# Introduction to the Plant Metabolic Network: Data and Tools for Analysis and Discovery

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#### **Plant metabolism**

- Plants provide crucial benefits to humanity and the ecosystem
- A better understanding of plant metabolism may contribute to:
  - More nutritious foods
  - More pest-resistant plants
  - Higher photosynthetic capacity and yield in agricultural and biofuel crops
  - New medicines
  - ... many more applications
- These efforts benefit from access to high quality plant metabolism data



#### Introduction

The Plant Metabolic Network (PMN) provides a broad network of plant metabolic pathway databases that contain curated information from the iterature and computational analyses about the genes, enzymes, compounds, reactions, and pathways involved in primary and secondary metabolism in plants.

The PMN is funded by the National Science Foundation (Grant #: 102600) and 0640769), governed by an Editorial Board composed of internationally renowned scientists, and executed at the Camegie Institution for Science, Department of Plant Biology.

SCIENCE





#### Plant Metabolic Pathway Databases

The PMN currently houses one multi-species reference database called PlantCyc and ten species/taxon-specific databases.

#### News

Come see the PMN at PAG in January

The PMN invites you to come to our workshop at the Plant and Animals Genome Conference (IR.G XXI) on Sunday, January 13 in San Diego.

The PMN, the Sol Genomics Network (SolCyc), and PMN users will present an overview of our databases and examples of their applications to ongoing research.

Early registration ends on November 1.

We hope to see you there!

Additional exciting news ....

#### Outline

- PMN overview
- New metabolic database creation at the PMN
- Community data submissions
- PMN data analysis tools
- Downloadable software

### **Plant Metabolic Network goals**

- **Transform published results into data-rich metabolic pathways**
- Create and deploy improved methods for predicting enzyme function and metabolic capacity using plant genome sequences
- Facilitate data analysis
- Support research, breeding, and education
- Provide public resources :
  - PlantCyc
  - AraCyc
  - 9 additional species-specific databases



### Plant Metabolic Network collaborators

- SRI International BioCyc project
- Provide Pathway Tools Software
- Maintain and update MetaCyc
- Other collaborators / contributors include:
  - MaizeGDB
  - **GoFORSYS**
  - SoyBase
  - Sol Genomics Network (SGN) / Boyce Thompson Institute
  - Gramene
  - MedicCyc / Nobel Foundation
  - PlantMetabolomics group
  - ... and more





#### **PMN data content statistics**

#### □ Latest PMN release – August 2012

	Pathways	Enzymes *	Reactions	Compounds
PlantCyc 7.0	978	34663	3617	3455

**Over 400 species of plants appear in PlantCyc** 

#### **PMN data content statistics**

#### New and updated species-specific databases

		Pathways	Enzymes *	Reactions	Compounds
	AraCyc 10.0	540	7127	3418	3323
	CassavaCyc 2.0	351	7178	2137	1538
New at the PMN!	ChlamyCyc 2.0	283	2157	1688	1130
	CornCyc 2.0	373	10527	2198	1752
	GrapeCyc 2.0	359	5341	2143	1571
New!	MossCyc 1.0	335	5664	2018	1409
New!	PapayaCyc 1.0	370	3898	2165	1557
	PoplarCyc 5.0	381	8691	2256	1613
New!	SelaginellaCyc 1.0	329	3958	1986	1403
	SoyCyc 3.0	441	13055	2566	2007

\* The term "enzyme" refers to both monomers and complexes found in the databases.

#### **PMN data sources**

□ In PlantCyc and AraCyc, many enzymes have experimental evidence



New databases rely primarily on computational predictions



- E2P2 = Ensemble Enzyme Prediction Pipeline
  - Used to predict enzyme function from protein sequence
  - Developed and maintained at the PMN

 1) Relies on an in-house, manually curated gold-standard set of proteins called the Reference Protein Sequence Data Set (RPSD)







- Proteins with known enzymatic function
- Proteins with NO enzymatic activity



#### **2**) Train the pipeline

- Use protein functional prediction programs on sampled data from RPSD
- Current programs:
  - BLAST
  - PRIAM
  - CatFam

- Predict the function of known proteins in the RPSD
- Learning consists of quantifying how well each program can predict each EC class



ie individual

Integrating predictions: simplified hypothetical example:



E2P2 decision: Protein A = 2.4.1.116

#### **E2P2** implementation and PGDB creation

- Retrieve proteome sequence from an annotated genome
  - Phytozome is the primary source
- Run E2P2 pipeline on proteome data to identify enzyme sequences and classify them with EC numbers.
- Load the proteins and EC assignments into Pathologic to predict metabolic pathways
- Generate an "unvalidated" species-specific database

Semi-automated validation / incorporation (SAVI) pathway review

Step 1: Check for UPPs ("Universal" Plant Pathways)

- Pathways believed to be found in "all" land plants
  - e.g. Photosynthesis, glycolysis, etc.
- 215 UPP pathways during PMN 7 release (August 2012)
- UPP decision rules
  - If the pathway was predicted -> KEEP it
  - If the pathway was not predicted -> ADD it

Step 2: Check for NPPs (non-plant/non-PMN pathways)

- Pathways believed to be present only outside of the plant kingdom
  - Glycogen biosynthesis
- Pathways describing processes not covered by the PMN
   protein ubiquitination, etc.
- 164 NPP pathways used during PMN 7 release (August 2012)
- NPP decision rule:
  - If the pathway was predicted -> REMOVE it

- Step 3: Manually validate remaining pathways
  - Keep pathways with experimental evidence for enzymes or key compounds in the given species
  - Keep pathways with enzymes catalyzing "unique" reactions
    - Sometimes results in the inclusion of biologically unlikely pathways
    - Clearly noted with a computational evidence code
    - \*\* May be removed as a criteria for pathway retention in future PMN releases

- **Future SAVI pipeline improvements** 
  - Add more automated decision rules:
    - Reactions that distinguish between two pathway variants (Primary metabolism)
    - Taxonomic range (Secondary metabolism)

### Expert input welcome!!

□ To submit data, report an error, volunteer to validate or ask a question

- Send an e-mail: <u>curator@plantcyc.org</u>
- Use our feedback form:

					Play	nge 🚽	search
About Plan	Search	Toole	Downloads	Useful Sites	Salared Data		Feedback
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- Visit the PMN poster P0929 Monday 3:00 4:30 PM
- Meet with me at the end of the workshop
- Schedule an individual meeting with me at PAG (or ASPB)



Together, we can make valuable, high quality databases

#### **PMN** databases - part of the BioCyc / MetaCyc family

#### Databases at the PMN have:

- Standard BioCyc display features
- Standard BioCyc analyses tools
- PMN-specific features



### **General searching at the PMN**

Pathway Tools quick search bar



Arabidopsis thaliana col	
Carica papaya	
Chlamydomonau reinhardhi	
Glycine max	
Manihot esculenta esculenta	
Physcomitrella patens	
PlantCyc	
Populus trichocarpa	
Selaginella moellendorffi	
Vitia vinifera	
Zea mays mays	

### **Specialized search options**





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

- Organism: breakdown by principal data types
- III Reactions: breakdowns by type of substrate; by EC Number, by number of isosymes, etc.
- E Pathways: breakdown by pathway class, information on pathway holes.
- El Compounds: small molecules that act as substrates, enzyme activators/inhibitors/cofactors
- Cenes/Proteins: breakdown of genes by product type, ontology, annotations; breakdown of pensymes, number of enzymes with activators/leit/biturs/cofactors, multifunctional enzymes.

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#### **Sequence-based search options**





### **Working with Groups**

#### Opportunities

- Create custom data sets
- Examine experimental results
- Perform enrichment analyses
- Share data
- Requires free registration

### **Register at the PMN**

- Registration and login available from every data and search page
  - \*\* Not available on the home page yet.

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### **Register at the PMN**

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Login . . .and start working with groups!!

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### Work with groups

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### Work with groups





## **Create groups from searches**

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# **Create groups from searches**

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#### **Create groups from searches**



### **Upload groups**



# **Upload groups**

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### **Perform enrichment analyses**

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### **Download and share groups**

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### Data analysis with the Metabolic Map / Omics Viewer

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#### Data and software downloads

Install a local copy of the Pathway Tools software



#### **Data and software downloads**

Download the complete database files with a FREE license







# Plant metabolic NETWORKING

- 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!



curator@plantcyc.org



www.plantcyc.org

# **PMN Acknowledgements**

#### Curator:

- kate dreher

#### Post-docs:

- Lee Chae
- Ricardo Nilo Poyanco
- Chuan Wang

#### Interns

- Caryn Johansen

#### Tech Team Members:

- Bob Muller (*Manager*)
- Larry Ploetz (Sys. Admin)
- Shanker Singh
- Bill Nelson

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- Flavia Bossi
- Hye-in Nam
- Taehyong Kim
- Meng Xu

#### Peifen Zhang (Director and curator)

#### PMN Alumni:

- A. S. Karthikeyan (curator)
- Christophe Tissier (curator)
- Hartmut Foerster (curator)
- Eva Huala (co-Pl)
- Tam Tran (intern)
- Varun Dwaraka (intern)
- Damian Priamurskiy (intern)
- Ricardo Leitao (intern)
- Michael Ahn (intern)
- Purva Karia (intern)
- Anuradha Pujar (SGN curator)

#### Tech Team Alumni

- Anjo Chi
- Cynthia Lee
- Tom Meyer
- Vanessa Kirkup
- Chris Wilks
- Raymond Chetty

#### Collaborators:

#### <u>SRI</u>

- Peter Karp
- Ron Caspi
- Hartmut Foerster
- Suzanne Paley
- SRI Tech Team

#### **MaizeGDB**

- Mary Schaeffer
- Lisa Harper
- Jack Gardiner
- Taner Sen

#### <u>ChlamyCyc</u>

- Patrick May
- Dirk Walther
- Lukas Mueller (SGN)
- Gramene and MedicCyc









We're here to help . . .

PIAnt Metabolic Network



curator@plantcyc.org

www.plantcyc.org

Poster **P0929**: Monday: 3:00 – 4:30 PM