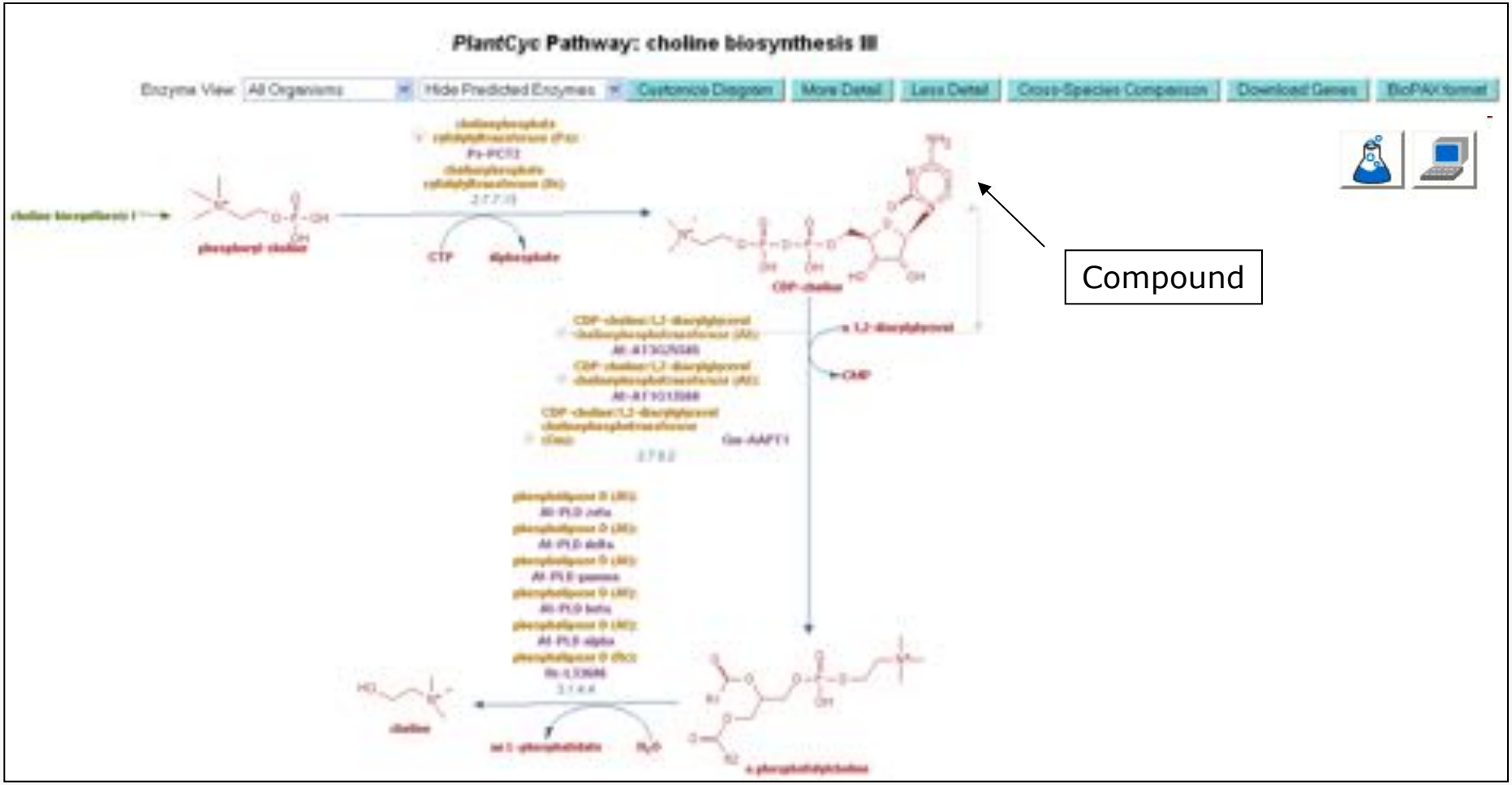
Hitz81: Hitz WD, Rhodes D, Hanson AD. (1981) "Radiotracer evidence implicating phosphoryl and phosphatidyl bases as intermediates in betaine synthesis by water-stressed barley leaves." Plant Physiol. (1981). 68. 814-822.

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). 259-284.

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

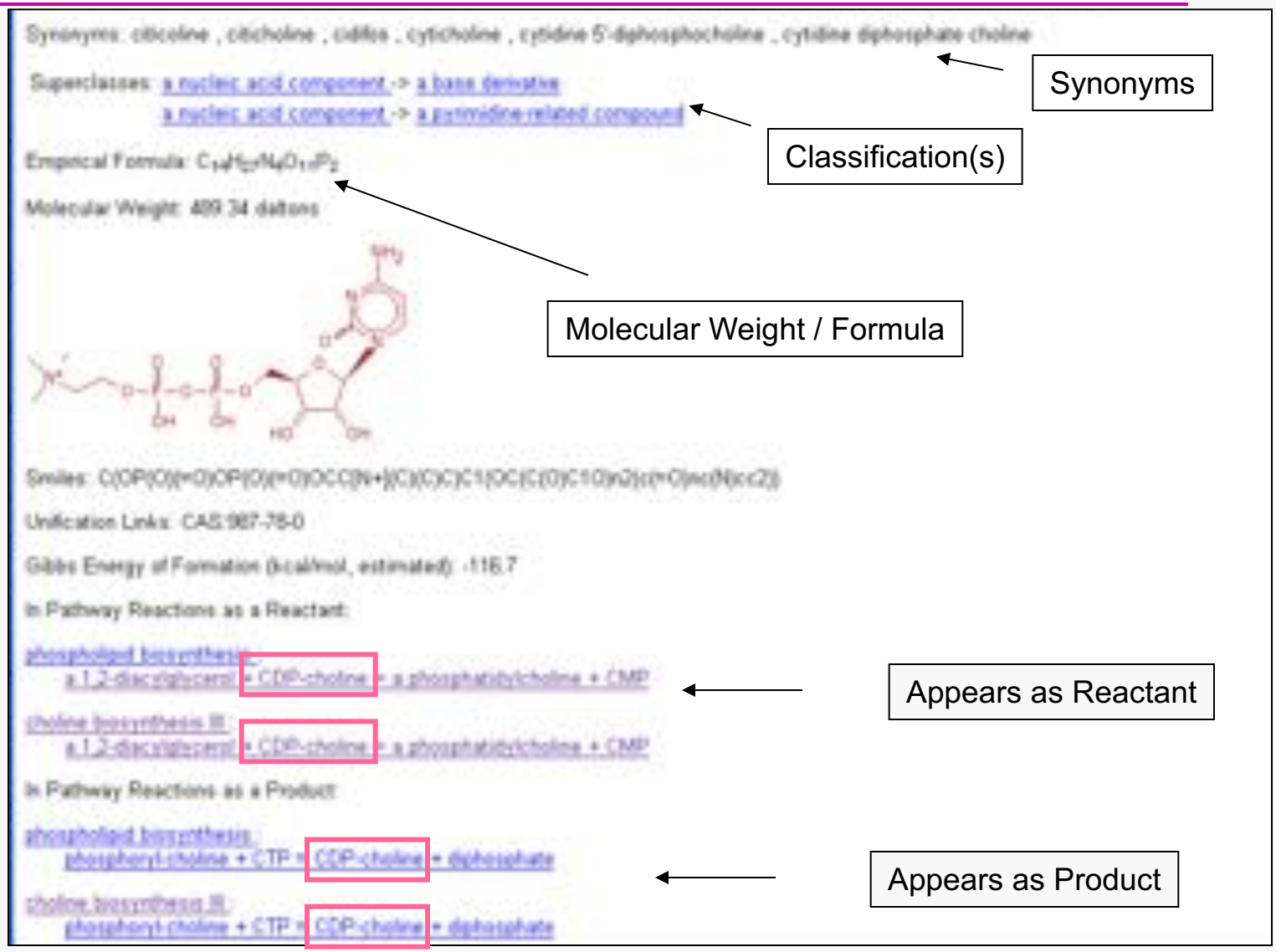
McNeil00: McNeil SD, Nuccio ML, Rhodes D, Shachar-Hill Y, Hanson AD (2000). "Radiotracer and computer modeling evidence that phospho-base methylation is the main route of choline synthesis in tobacco." Plant Physiol 123(1):371-80. PMID: 10806254

Getting information from PMN pathway pages

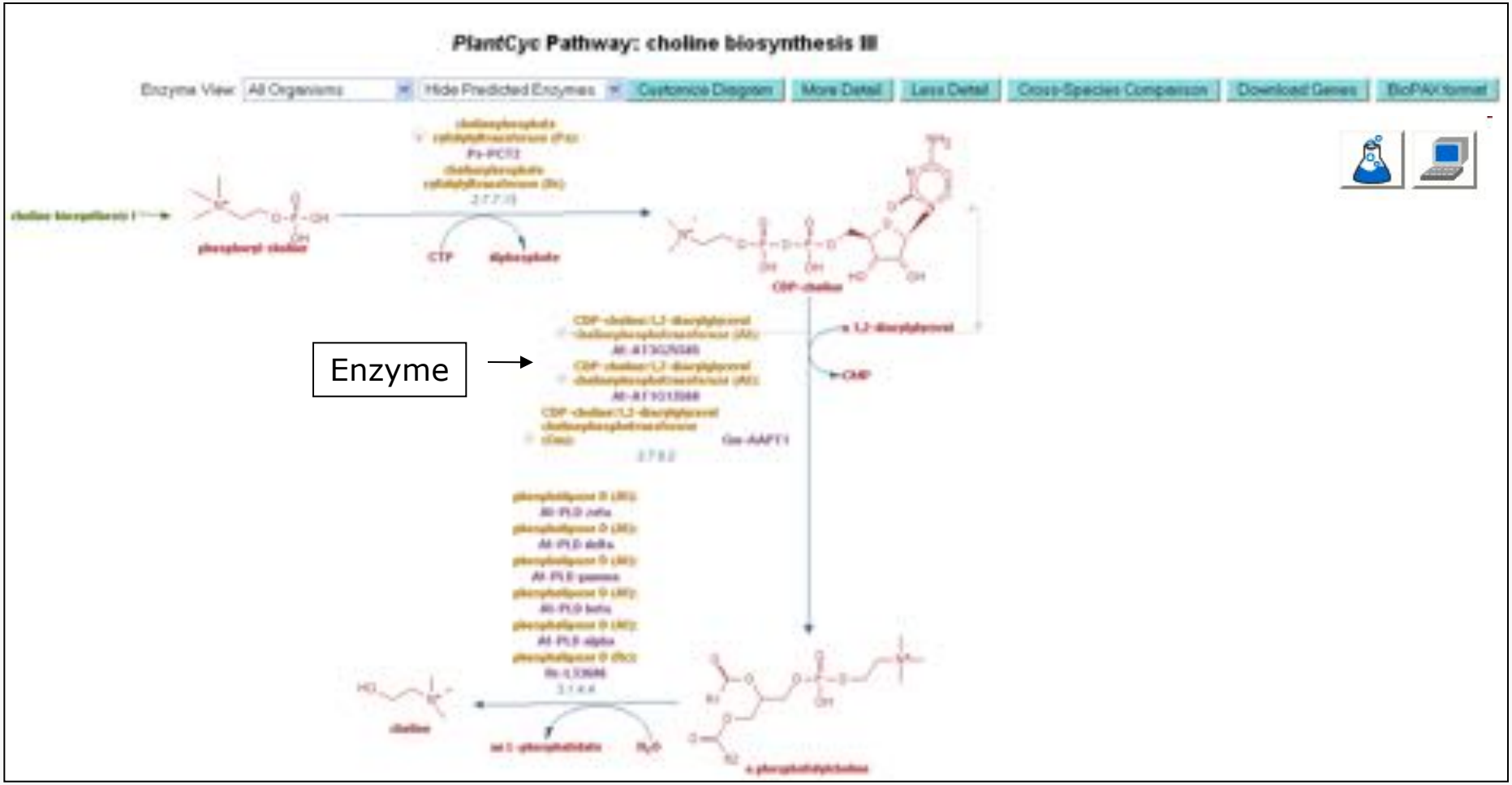


PMN compound pages

Compound:
CDP-choline



Getting information from PMN pathway pages



PMN enzyme pages

Arabidopsis **Enzyme: phosphatidyltransferase**

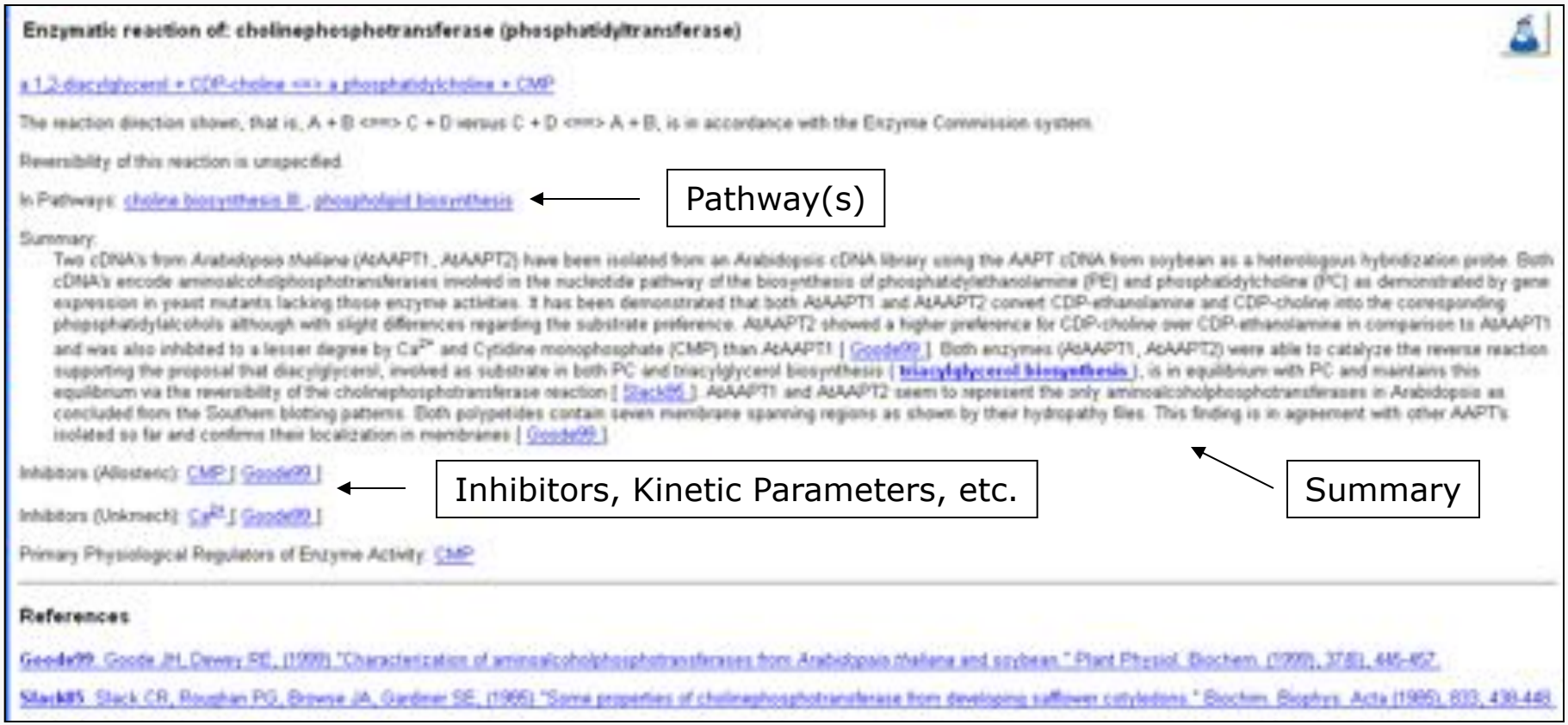
Multifunctional protein

*

*

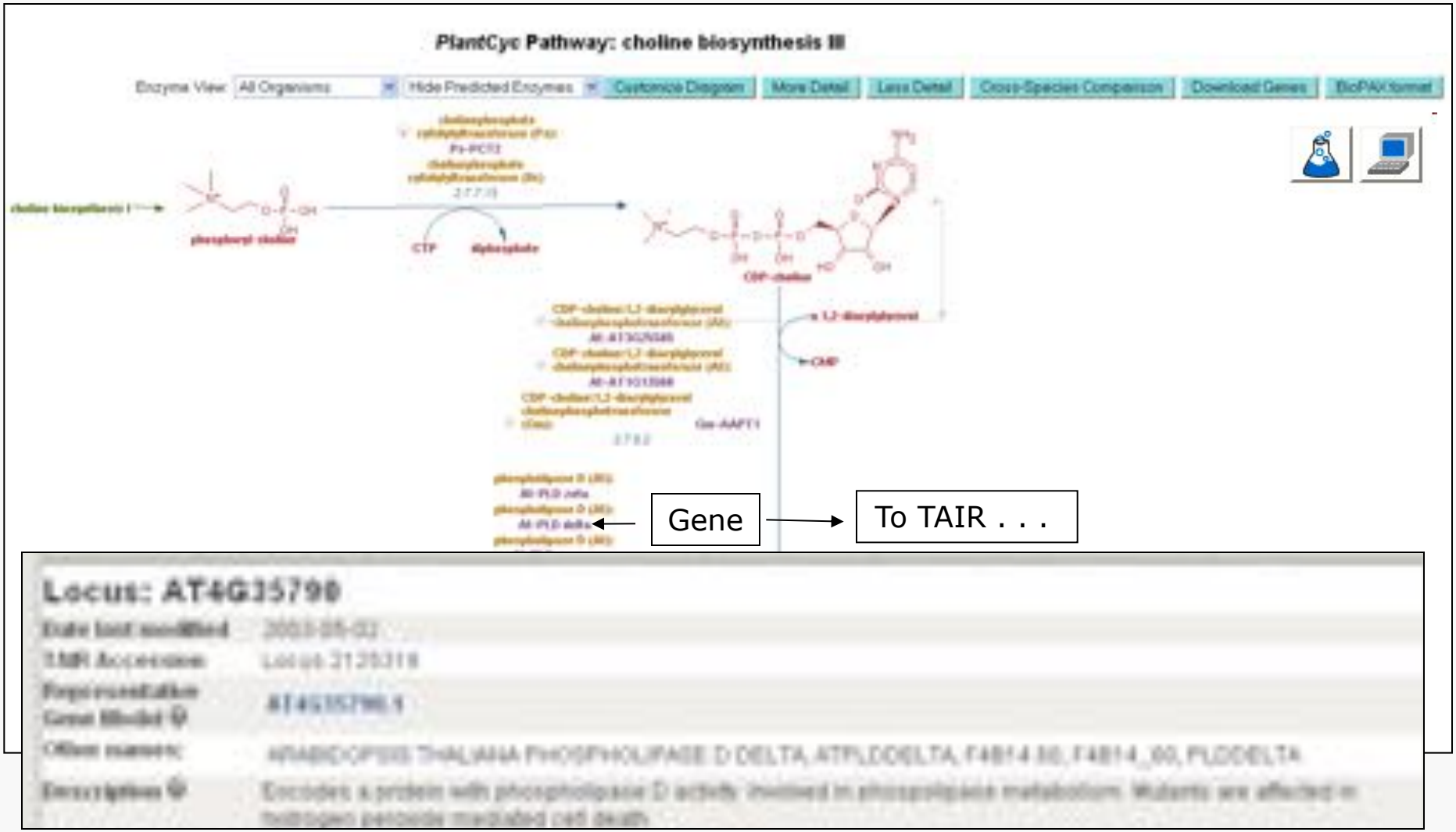
PMN enzyme pages

Arabidopsis **Enzyme: phosphatidyltransferase**



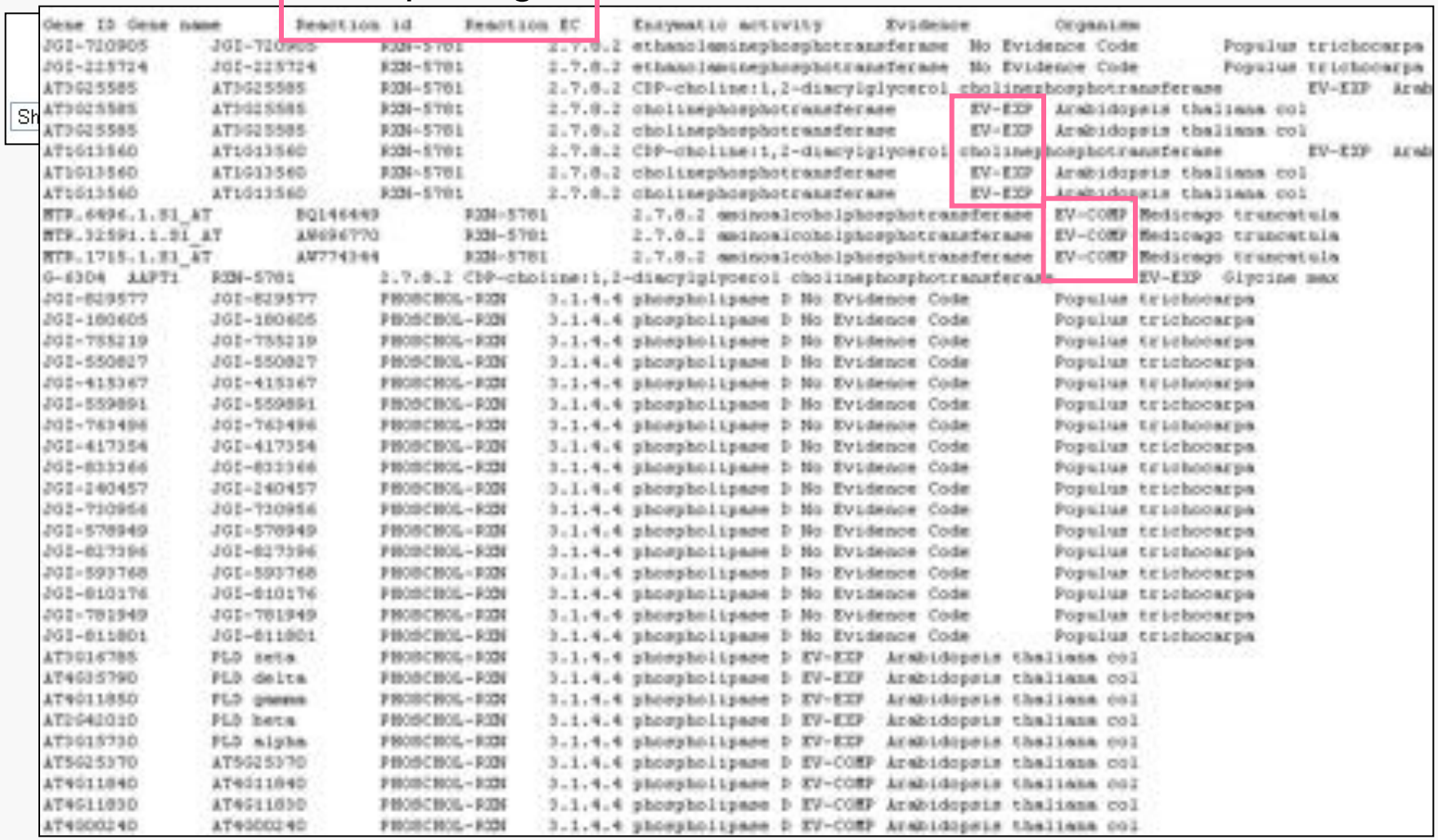
References

Getting information from PMN pathway pages



Getting information from PMN pathway pages

- Download a complete gene list



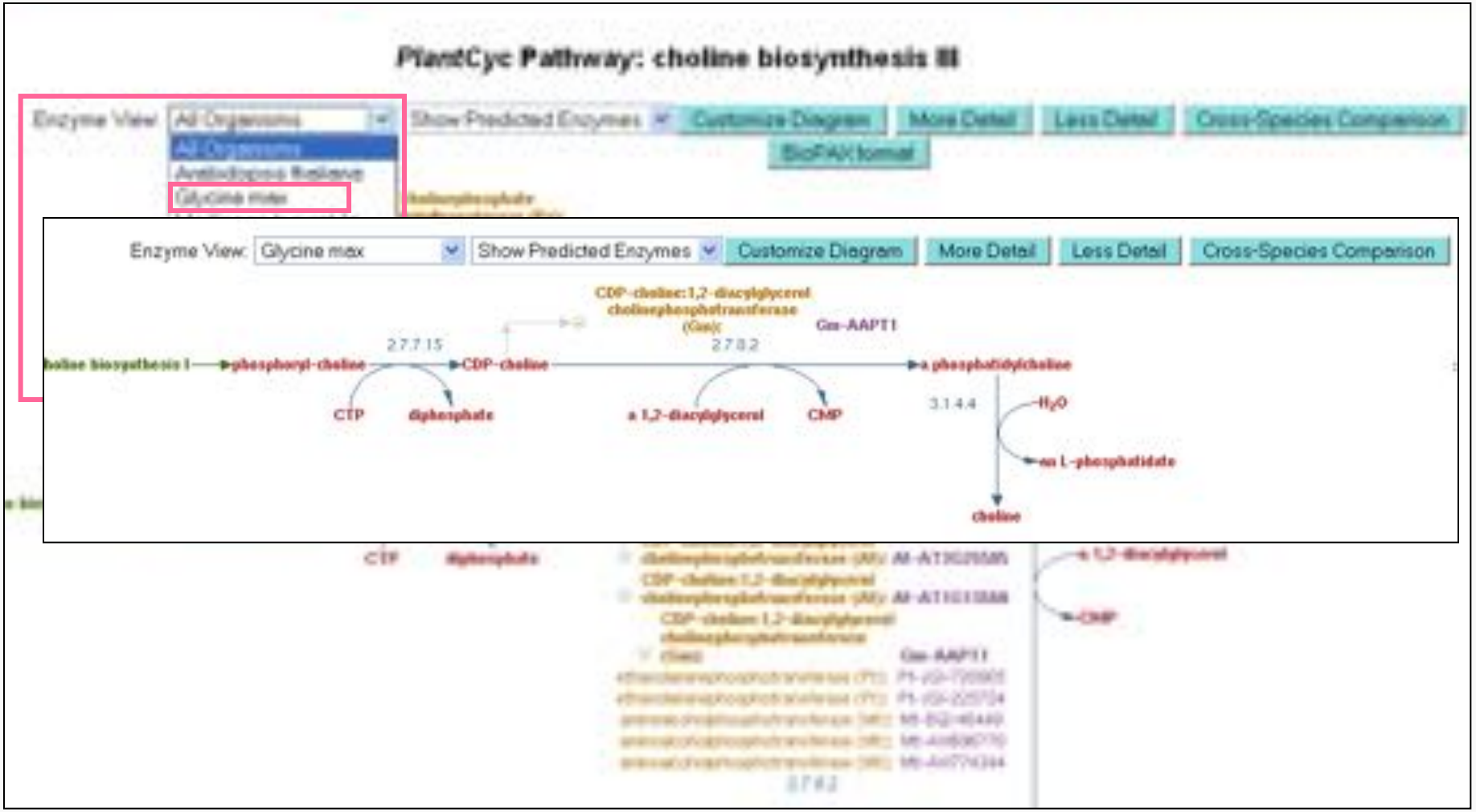
Gene ID	Gene name	Reaction id	Reaction EC	Enzymatic activity	Evidence	Organism
JGI-710905	JGI-710905	RXN-5701	2.7.8.2	ethanolaminephosphotransferase	No Evidence Code	Populus trichocarpa
JGI-225724	JGI-225724	RXN-5701	2.7.8.2	ethanolaminephosphotransferase	No Evidence Code	Populus trichocarpa
AT3G25585	AT3G25585	RXN-5701	2.7.8.2	CDP-choline:1,2-diacylglycerol cholinephosphotransferase	EV-EXP	Arab
AT3G25585	AT3G25585	RXN-5701	2.7.8.2	cholinephosphotransferase	EV-EXP	Arabidopsis thaliana col
AT3G25585	AT3G25585	RXN-5701	2.7.8.2	cholinephosphotransferase	EV-EXP	Arabidopsis thaliana col
AT1G13560	AT1G13560	RXN-5701	2.7.8.2	CDP-choline:1,2-diacylglycerol cholinephosphotransferase	EV-EXP	Arab
AT1G13560	AT1G13560	RXN-5701	2.7.8.2	cholinephosphotransferase	EV-EXP	Arabidopsis thaliana col
AT1G13560	AT1G13560	RXN-5701	2.7.8.2	cholinephosphotransferase	EV-EXP	Arabidopsis thaliana col
MTR.6896.1.S1_AT	BQ146449	RXN-5701	2.7.8.2	aminoalcoholphosphotransferase	EV-COMP	Medicago truncatula
MTR.32591.1.S1_AT	AW696770	RXN-5701	2.7.8.2	aminoalcoholphosphotransferase	EV-COMP	Medicago truncatula
MTR.1715.1.S1_AT	AW774399	RXN-5701	2.7.8.2	aminoalcoholphosphotransferase	EV-COMP	Medicago truncatula
G-6304	AAPT1	RXN-5701	2.7.8.2	CDP-choline:1,2-diacylglycerol cholinephosphotransferase	EV-EXP	Glycine max
JGI-829577	JGI-829577	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-180605	JGI-180605	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-755219	JGI-755219	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-550827	JGI-550827	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-415367	JGI-415367	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-559891	JGI-559891	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-763496	JGI-763496	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-417356	JGI-417356	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-833366	JGI-833366	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-240457	JGI-240457	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-710956	JGI-710956	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-570949	JGI-570949	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-827396	JGI-827396	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-593768	JGI-593768	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-810176	JGI-810176	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-781949	JGI-781949	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
JGI-811801	JGI-811801	PWY0C80L-RXN	3.1.4.4	phospholipase D	No Evidence Code	Populus trichocarpa
AT3G16785	PLD zeta	PWY0C80L-RXN	3.1.4.4	phospholipase D	EV-EXP	Arabidopsis thaliana col
AT4G35790	PLD delta	PWY0C80L-RXN	3.1.4.4	phospholipase D	EV-EXP	Arabidopsis thaliana col
AT4G11850	PLD gamma	PWY0C80L-RXN	3.1.4.4	phospholipase D	EV-EXP	Arabidopsis thaliana col
AT2G42010	PLD beta	PWY0C80L-RXN	3.1.4.4	phospholipase D	EV-EXP	Arabidopsis thaliana col
AT3G15730	PLD alpha	PWY0C80L-RXN	3.1.4.4	phospholipase D	EV-EXP	Arabidopsis thaliana col
AT5G25370	AT5G25370	PWY0C80L-RXN	3.1.4.4	phospholipase D	EV-COMP	Arabidopsis thaliana col
AT4G11840	AT4G11840	PWY0C80L-RXN	3.1.4.4	phospholipase D	EV-COMP	Arabidopsis thaliana col
AT4G11830	AT4G11830	PWY0C80L-RXN	3.1.4.4	phospholipase D	EV-COMP	Arabidopsis thaliana col
AT4G00240	AT4G00240	PWY0C80L-RXN	3.1.4.4	phospholipase D	EV-COMP	Arabidopsis thaliana col

Getting information from PMN pathway pages

- Download the pathway in BioPAX format

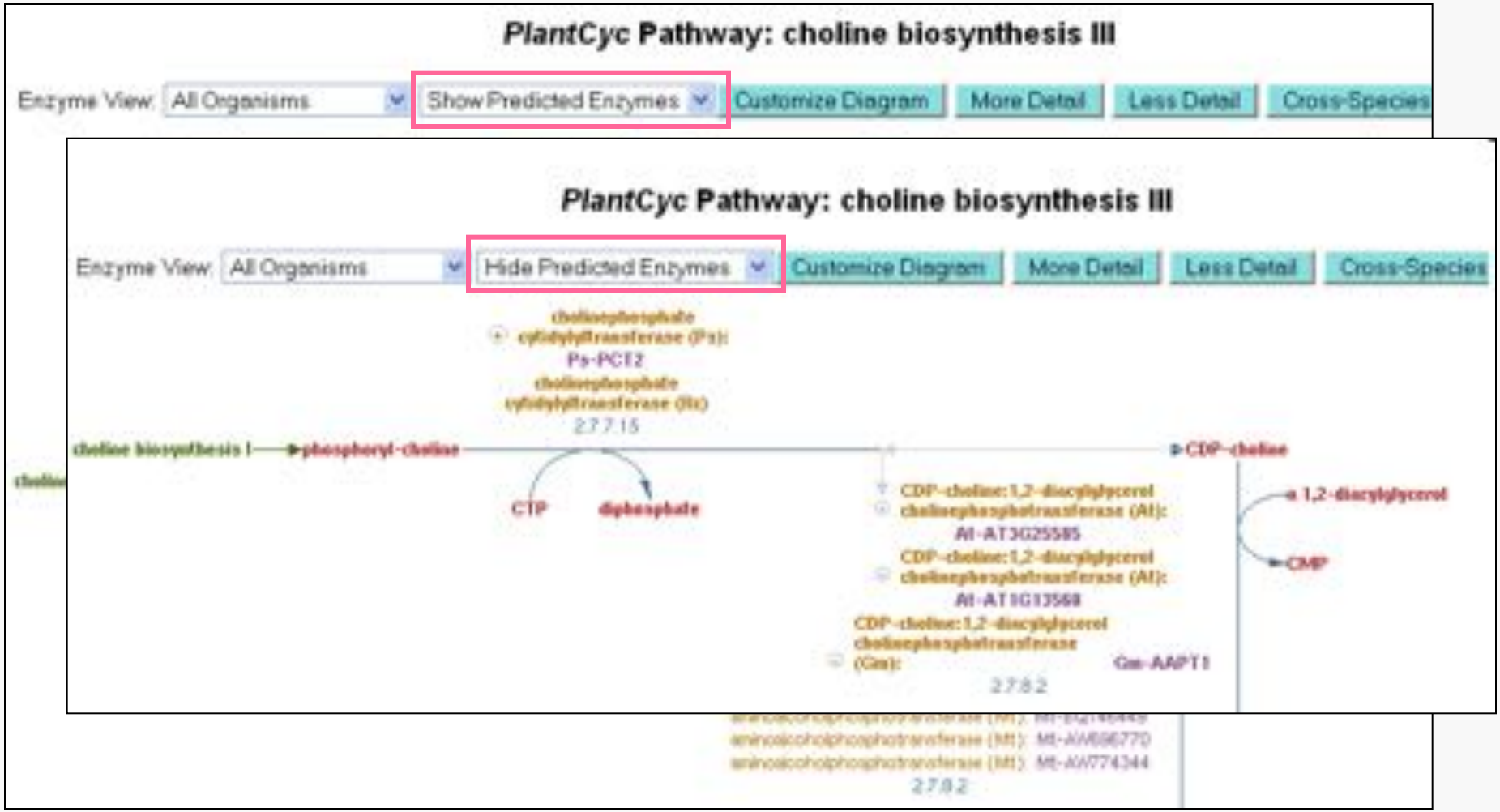
Getting information from PMN pathway pages

- Set organism viewing preferences on PlantCyc pages



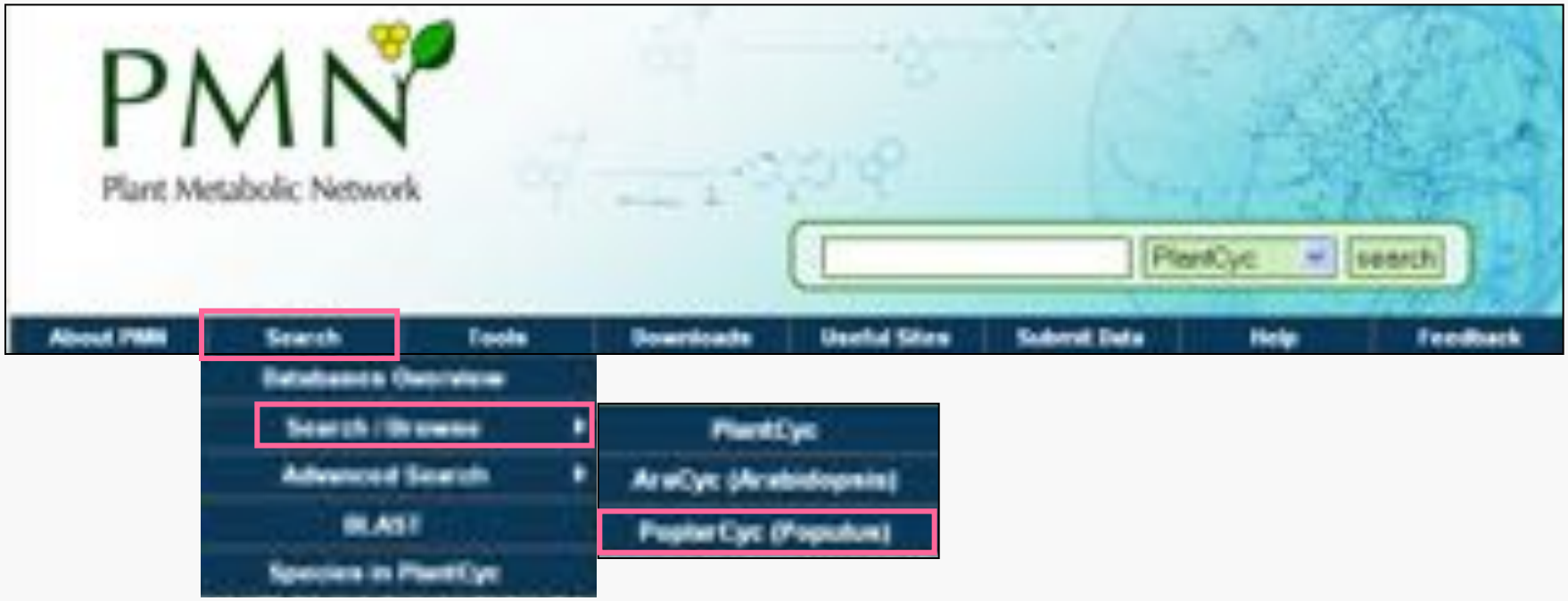
Getting information from PMN pathway pages

- View predicted or experimentally supported enzymes

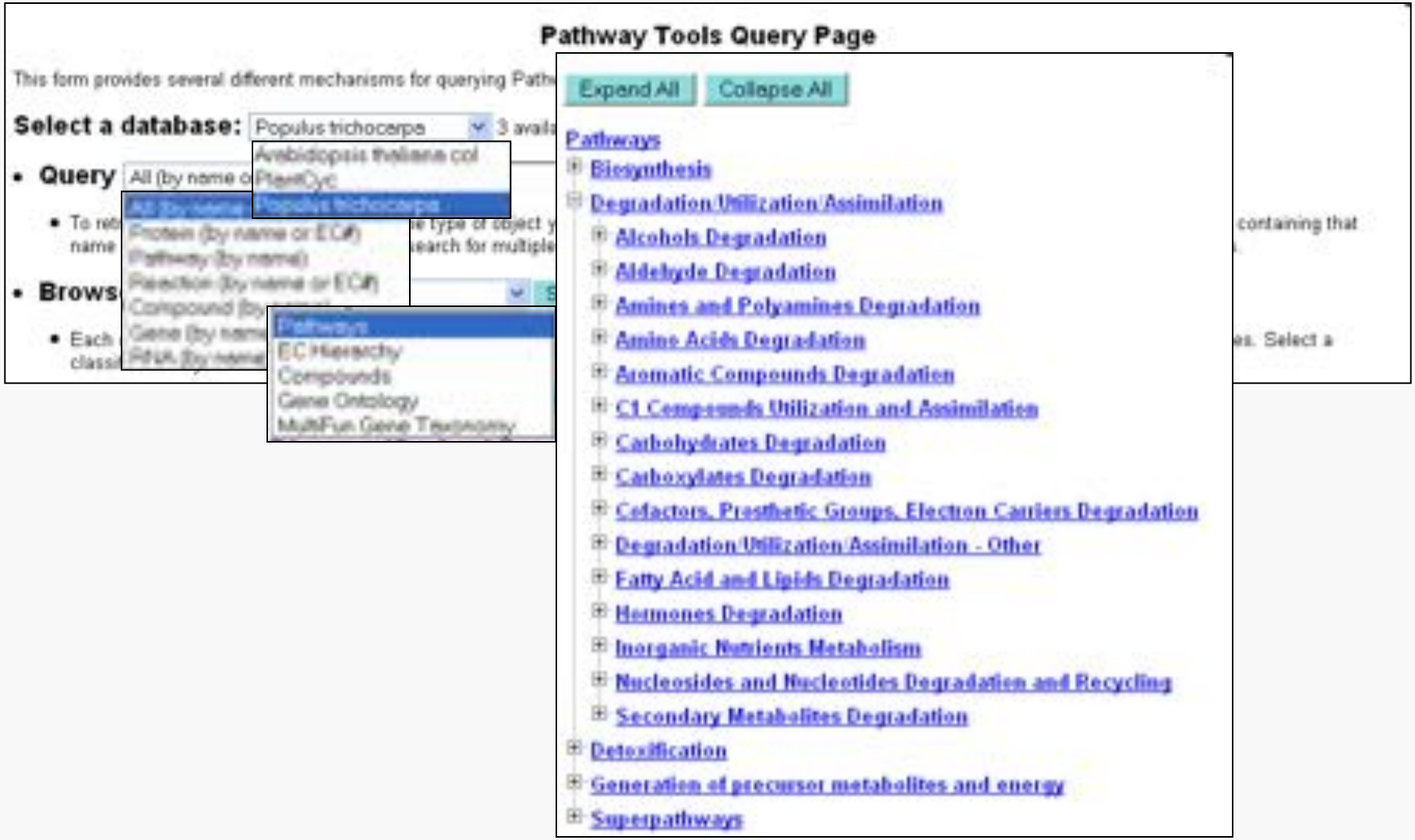


Searching in PMN databases

- Search page
  - Provides more selective searches
  - Allows browsing

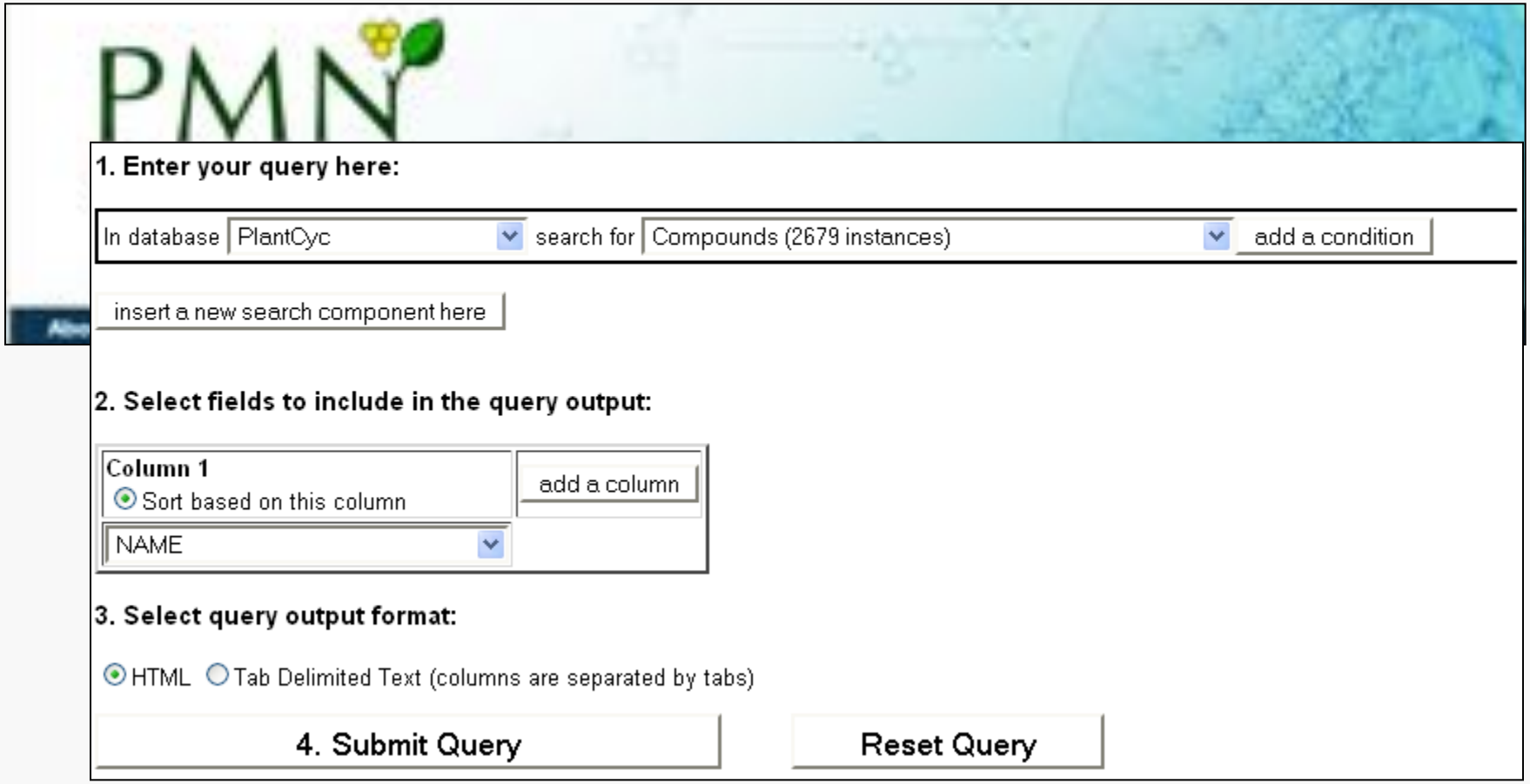


Searching in PMN databases



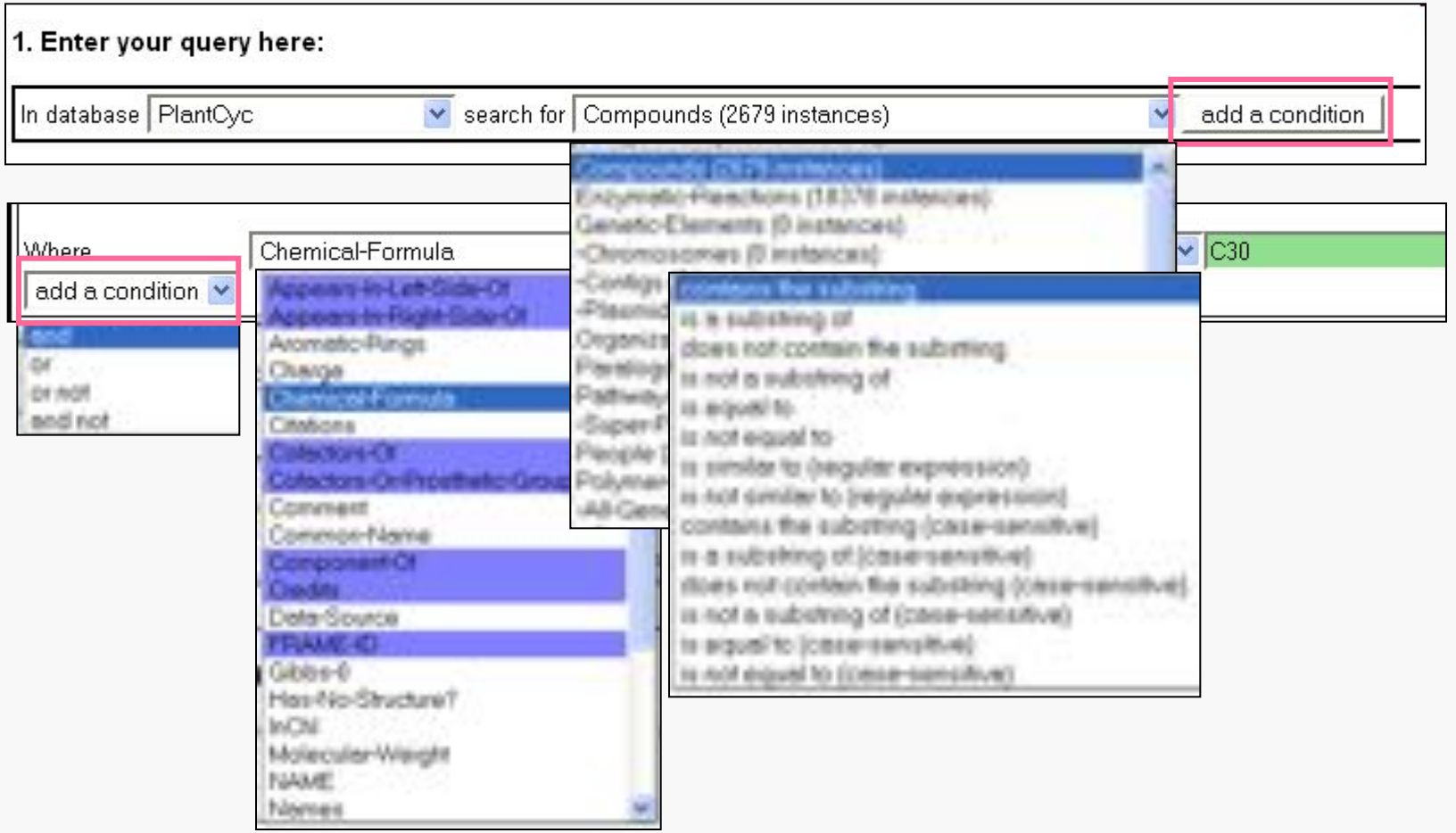
Advanced searching in PMN databases

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



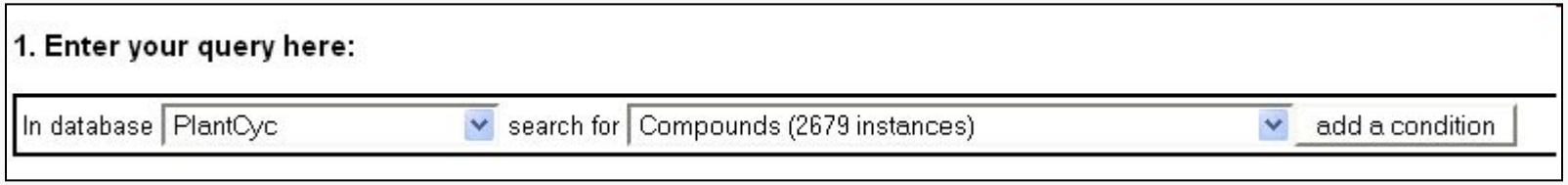
Advanced searching in PMN databases

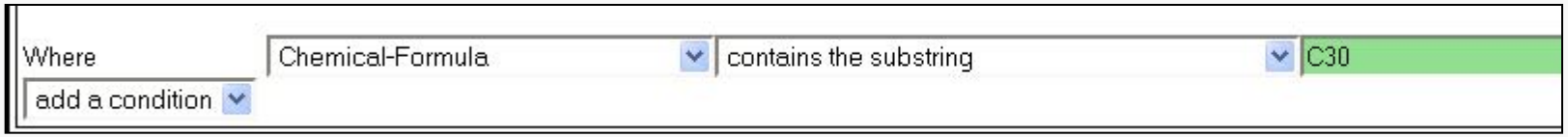
- Find all of the 30-carbon compounds that appear as products in reactions
  - Construct query

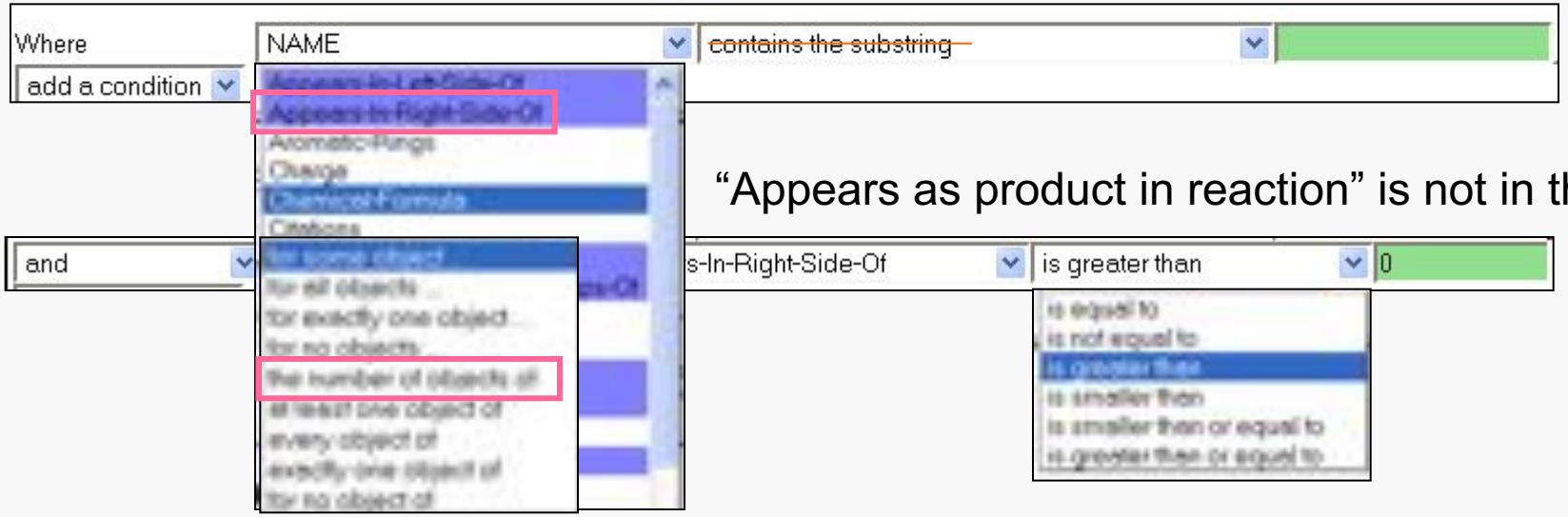


Advanced searching in PMN databases

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



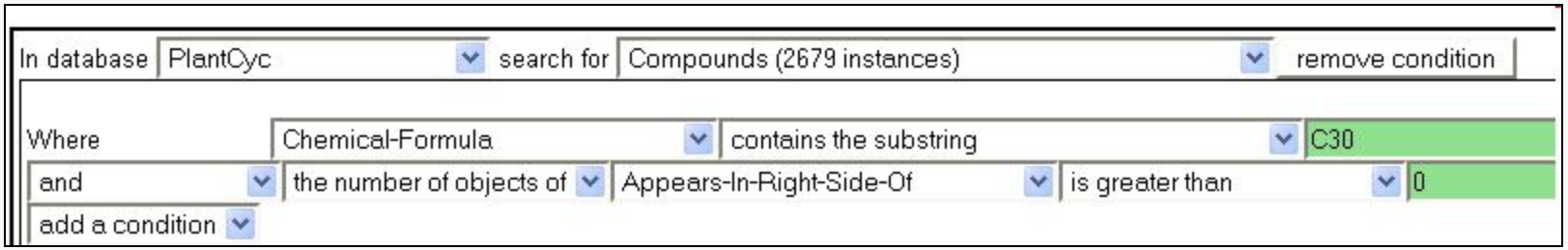




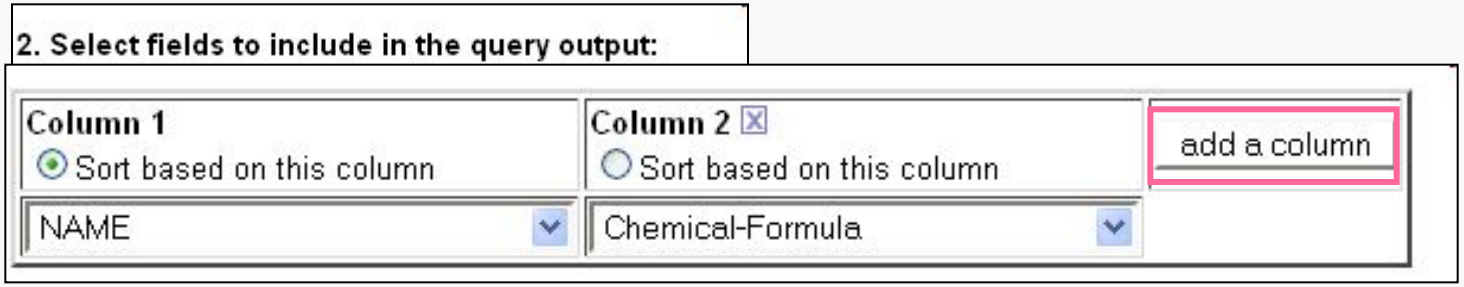
"Appears as product in reaction" is not in the list

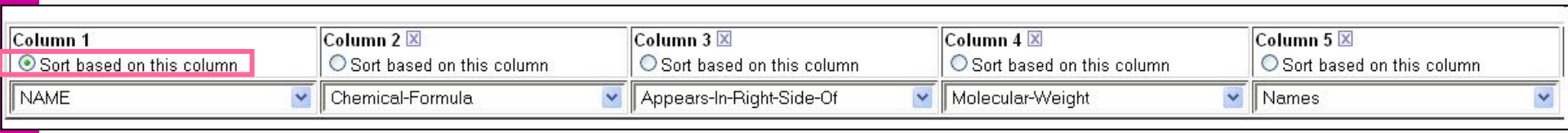
Advanced searching in PMN databases

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



  - Select desired data outputs





Advanced searching in PMN databases

Advanced Query Results

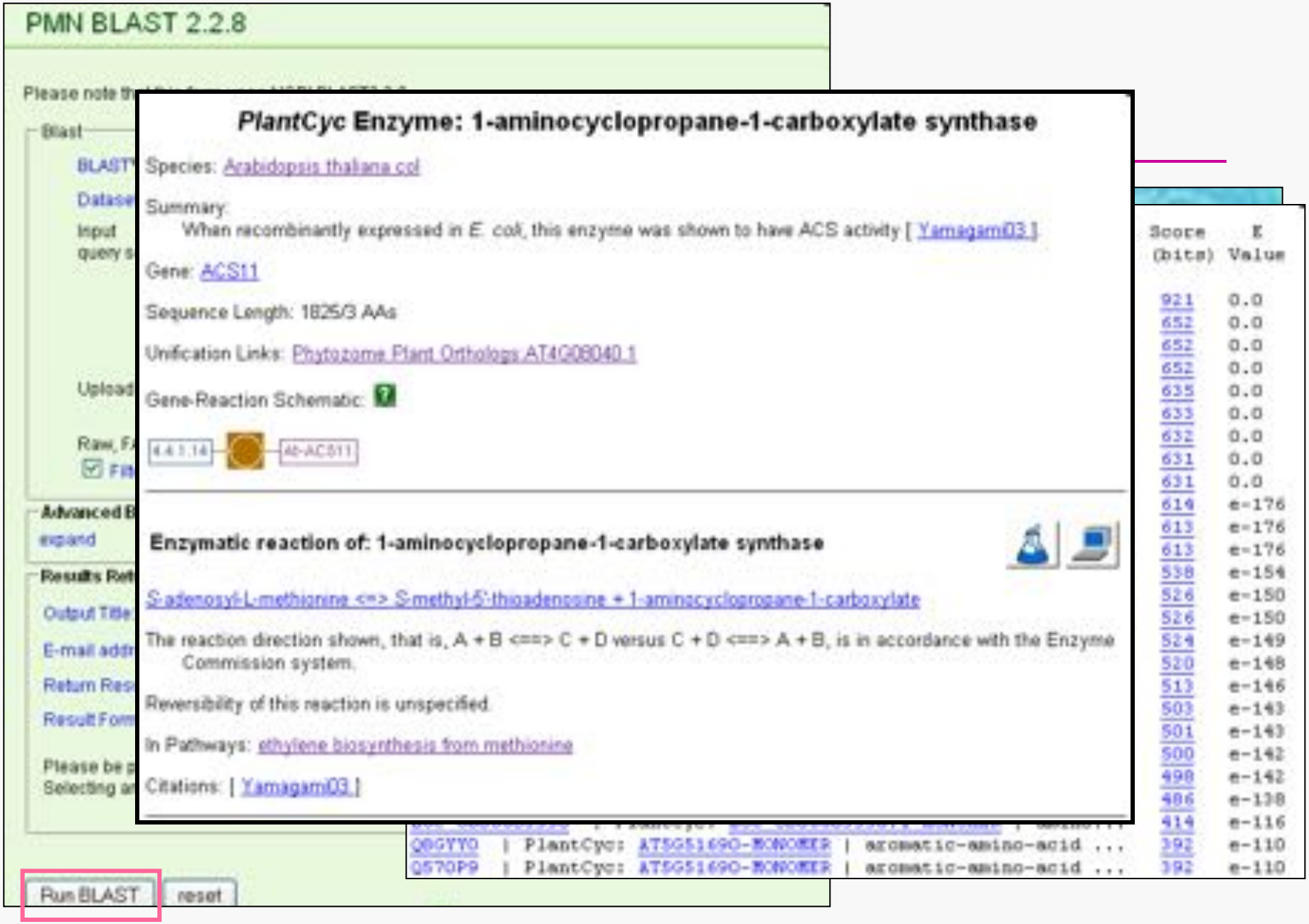
Your query in BioVelo is sort ([(x1^?NAME, x1^?CHEMICAL-FORMULA, x1^?APPEARS-IN-RIGHT-SIDE-OF, x1^?MOLECULAR-WEIGHT, x1^?NAMES) : x1<-PLANT^^Compounds, ("C30" instringci x1^CHEMICAL-FORMULA) & ((#x1^APPEARS-IN-RIGHT-SIDE-OF) > 0)],1)

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)
α-amyrin	C30H50O1	(S)-2,3-epoxysqualene = α-amyrin	426.724	α-amyrin, viminalol, alpha-Amyrenol
β-amyrin	C30H50O1	(S)-2,3-epoxysqualene = β-amyrin	426.724	β-amyrin, β-amyrenol
(E)-cinnamoyl-CoA	C30H42N7O17P3S1	trans-cinnamate + coenzyme A = (E)-cinnamoyl-CoA + H_2O	897.68	(E)-cinnamoyl-CoA
(S)-2,3-epoxysqualene	C30H50O1	squalene + NADPH + O_2 = (S)-2,3-epoxysqualene + $NADP^+$ + H_2O, O_2 + a reduced acceptor + squalene = (S)-2,3-epoxysqualene + H_2O + an acceptor	426.724	(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
24-ethylidenelophenol	C30H50O1	24-methylenelophenol + S-adenosyl-L-methionine = 24-ethylidenelophenol + S-adenosyl-L-homocysteine	426.724	24-ethylidenelophenol, (Z)-24-ethylidenelophenol, citrostadienol
4,4-dimethyl-14α-formyl-5α-cholesta-8,24-dien-3β-ol	C30H48O2	4,4-dimethyl-14α-hydroxymethyl-5α-cholesta-8,24-dien-3β-ol + NADPH + O_2 = 4,4-dimethyl-14α-formyl-5α-cholesta-8,24-dien-3β-ol + $NADP^+$ + 2 H_2O	440.708	4,4-dimethyl-14α-formyl-5α-cholesta-8,24-dien-3β-ol
4,4-dimethyl-14α-hydroxymethyl-5α-cholesta-8,24-dien-3β-ol	C30H50O2	lanosterol + NADPH + O_2 = 4,4-dimethyl-14α-hydroxymethyl-5α-cholesta-8,24-dien-3β-ol + $NADP^+$ + H_2O	442.724	4,4-dimethyl-14α-hydroxymethyl-5α-cholesta-8,24-dien-3β-ol
4-(1-methyl-2-pyrrolidinyl)-3-oxobutanoyl-CoA	C30H49N8O18P3S1	1-methylpyrrolidine-2-acetyl-CoA + acetyl-CoA = 4-(1-methyl-2-pyrrolidinyl)-3-oxobutanoyl-CoA + coenzyme A	934.741	4-(1-methyl-2-pyrrolidinyl)-3-oxobutanoyl-CoA, N-methylpyrrolidineacetoacetyl-CoA
4-coumaroyl-CoA	C30H42N7O18P3S1	coenzyme A + 4-coumarate + ATP = 4-coumaroyl-CoA + diphosphate + AMP	913.679	4-coumaroyl-CoA, p-coumaryl-CoA, 4-coumaryl-CoA, coumaroyl-CoA, p-coumaroyl-CoA

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 th
Blast
BLAST
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Raw, FA
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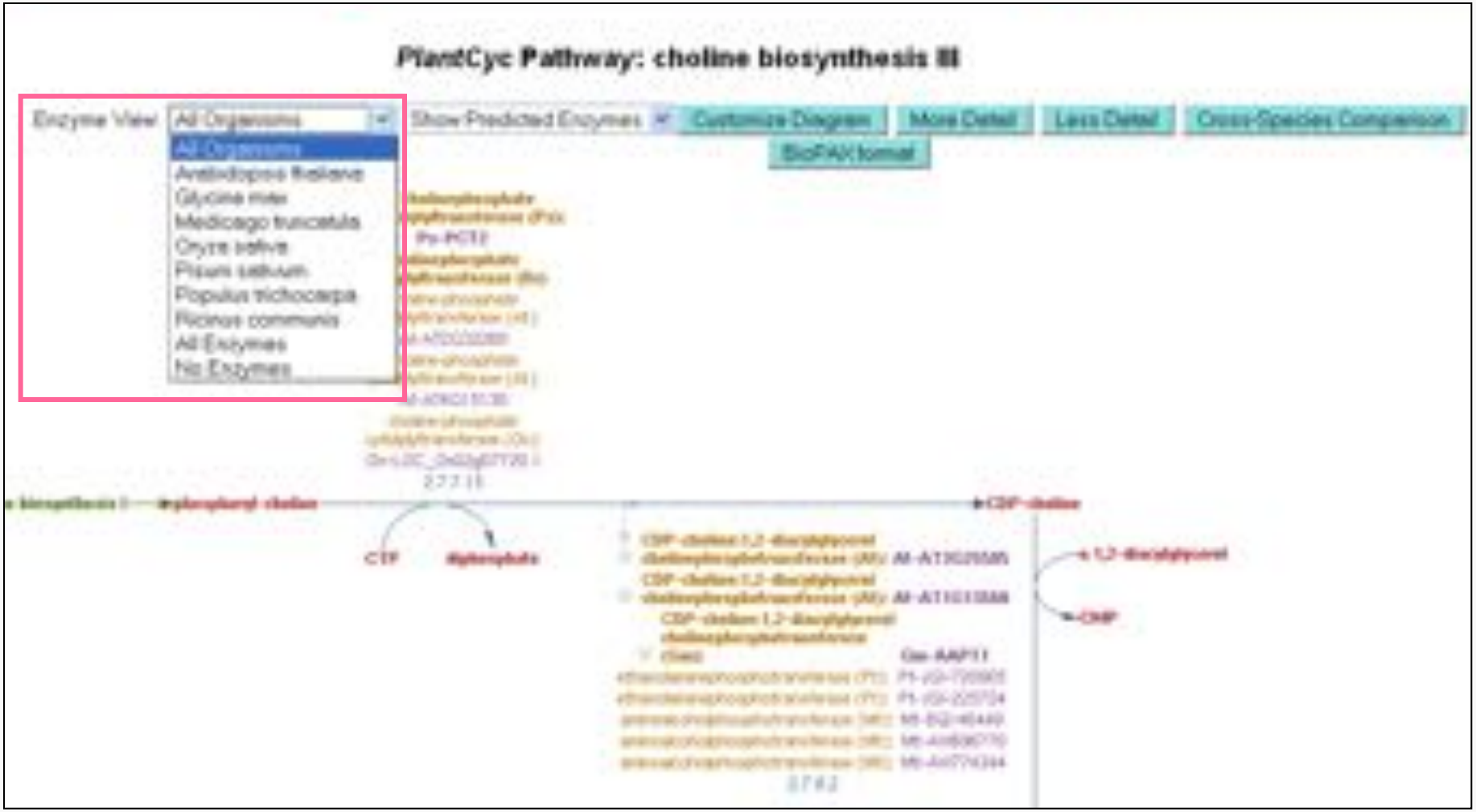
expand
Results Ret
Output Title
E-mail addr
Return Res
Result Form
Please be p
Selecting ar
Run BLAST
reset
PlantCyc Enzyme: 1-aminocyclopropane-1-carboxylate synthase
Species: Arabidopsis thaliana col
Summary:
When recombinantly expressed in E. coli, this enzyme was shown to have ACS activity [Yamagami03]
Gene: ACS11
Sequence Length: 1825/3 AAs
Unification Links: Phytozome Plant Orthologs AT4G08040.1
Gene-Reaction Schematic:
4.4.1.14
Ab-ACS11
Enzymatic reaction of: 1-aminocyclopropane-1-carboxylate synthase
S-adenosyl-L-methionine <=> S-methyl-5'-thioadenosine + 1-aminocyclopropane-1-carboxylate
The reaction direction shown, that is, A + B <==> C + D versus C + D <==> 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 (bits) E Value
921 0.0
652 0.0
652 0.0
652 0.0
635 0.0
633 0.0
632 0.0
631 0.0
631 0.0
614 e-176
613 e-176
613 e-176
538 e-154
526 e-150
526 e-150
524 e-149
520 e-148
513 e-146
503 e-143
501 e-143
500 e-142
498 e-142
486 e-138
414 e-116
392 e-110
392 e-110
Q0GYY0 | PlantCyc: AT5G51690-MONOMER | aromatic-amino-acid ...
Q570P9 | PlantCyc: AT5G51690-MONOMER | aromatic-amino-acid ...

Comparing across species

- Use species selection tool on pathway pages



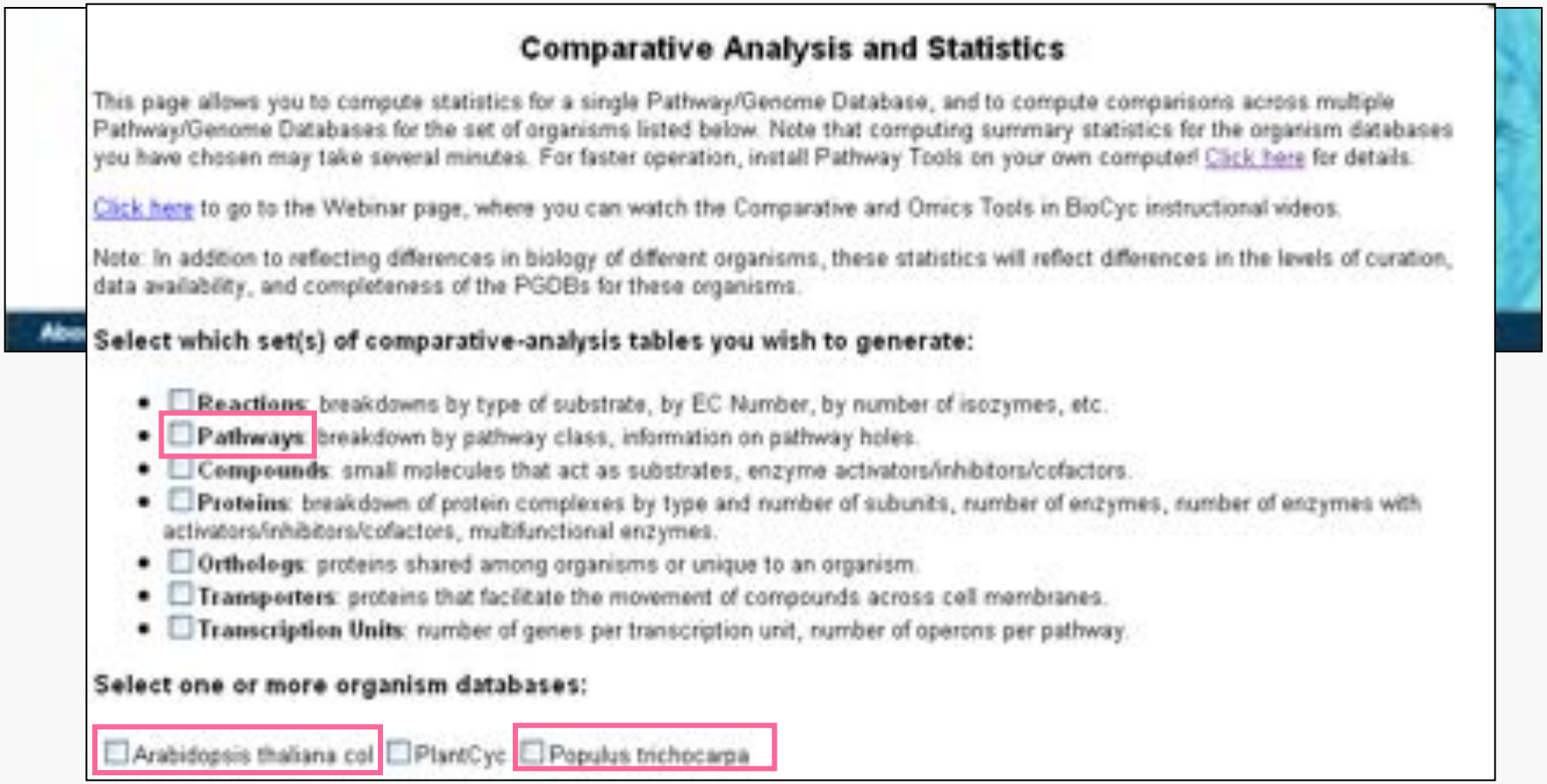
Compa

- Us

Organism	Evidence Glyph	Enzymes and Genes for choline biosynthesis III	
AraCyc col		EC# 2.7.7.15	choline-phosphate cytidylyltransferase: AT4G15130 choline-phosphate cytidylyltransferase: AT2G32260
		EC# 2.7.8.2	phosphatidyltransferase: AT3G25585 phosphatidyltransferase: AT1G13560
		EC# 3.1.4.4	phospholipase D: AT1G52570 phospholipase D: AT1G55180 phospholipase D: AT3G05630 phospholipase D: AT4G00240 phospholipase D: AT4G11830 phospholipase D: AT4G11840 phospholipase D: AT5G25370 phospholipase D: PLD alpha phospholipase D: PLD beta phospholipase D: PLD gamma phospholipase D: PLD delta phospholipase D: PLD zeta
P. trichocarpa		EC# 2.7.7.15	None
		EC# 2.7.8.2	diacylglycerol cholinephosphotransferase: JGI-225724 diacylglycerol cholinephosphotransferase: JGI-720905
		EC# 3.1.4.4	phospholipase D: JGI-811801 phospholipase D: JGI-781949 phospholipase D: JGI-810176 phospholipase D: JGI-593768 phospholipase D: JGI-827396 phospholipase D: JGI-578949 phospholipase D: JGI-730956 phospholipase D: JGI-240457 phospholipase D: JGI-833366 phospholipase D: JGI-417354 phospholipase D: JGI-763496 phospholipase D: JGI-558891 phospholipase D: JGI-415367 phospholipase D: JGI-550827 phospholipase D: JGI-755219 phospholipase D: JGI-180605 phospholipase D: JGI-829577

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.

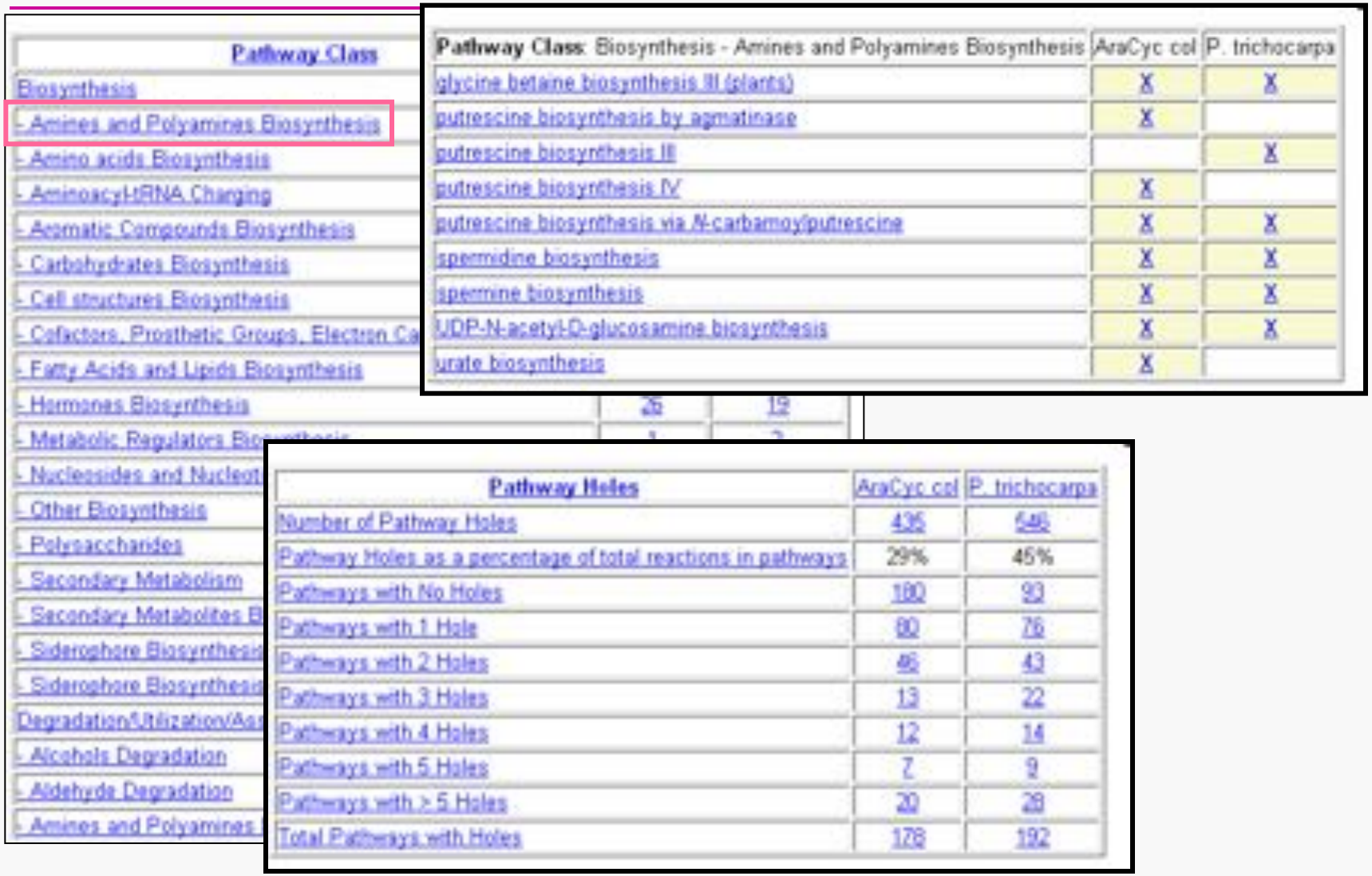
Select which set(s) of comparative-analysis tables you wish to generate:

- ☐ **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
Biosynthesis
- Amines and Polyamines Biosynthesis
- Amino acids Biosynthesis
- Aminoacyl-tRNA Charging
- Aromatic Compounds Biosynthesis
- Carbohydrates Biosynthesis
- Cell structures Biosynthesis
- Cofactors, Prosthetic Groups, Electron Ca
- Fatty Acids and Lipids Biosynthesis
- Hormones Biosynthesis
- Metabolic Regulators Bio
- Nucleosides and Nucleot
- Other Biosynthesis
- Polysaccharides
- Secondary Metabolism
- Secondary Metabolites B
- Siderophore Biosynthesis
- Siderophore Biosynthesis
Degradation/Utilization/As
- Alcohols Degradation
- Aldehyde Degradation
- Amines and Polyamines

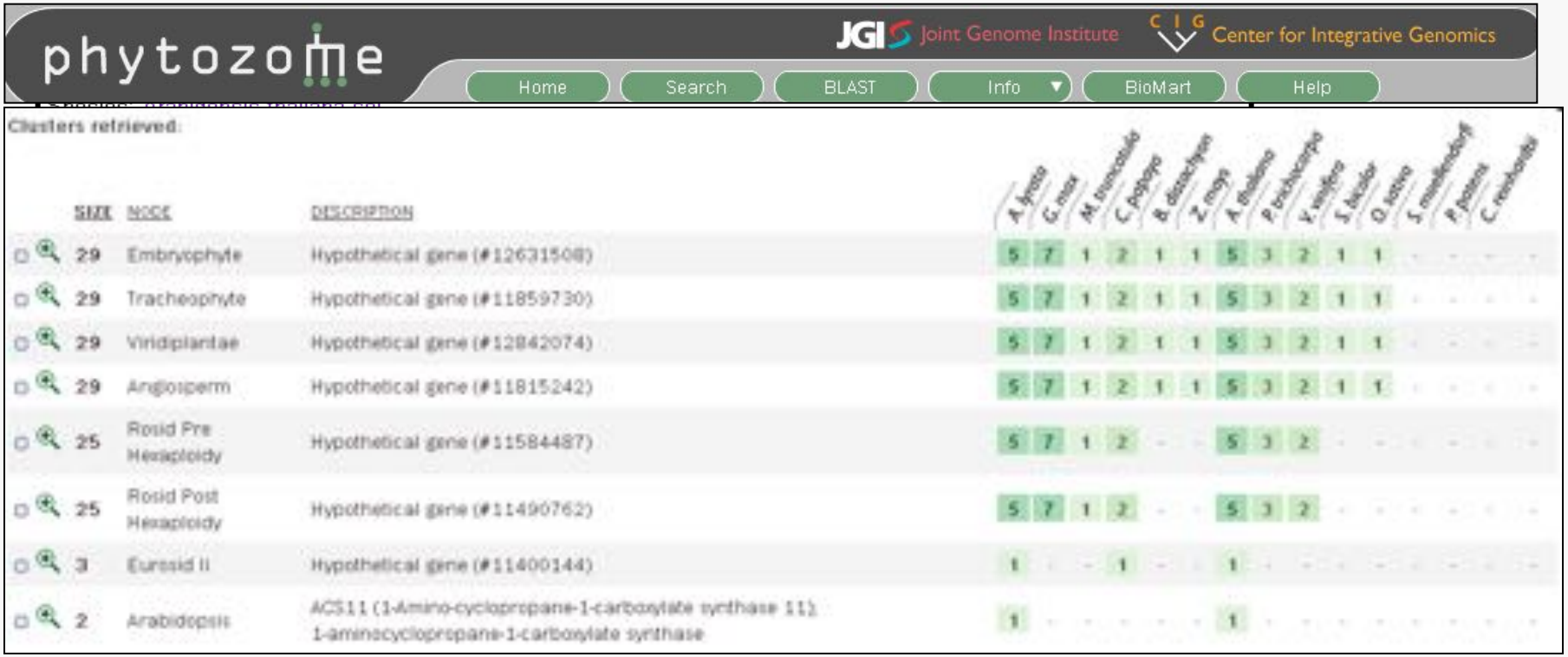
	26	19

Pathway Class: Biosynthesis - Amines and Polyamines Biosynthesis	AraCyc col	P. trichocarpa
glycine betaine biosynthesis III (plants)	X	X
putrescine biosynthesis by agmatinase	X	
putrescine biosynthesis III		X
putrescine biosynthesis IV	X	
putrescine biosynthesis via N-carbamoylputrescine	X	X
spermidine biosynthesis	X	X
spermine biosynthesis	X	X
UDP-N-acetyl-D-glucosamine biosynthesis	X	X
urate biosynthesis	X	

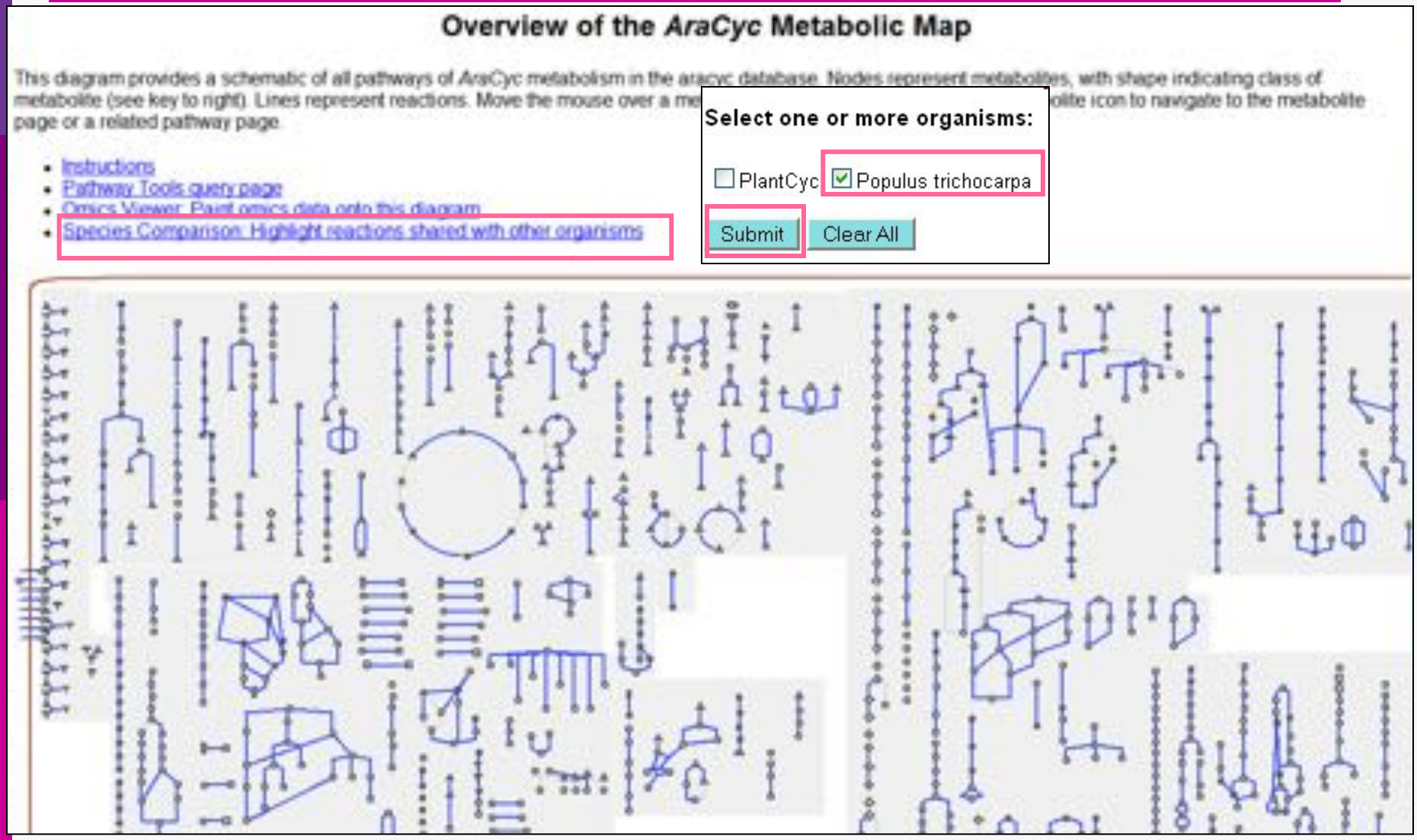
Pathway Holes	AraCyc col	P. trichocarpa
Number of Pathway Holes	436	646
Pathway Holes as a percentage of total reactions in pathways	29%	45%
Pathways with No Holes	180	93
Pathways with 1 Hole	80	76
Pathways with 2 Holes	46	43
Pathways with 3 Holes	13	22
Pathways with 4 Holes	12	14
Pathways with 5 Holes	7	9
Pathways with > 5 Holes	20	28
Total Pathways with Holes	178	192

Comparing across species

- Use Phytozome links on enzyme pages



Comparing across species



Comparing across species

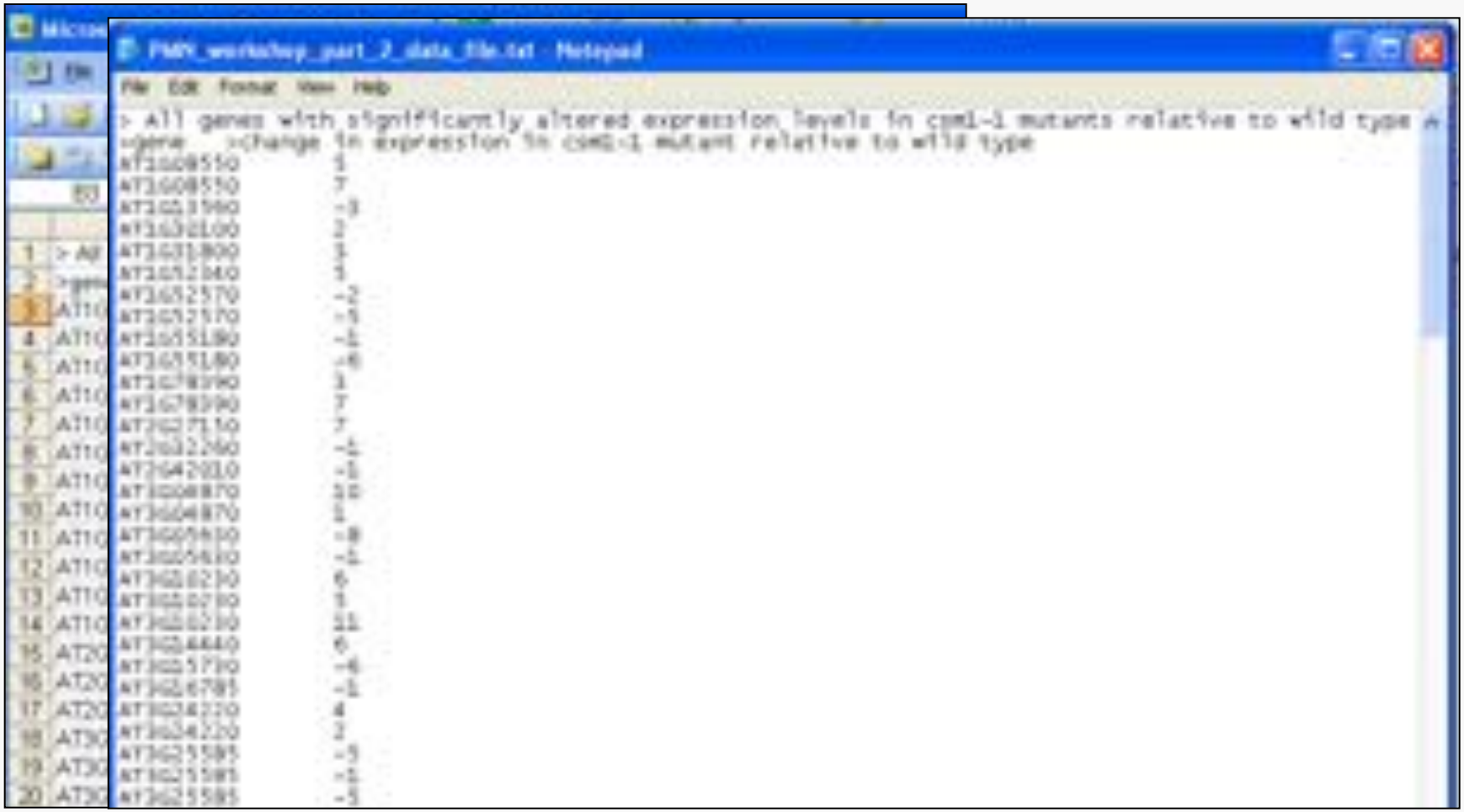
Visualizing OMICs data

- 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

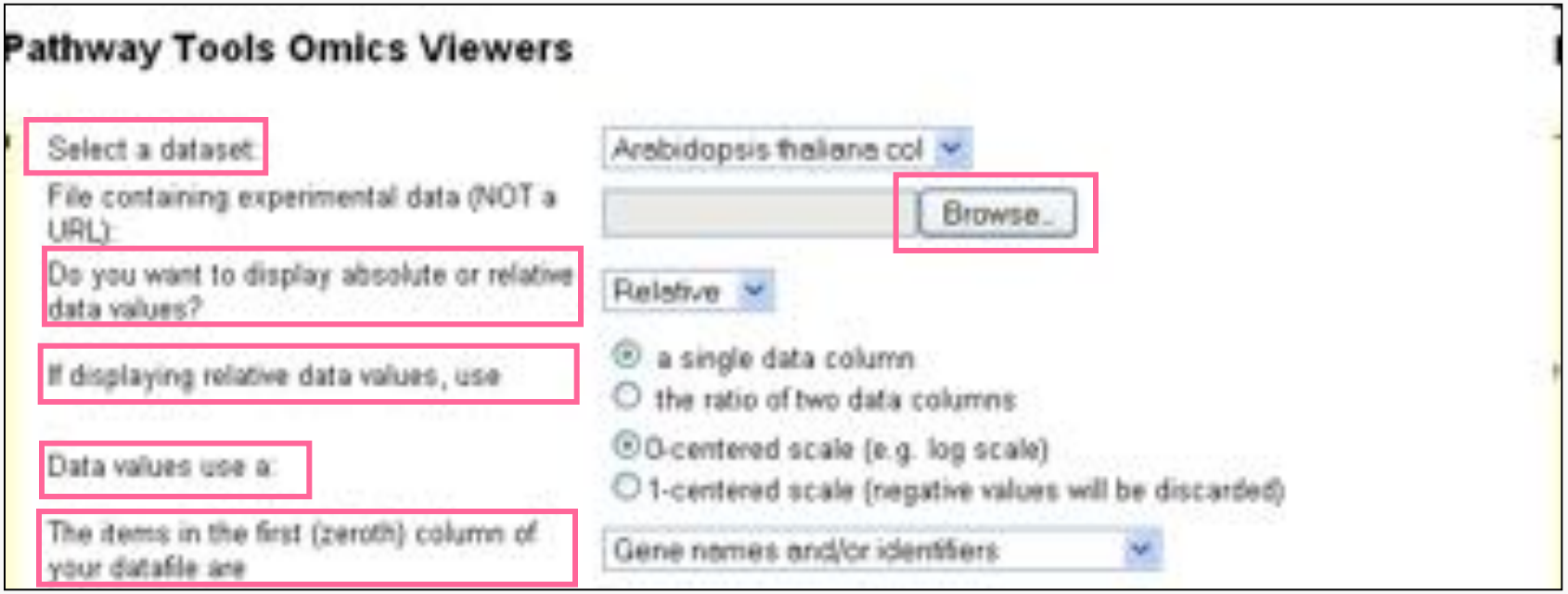


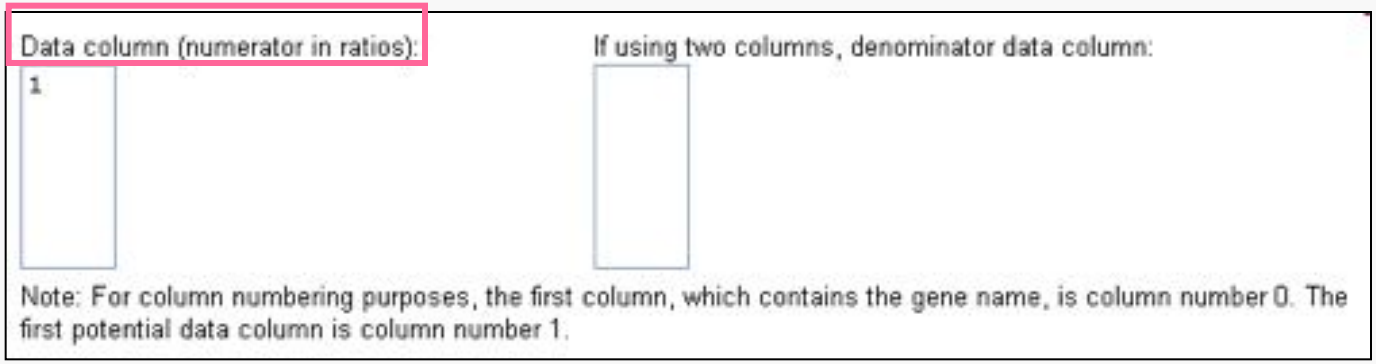
Visualizing OMICs data

- Upload data in the OMICs viewer

Visualizing OMICs data

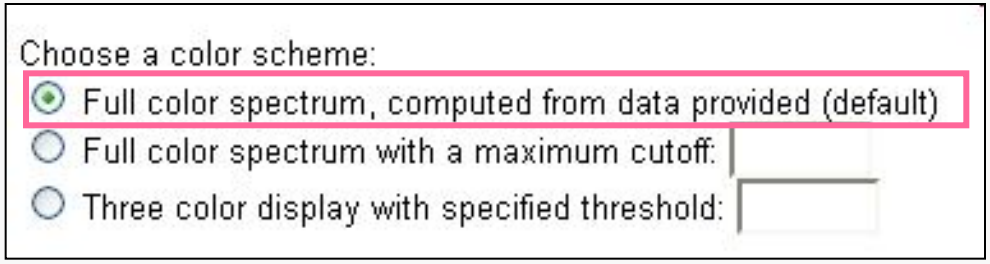
- Upload data in the OMICs viewer

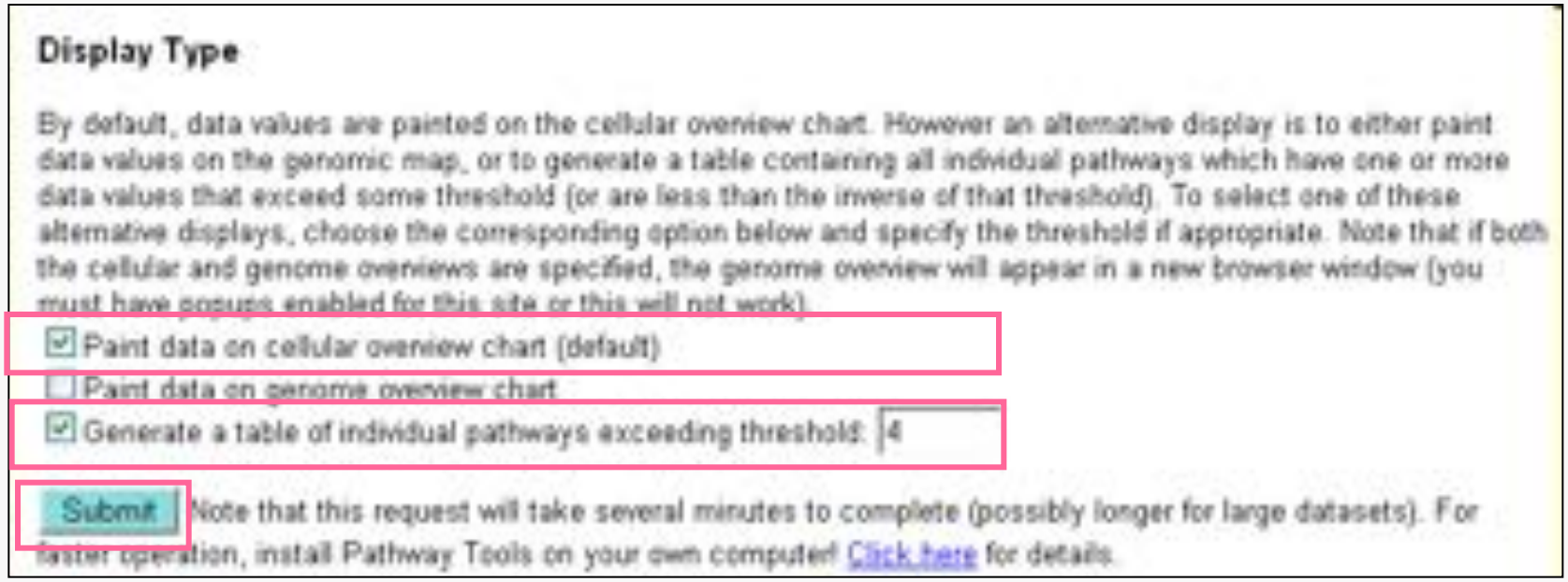




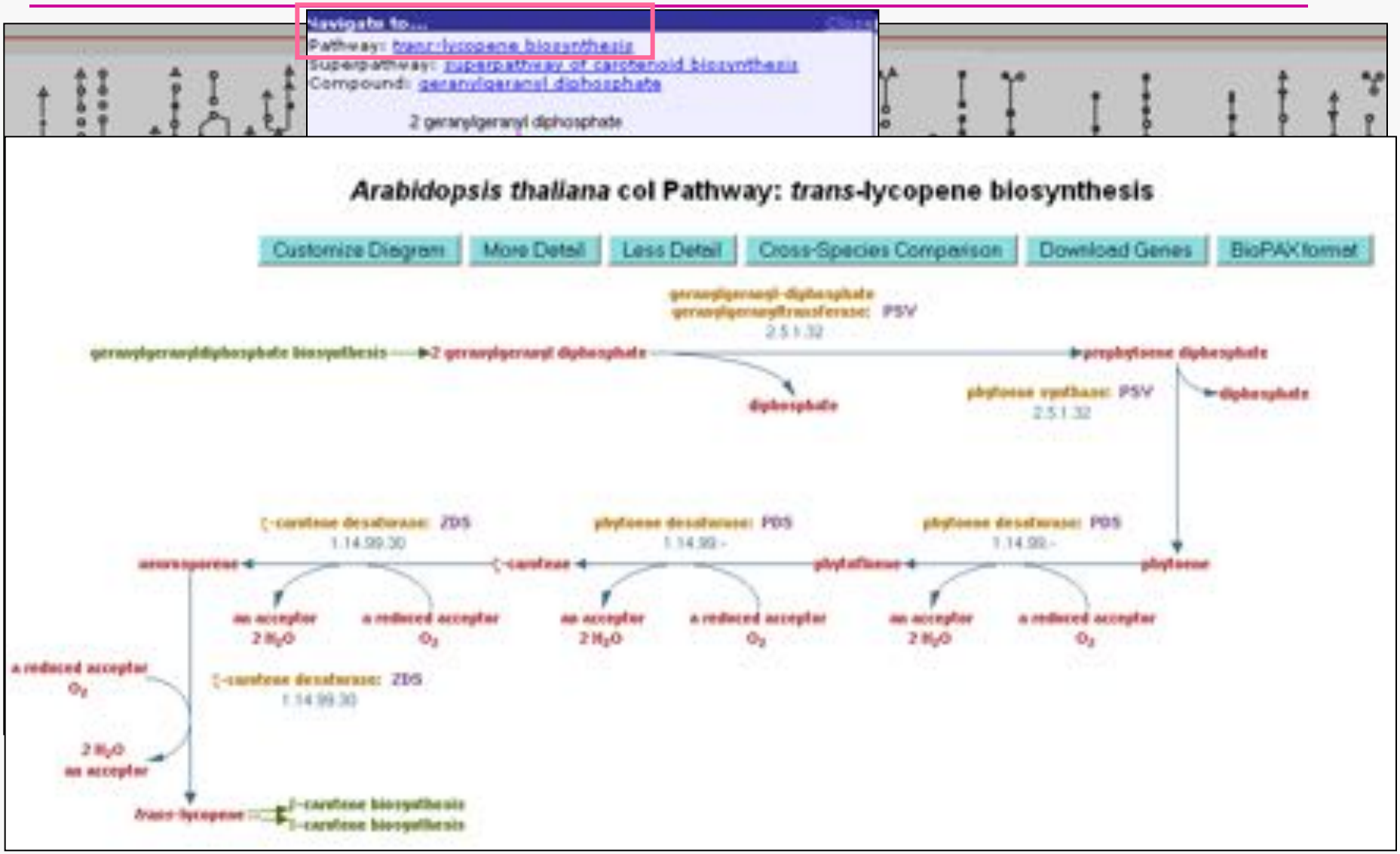
Visualizing OMICs data

- Set display parameters in the OMICs viewer

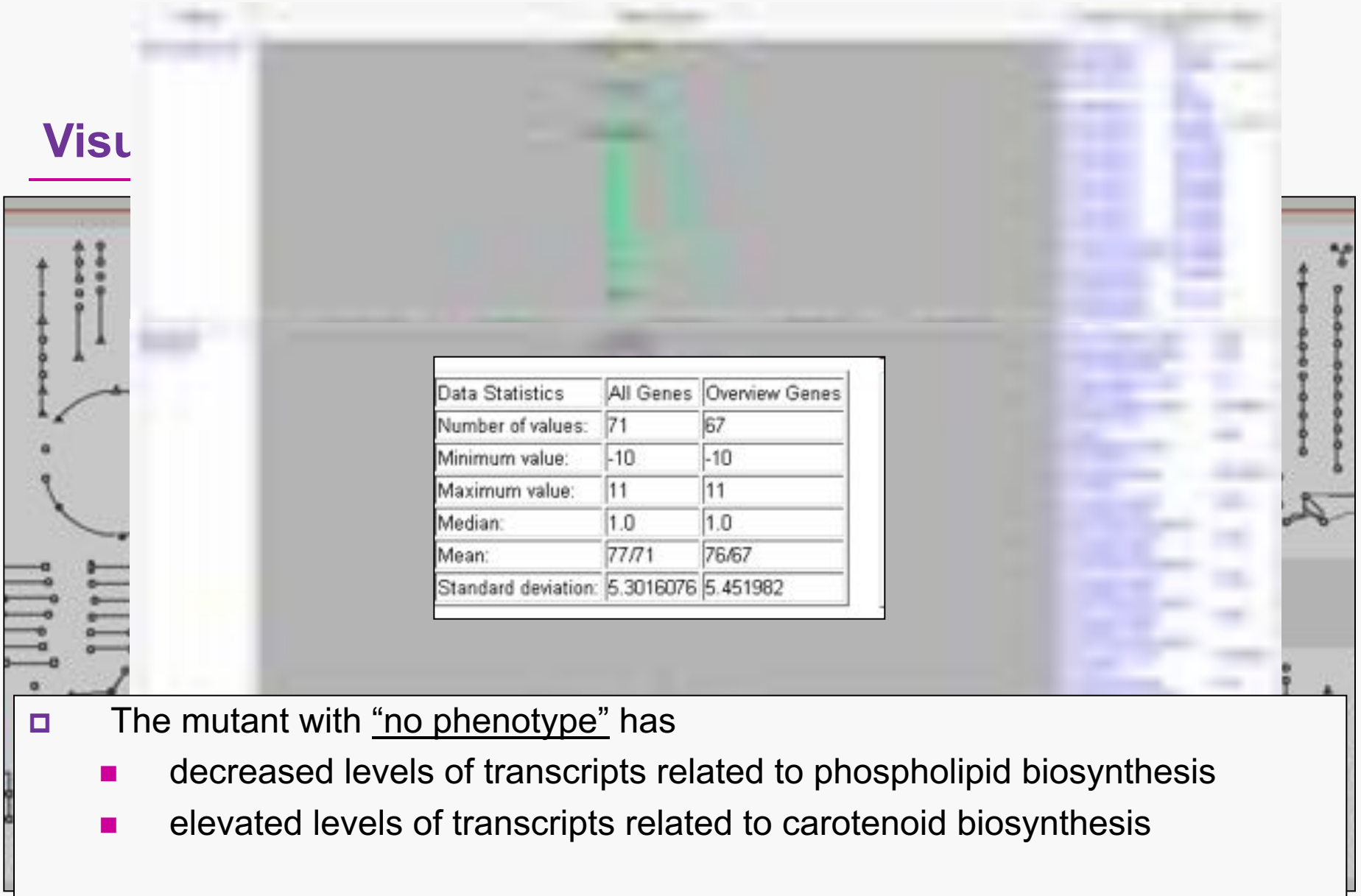




Visualizing OMICs data



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

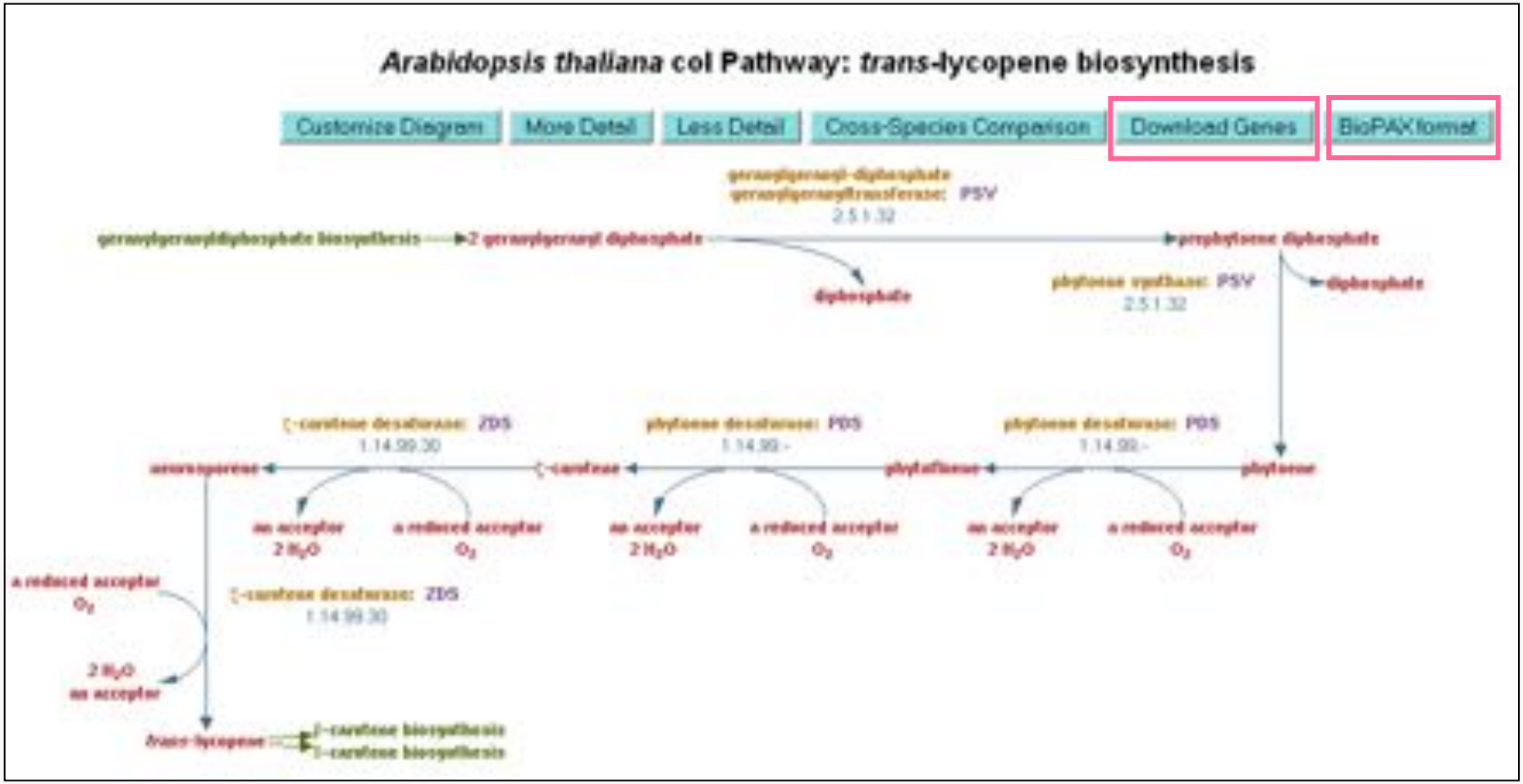
- Many applications

- 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

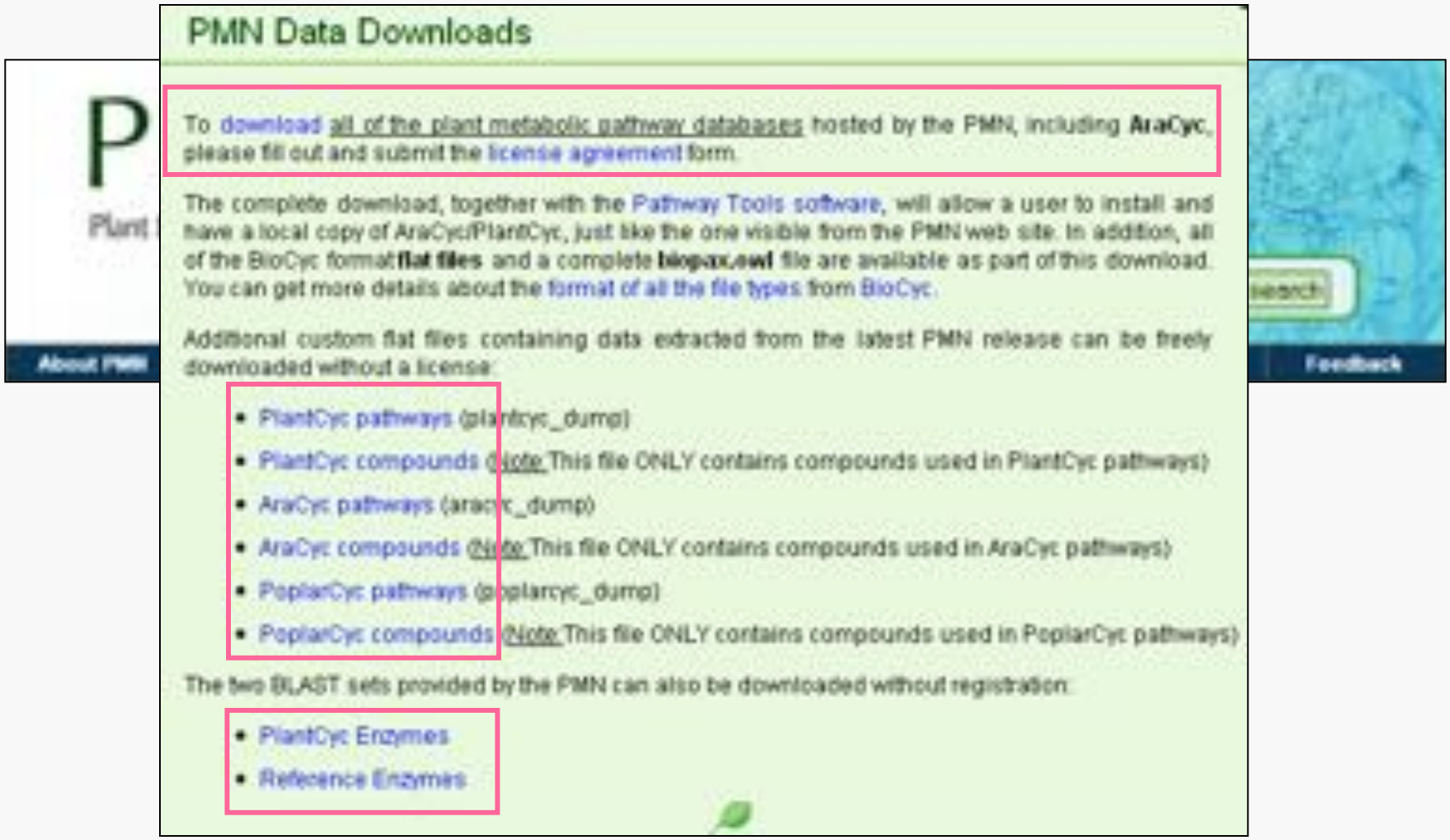
Data and software downloads

- Get pathway data sets from pathway pages



Data and software downloads

- Obtain large data sets

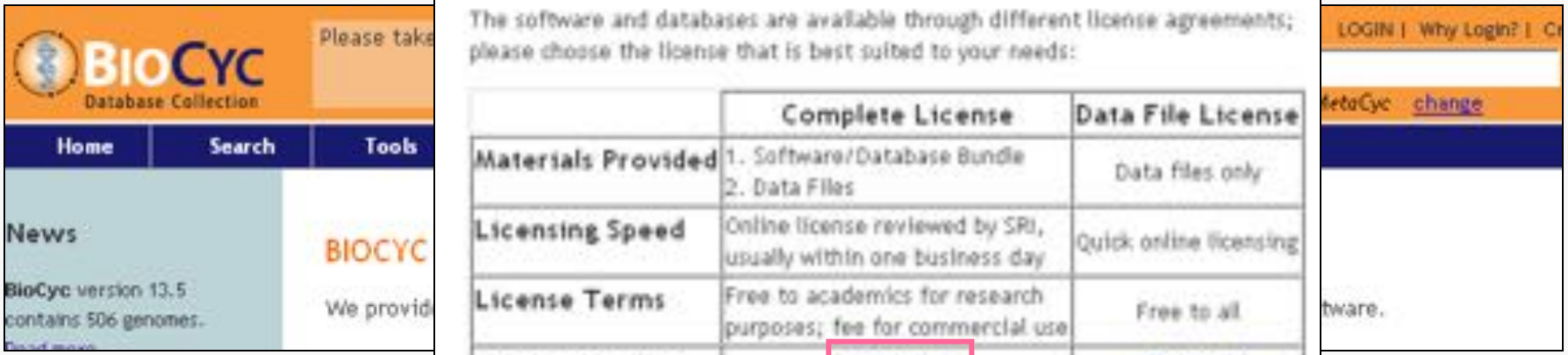


Data and software downloads

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

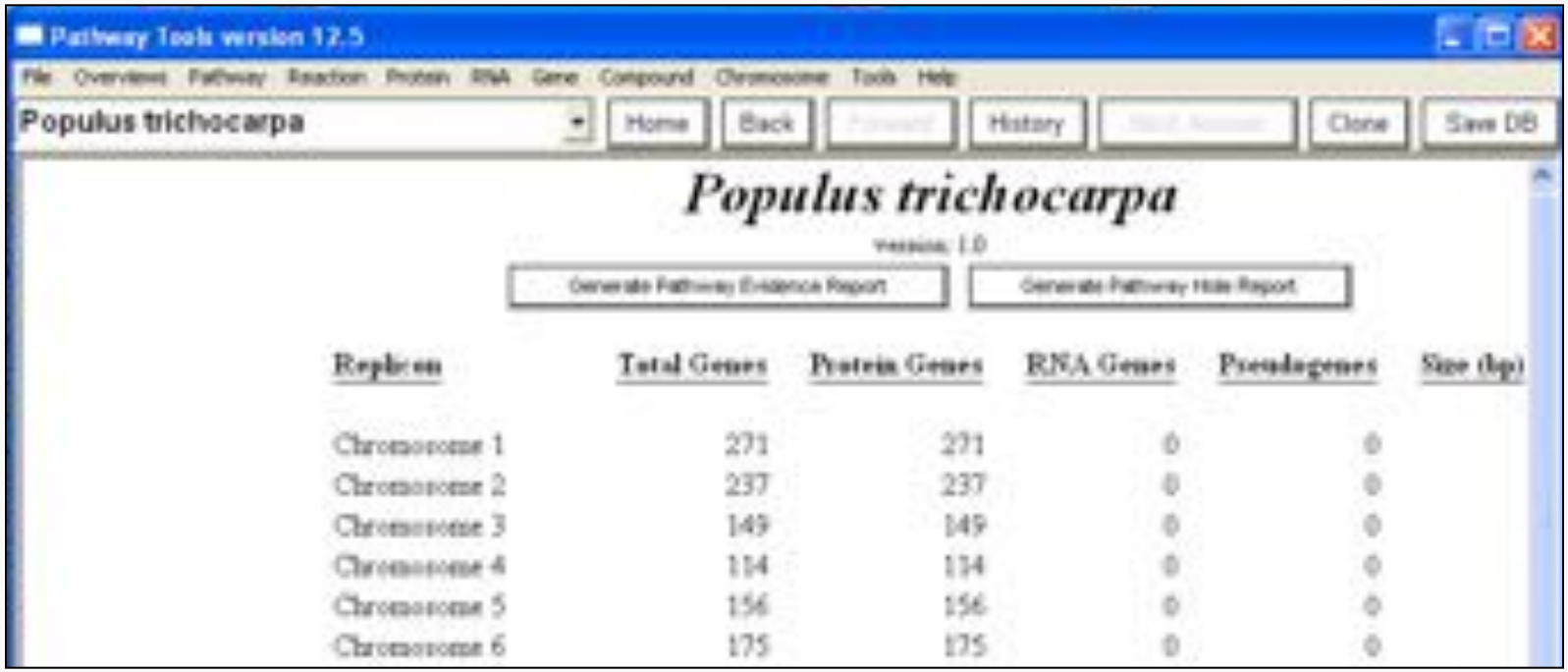
Data and software downloads

- Install a local copy of the Pathway Tools software

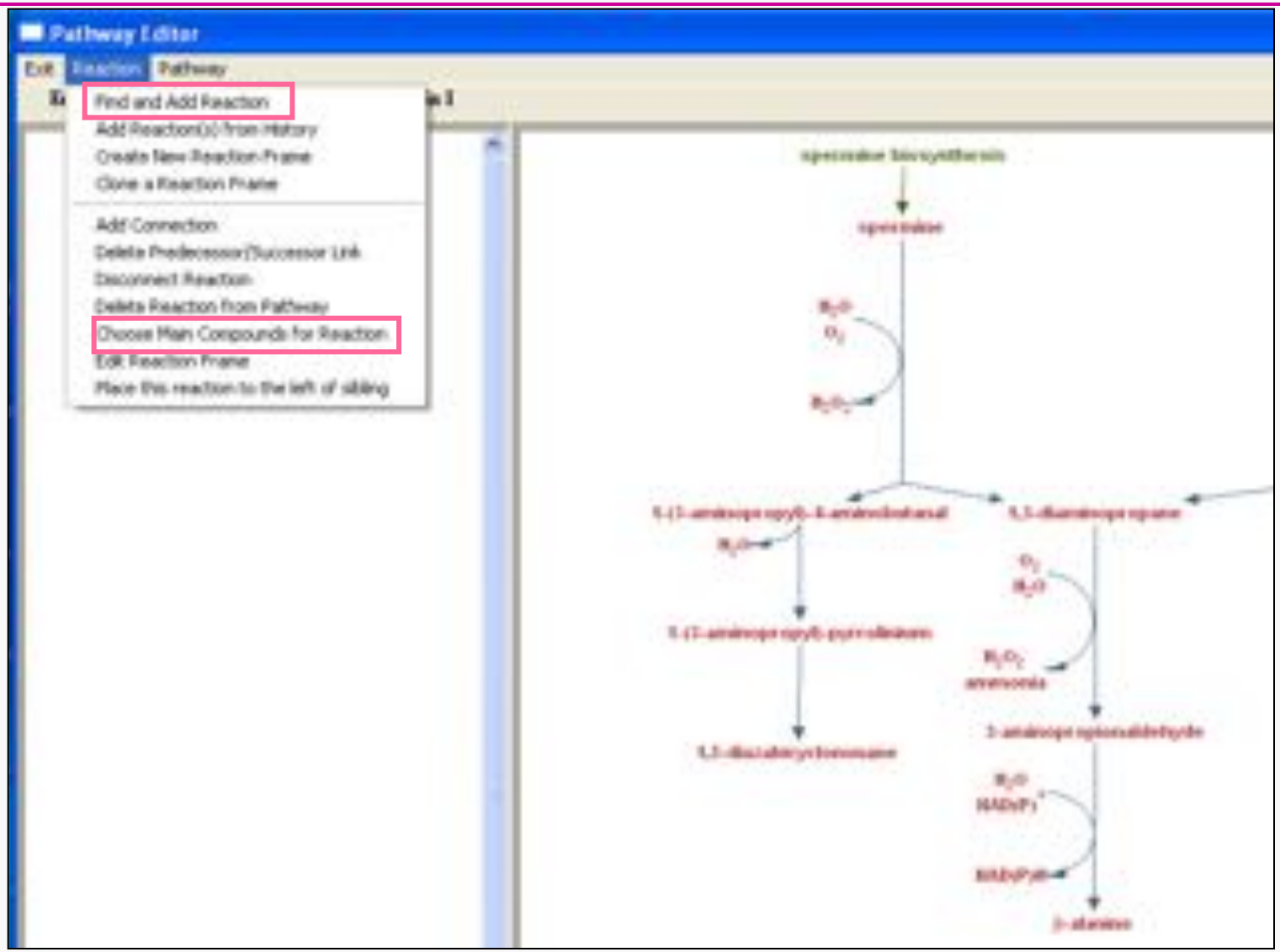


Data and software downloads

- Desktop version offers additional features

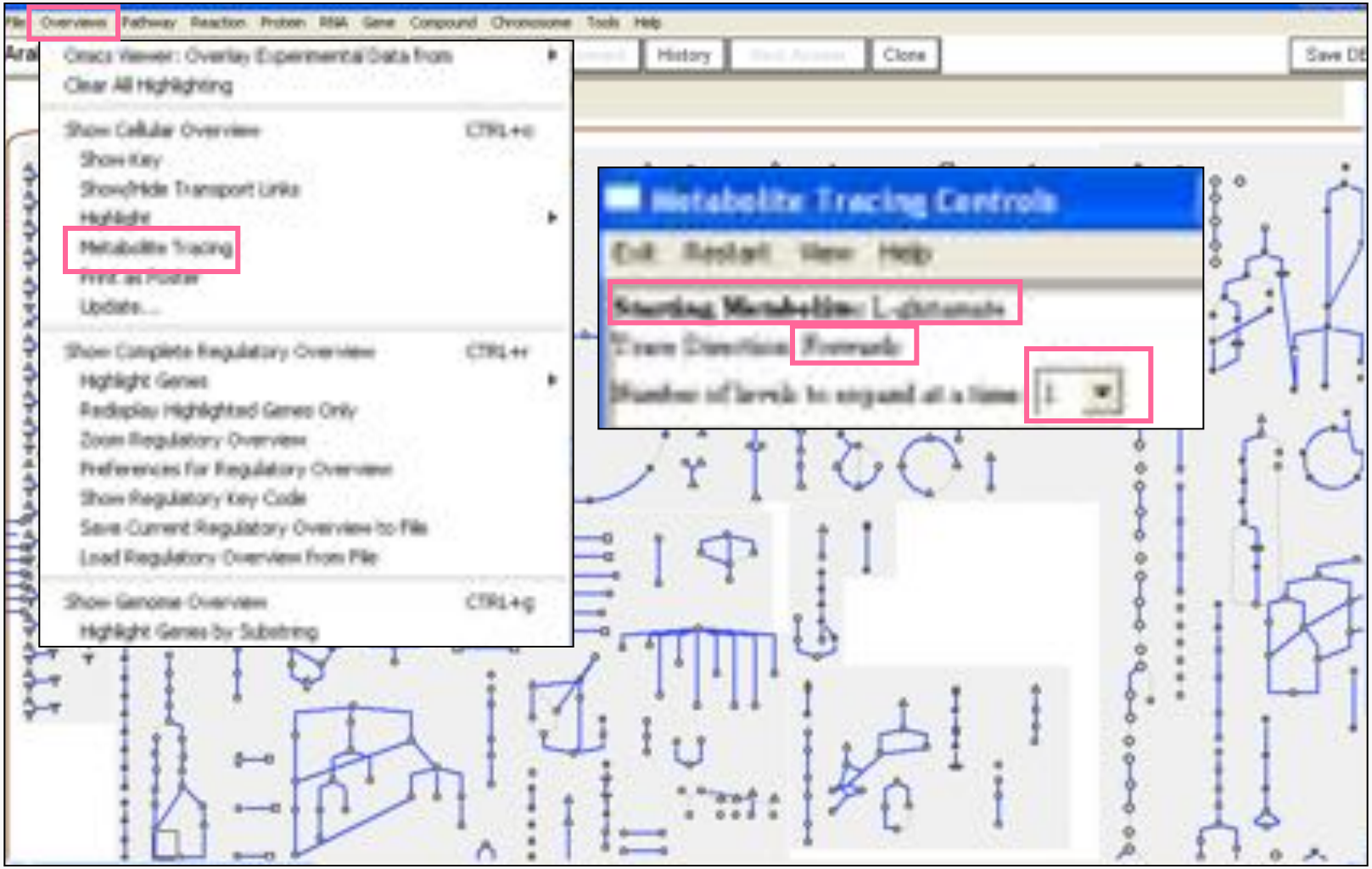


Data and software downloads



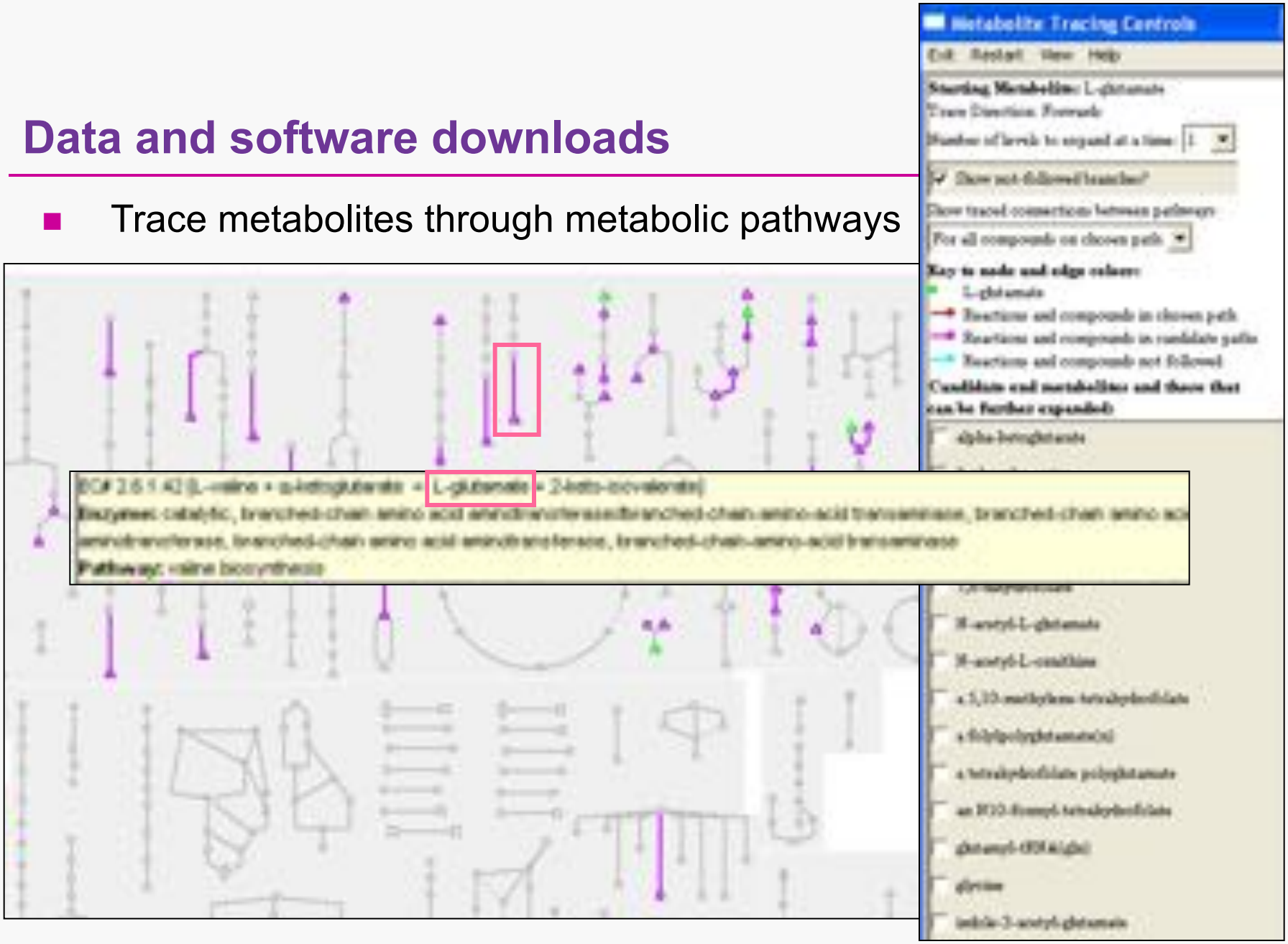
Data and software downloads

- Trace metabolites through metabolic pathways



Data and software downloads

- Trace metabolites through metabolic pathways



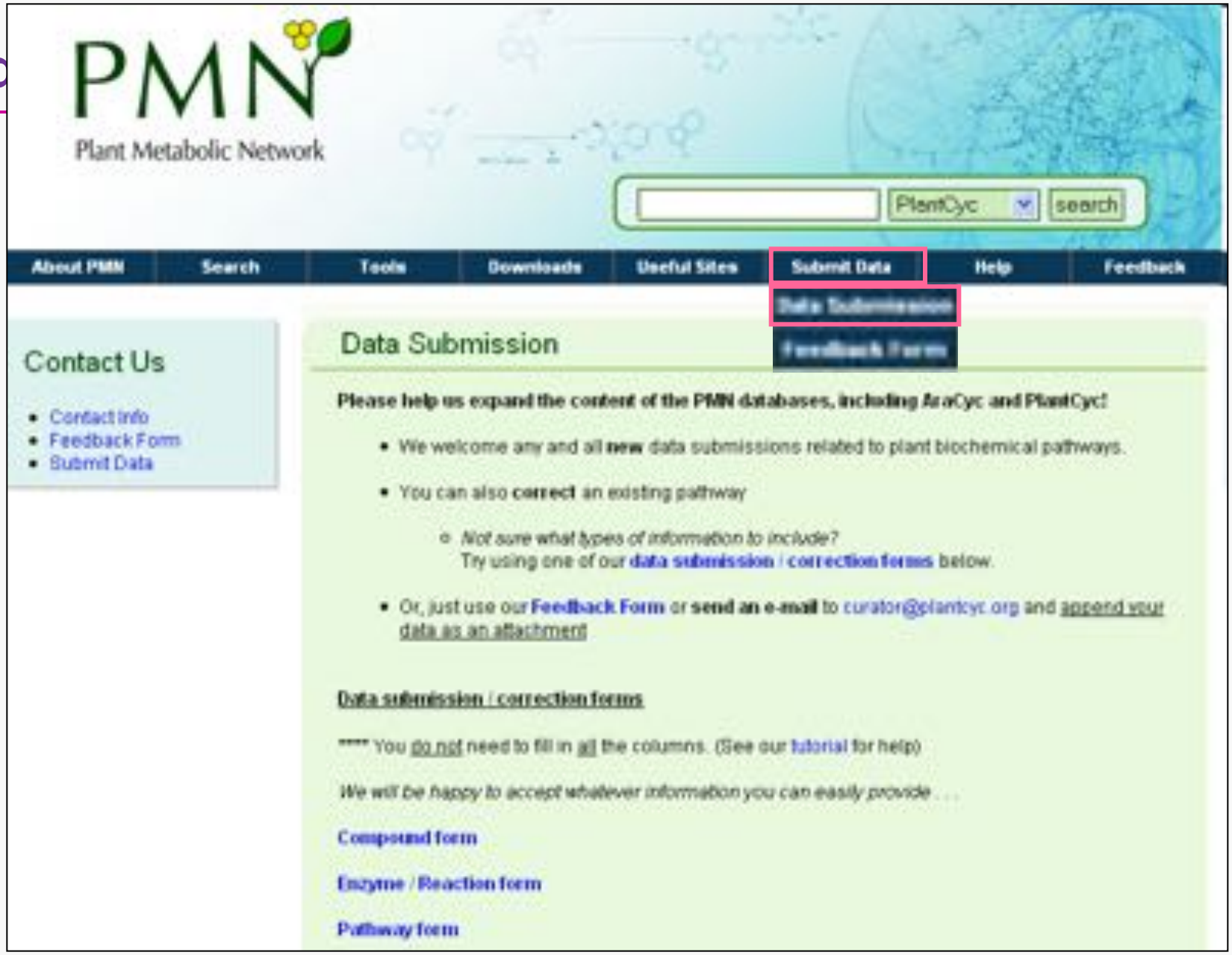
Data and software downloads

- 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

Creating new PMN content

- Manual curation
  - Entering experimental data
- Computational prediction

Ac


PMN
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PlantCyc
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Help
Feedback
Contact Us
Contact Info
Feedback Form
Submit Data
Data Submission
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 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


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In addition to the active contributors 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
EJ Blom - Aalgerie, The Netherlands
Mark Poolman - Oxford Brookes University, UK
Bryan Reinicke - Universidad de Chile, Chile
Contributors to Pathways of Primary and Secondary Metabolism
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Amines and Polyamines
John Jelesko - Virginia Tech, USA
Amino Acids
Vijay Joshi - Cornell University, USA
Carbohydrates
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Cofactors, Prosthetic Groups, and Electron Carriers
Imad Ajawi - Michigan State University, USA
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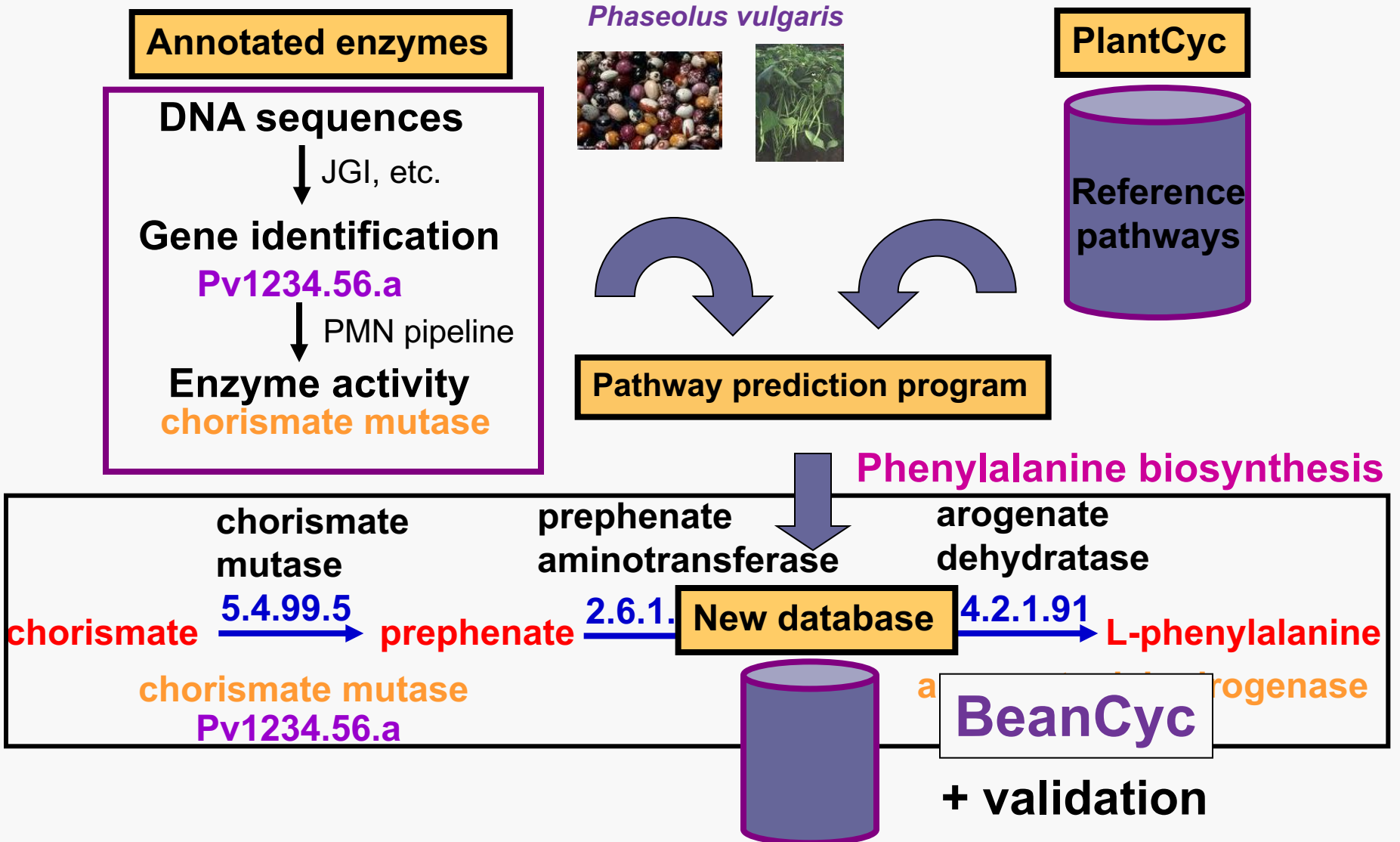
Carlos Menck - Universidade de São Paulo, Brazil
David Oliver - Iowa State University, USA
Stephane Ravanel - Institut de Recherches en Technologies et Sciences pour le Vivant, France

Creation of new PMN databases

- 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?

- 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

- 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

PMN
Plant Metabolic Network

AraCyc

curator@plantcyc.org

www.plantcyc.org

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PMN Acknowledgements

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- Hartmut Foerster *(curator)*

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- Ron Caspi (SRI)
- SRI Tech Team
- Lukas Mueller (SGN)
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- Gramene and MedicCyc

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- Cynthia Lee
- Tom Meyer
- Shanker Singh
- Chris Wilks

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What is in the PMN?

- 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