Building Better Biological Databases Together: Part 3:

Accessing the Data You Need at the Plant Metabolic Network

kate dreher curator

PMN/TAIR

The Carnegie Institution for Science Stanford, CA

Accessing the data you need at the PMN

- Introduction
- Data Overview
- Basic and Advanced Searching
- New and Improved Features
- Desktop Capabilities
- Acknowledgments

Plant metabolism

- Plants provide crucial benefits to the ecosystem and humanity
- A better understanding of plant metabolism may contribute to:
 - More nutritious foods
 - New medicines
 - More pest-resistant plants
 - Higher photosynthetic capacity and yield in crops
 - Better biofuel feedstocks
 - Improved industrial inputs (e.g. oils, fibers, etc.)
 - . . . many more applications

□ These efforts require access to high quality plant metabolism data

Plant Metabolic Network goals

- Capture and organize published data to create metabolic pathways
- Facilitate data analysis
- Make proteome-based metabolic pathway predictions for many plant species
- Support research and education
- Provide public resources : www.plantcyc.org
 - PlantCyc
 - AraCyc
 - PoplarCyc
 - more on the way



Plant Metabolic Network collaborators

- SRI International BioCyc project
 - Created Pathway Tools software



Maize Genetics and Genomics Database



- Provide on-going Pathway Tools software support and development
- Maintain and update MetaCyc (multi-kingdom) reference metabolic pathway database
- Other collaborators / contributors include:
 - Sol Genomics Network (SGN) / Boyce Thompson Institute
 - Gramene
 - Maize GDB
 - MedicCyc / Nobel Foundation
 - SoyBase
 - ChlamyCyc
 - PlantMetabolomics group
 - . . . and more



Plant Metabolic Network data

Pathway-based access to multiple data types





PMN data content statistics

Latest PMN release – April 2011

	PlantCyc 5.0	AraCyc 8.0	PoplarCyc 3.0
Pathways *	737	393	309
Enzymes **	11217	5520	3422
Reactions	3142	2525	1758
Compounds	3146	2825	1406
Organisms	366	1	1***

* These represent "base pathways" that are composed entirely of reactions. A base pathway may be joined with additional base pathways and/or reactions to create a superpathway. Superpathways are not included in this statistic.

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

*** The vast majority of the enzymes present in the database are from *Populus trichocarpa* but experimentall supported enzymes and pathways from other species or hybrids in the *Populus* genus can be included in PoplarCyc.

Searching at the PMN

Pathway Tools quick search bar

PMN	Select a Database:	Choline Search Database PlantCyc <u>change</u>	Quick Search
	Arabidopsis thaliana col PlantCyc Populus trichocarpa		

Quick search results



Specific search pages

PMN	P q	and the second	ten de	1-1	Search Database	PlantCyc <u>cha</u>	Quick	Search
About PMN	Search	Tools	Downloads	Useful Sites	Submit Data	Help	Feedback	
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PlantCy	c Comp	bound Se	arch	lear Form	All Compounds			
	compound by r	same or ID						
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Search/Filt	ter by molecula	r weight					(ina	ctive)
► Search/Fit	ter by chemical	formula (partial	or full)				(ina	ctive)
Search by I	nchi string						{ina	ctive)
		5	ubmit Query C	lear Form List of	All Compounds			

Specific search pages

antCyc Gene/Prot	ein/RNA Search			
Submit Query	Clear Form List of All Gen	es List of All Polypeptides	List of All Protein Complexes	List of All RNAs
Search by gene name or database id	entifier .			
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nter a gave name, or a database identifier from	this database or from an external databa	GENE		
ontain Noko. Partial nameo will generate a subotr	ing search on game names only (not on data	abare identifiers).		
enpler: "trp#", "trp", "b13%"				
Search by protein name, EC number,	or database identifier	12		
cytokinin		DPO	TEINI	
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cytokindo contesa - Das mayo	able collector substrate or Ka	so d	1	inactive]
Sparsh/Ellter by evidence code	ator, conscient, subscrate of me	ente -		inactive]
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Specific search pages

10000	Submit Query	Clear Form List of All	Genes List of All Polyp	eptides List of All Protein Complexes List of All		
Search by ge	me name or database id	entifier.				
rtar a gane nan orrain Inko. Pa omples: "Trpk" Selarch bly p	PlantCyc You searched for a Your query returne	Query Res Il gene products who d 2 results.	ults se name contains the	string "cytokinin oxidase" , and that I		
cvtokir	Gene Name 🔺 🔻	Product Name △ ▽	Organism △ ▽	Evidence 🛆 🛡		
iter a protein a	CKX(1	cytokinin oxidase	Arabidopsis thaliana	Reaction enhanced in mutant		
ration to which	CKX1	cytokinin oxidase	Zea mays	Assay of partially-purified protein		
anple: "Fight Search/Filte Search/Filte Search/Filte Search/Filte	plan rymaus", "Pl ir by product m ir by pl ir by small mole ir by evidence ir by cell compo	Cytokinin oxidase Zea mays Assay or partially-purified protein Assay or partially-purified protein Inferred by computational analysis (6850) Inferred by curator (7) Inferred from experiment (2204) Select one or more evidence codes to filter the result to only include gene products that have the corresponding evidence for their function. Deselecting all evidence codes has the same effect as selecting all evidence codes no filtering will be done based on evidence code.				

Sequence-based search options



PMN BLAST 2.2.8



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

databasa PlantQvs	coarch for Compounds (2679 instances)	edd e condition
	search for pounds (2073 Instances)	
Select fields to include	in the query output:	
olumn 1		
Sort based on this column		

□ Find all of the <u>30-carbon compounds</u> that appear as products in reactions

Construct query

n database PlantCyc	💌 search for	Compounds (2679 instances)	~	add a condition
		Enzymetic Paesthons (18378 instencies) Genetic-Elements (18378 instencies) -Chromosomes (1 instences) -Contigs (2 instences) -Plasmids (3 instences) -Plasmids (3 instences) Organizations (11 instences) Partilogous-Gene-Groups (3 instences) Pattweys (714 instences) -Super-Pattways (72 instances) Playmer-Segments (18010 instences) -Al-Genes (10010 instences)		

n database	PlantCyc	💌 sea	arch for	Сотроі	unds (2679 instances)		*	remo∨e condition]
Where		Chemical-Formula		*	contains the substring		*	C30	
and	*	the number of objects	s of 🔽 🖌	Appears	-In-Right-Side-Of	💌 🛛 is greater than		✓ 0	
add a conc	dition 🔽								

Select output fields

Column 1 ⓒ Sort based on this column	add a column
NAME	~

Column 1	Column 2 ⊠	Column 3 ⊠	Column 4 ⊠
	○ Sort based on this column	○ Sort based on this column	○ Sort based on this column
NAME	Chemical-Formula 💌	Appears-In-Right-Side-Of	Molecular-Weight

Select file format and retrieve

3. Select query output format:
⊙ HTML ○ Tab Delimited Text (columns are separated by tabs)
4. Submit Query

■ A list of **30-carbon compounds that appear as products in reactions**

his query resulted in a single	e fable 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 fee (x1 *? MOLECULAR- WEIGHT)
a-amyrin	C30H5001	(S)-2.3-epoxysqualene = o-amyrin	426.724
<u> P-amyrin</u>	C30H5001	(S)-2.3-epoxysqualene = β-amyrin	426.724
(E)-cinnamoyl-Coð	C30H42N7.017P3S1	trana-cinnamate + coanzyme A = (£)-cinnamoyi-CoA + H ₂ O	897.68
(S)-2.3-epoxysqualene	C30H5001	squalene + NADPH + O ₂ = (S)-2.3- epoxysqualene + NADP ⁴ + H ₂ O, O ₂ + a reduced acceptor + squalene = (S)-2.3- epoxysqualene + H ₂ O + an acceptor	426.724
24 ethylidenelophenal	C30H5001	24-methylenelophenol + S-adenosyl- L-methionine = 24-ethylidenelophenol + S-adenosyl-L-homocysteine	426.724
4.A-dimethyl-14a-formyl- 5a-cholesta-8.24-dien-3p-ol	C30H4802	4.4-dimethyl-14a-hydroxymethyl- 5a-cholesta-8.24-dien-38-ol + NADPH + O2 = 4.4-dimethyl-14a-formyl-5a-cholesta- 8.24-dien-38-ol + NADP [±] + 2 H ₂ O	440.708
4,4-dimethyl- 14a-hydroxymethyl- 5a-cholesta-8,24-dien-38-ol-	C30H5002	lanosterol + NADPH + O ₂ = 4.4-dimethyl- 14o-hydroxymethyl-5o-cholesta- 8.24-dien-38-ol + NADP ⁴ + H ₂ O	442.724
4-(1-methyl-2-pymolidiny()-3- oxobutancyl-CoA	C30H49N8018P351	1-methylpyrrolidine-2-acetyl-CoA + acetyl-CoA = 4-(1-methyl-2-pyrrolidinyl)-3- oxobutanoyl-CoA + coenzyme A	934.741
4 coumaroy1-CoA	C30H42N7O18P3S1	coenzyme A + 4-coumarate + ATP = 4-coumaroyI-CoA + diphosphate + AMP	913.679

New search options at the PMN





New database analysis tools at the PMN



Improved Metabolic Map / Omics Viewer





PMN	-spiel	Searching Av	chikipola Mali	Quest 1 ene col shares o	Carlo Search	
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	From File	Highlight Co	mproved(s)		*
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Improved Metabolic Map / Omics Viewer



Data analysis with the Metabolic Map / Omics Viewer

Display experimental data a on metabolic map

- Data types:
 - Genes transcriptomics
 - Enzymes proteomics
 - Reactions fluxomics
 - Compounds metabolomics
- Data inputs:
 - Single or multiple values for each object
 - Absolute or relative values
- Data comparisons
 - Wild type vs. mutant
 - Stressed vs. unstressed
 - Time course after stimulus
 - Ecotype-specific responses
 - Development-driven changes
 - Organ / tissue based analyses
 - . . . and many more

Preparing the input files

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	811077760	1.15	1.2	2.2	2.11	1.53	1.75	
	At.2033340	4.7	-9.57		-9,73	0.08	-0.72	
	At1032214	-1.1	-0.05	1.08	1.18	1.28	9.98	
_	Ortifizetak	-0.45	-0.56	1.13	5.23	0.87	-0.10	
┛╽	At19011520	-1,08	-0.15	-118	-5.15	11.15	-9.58	
	A13001800	0.07	-0.72	-0.68	-1.8	-1.98	-9.21	
	A113402470	0.03	-0.51	0.58	1.30	0.55	1.4	
	At1902470	0.55	-0.12	0.61	0.48	-0.05	1.11	
_	A12002380	0.6	-0.88	0.08	0.18	-2.3	+2.45	
-	A13 (002 590)	1.15	0.7	0.03	-0.6	-2.4	-1.05	
	Art.1g12780	-1.15	0.05	0.1	-0.06	-0.57	-0.28	
	44.3 (04120)	-0.18	+1.35	0.13	+0.3	6.23	3.77	
	ALT004120	-0.15	-1.5	0.01	-0.35	0.28	1.7	
	Art3g04520	-0.07	+0.65	0.1	-0.78	4.2	1.55	
	At3004870	1.05	-1.08	-0.05	-1.1	4.08	+1.33	
	A13904940	-0.65	-0.1	-9.88	-1.3	-1.81	-2.3	
	kt3g07420	-0.48	-0.18	-9.7.	-ht:	÷	-0.1	
	#13g30850	-0.6	-0.78	-0.48	-0.72	-1.00	-1.67	
	A13g13790	-0.2	1.0	3.68	5.78	3.77.	2.05	
	.kt3y12790	1.1	1.75	1.95	5.95	1.05	2.92	
	#17054415	0.25	10.83	-0.85	1.6.1	+1.2	-1.03	
	A4.5g11240	+0.72	-0.6	-1.08	-0.8	1.5	1.47	

Displaying the data

Select a file containing experimental data:	Dowte,
Barris is the first calutes of the file are	Data polymor(a) to use
Gene names and/or identifiers 🛛 🗮 💽	
Data values una a D-centered scale 💌 🚺	Select type of values - Fistative 🛩 💽
Choose a color scheme:	For relative data volvers use:
Full color spectrum from data M	Nis ratio of data columnia 🤟 🚺



Data and software downloads

Install a local copy of the Pathway Tools software

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nt Metabolic Network		10				
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Pathway Tools westen 12.5				1000		C TH
Ple Overview Pathway Reacton Protein Rtv Populus trichocarpa	Game Compound Home	Bac	ome Tools Hele	tatary]	Clone	Sant
		Pop	ulus trick	trichocarpa		
	Cenerale Pat	ining Entaip	nce Report	Generate Pathway	taie Report	
Replicon	Total	Genes	Protein Genes	RNA Genes	Pseudagenes	Size (bg
Chromorome 1		271	271	0	0	
Chromosome 2		237	237	0	0	
Chromosome 3	1	149	149	0	0	
Chromosome 4		114	114	0	0	
Chromosome 5		156	156	0	0	
Chromosome 6		175	175	0		

Pathway Tools – desktop version

- Desktop version offers additional features
 - Create new pathways
 - Modify existing pathways
 - Generate and work with groups of items
 - Perform metabolite tracing on metabolic map
 - See Omics Viewer results on pathway pages
- **Demonstrations available throughout the conference**



On the horizon . . .

- Develop a better enzyme annotation pipeline
- Predict plant metabolic pathways for many species with predicted proteomes
 - First round candidates:

moss	Selaginella moellendorfi
papava	soybean
	maize
tomato	Medicago
Chlamvdomonas	□ poplar
wine grape	cassava

- Solicit help from experts for pathway validation
 - Remove mis-predictions
 - Add missed pathways
- Release new databases at the PMN

Questions, contributions, volunteering to validate?

- □ To submit data, report an error, or ask a question . . .
 - ... stay tuned for the next portion of my talk
 - Send an e-mail: <u>curator@plantcyc.org</u>
 - Use our feedback form:



- Stop by the Plant Genome Resources Outreach Booth (415)
- Visit the PMN poster P02029
- Schedule an individual meeting with me

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!



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www.plantcyc.org





PMN Acknowledgements



Current Tech Team Members:

- Bob Muller (Manager)
- Larry Ploetz (Sys. Administrator)
- Cynthia Lee
- Shanker Singh
- Chris Wilks

Tech Team: alumni

- Raymond Chetty
- Anjo Chi
- Vanessa Kirkup
- Tom Meyer

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



National Science Foundation



Other queries

- Identify all of the "glycosyltransferase" <u>enzymes</u> associated with no more than two reactions in AraCyc
 - List their:
 - name
 - subcellular localization
 - reactions catalyzed
- Find all of the <u>biochemical pathways</u> in PoplarCyc that have more than 5 reactions and where NADPH is used at least once in the pathway
 - List their:
 - name
 - reactions
 - citations and evidence codes

Improved Metabolic Map / Omics Viewer



1. Enter your query here:

.

uery database <u>Republic trichocarpe</u>	for Pathways (323 instances)	🔀 (let's call them 2	1) remove condition
there the number of objects of Reaction-List (323 values)	🥳 is greater than or equal to 😹 5	Switch to	variable entry
and 🦉 for some obj	ed	i) 🛛 🖉 of type: Generalized-Re	actions (lef) call them 22)
we have for some object	👻 in 22 💌 Enzymatic-Reaction (1134 v	slues) 🔟 of type Enzymatic-Reacti	ons (lat's call them 23)
we have for some object	💌 in 23 💌 Plenction (6138 values)	ef type Reaction	s (lefs call them 24)
we have for some object	💌 in 24 🐋 Let	💌 of type: Chemicals 🛛 🖼 (lefs call them 25)
we have 25 💌 Name add a condition 🐱	😿 is equal to	NADPH	Switch to veriable ent
or 💌 for som	ne object	ef type Chemicals	🦉 (lets call them 24)
we have 25 Manue add a condition M	😭 contains the substring	NADPH	Switch to veriable en
add a condition 💥			
add a condition 👱			
edd a condition 😒			
idd a condition 👻			

CHERT CHERT AND CONTRACT CONTRACT OF A CONTRACT

Advanced Query Results

This query resulted in a single table of 29 rows.

NAME A 🗸	Reaction-List 🛆 🔽	Citations 🛆 🗸
arginine biosynthesis II (acetyl cycle)	2 ATP + L-glutamine + bicarbonate + H ₂ O = L-glutamate + 2 ADP + phosphate + carbamoyl-phosphate + 4 H ⁴ , L-glutamate + acetyl-CoA = N-acetyl-L-glutamate + coenzyme A + H ⁴ , L-glutamate + N-acetyl-L-omithine = N-acetyl-L-glutamate + L-omithine, N-acetyl-L-glutamate + ATP = N-acetylglutamyl-phosphate + ADP + H ⁴ , N-acetyl-L-glutamate 5-semialdehyde + NADP ⁴ + phosphate + N-acetylglutamyl-phosphate + NADPH + H ⁴ , N-acetyl-L-omithine + 2-ketoglutarate = N-acetyl-L-glutamate 5-semialdehyde + L-glutamate, L-omithine + carbamoyl-phosphate = citrulline + phosphate + H ⁴ , L-arginino-succinate = L-arginine + fumarate, L-asgartate + citrulline + ATP = L-arginino-succinate + diphosphate + AMP + 2 H ⁴	curator09:EV- COMP-HENF: 3452886714: pelfenz
ascorbate giutathione cycle	L-ascorbate + O_2 + 5 H ⁺ = monodehydroascorbate + 2 H ₂ O, 2 monodehydroascorbate -> L-ascorbate + L-dehydro-ascorbate + 3 H ⁺ , 2 monodehydroascorbate = NADPH = 2 L-ascorbate = NADP ⁺ + 3 H ⁺ , 2 L-ascorbate + H ₂ O ₂ + 4 H ⁺ + 2 monodehydroascorbate + 2 H ₂ O, 2 glutathione + NADP ⁺ = glutathione disulfide + NADPH + H ⁺ , L-dehydro-ascorbate + 2 glutathione = glutathione disulfide + L-ascorbate + H ⁺	17899442:EV- EXP-IDA:3457189877:dreher, EDJOL001:EV- EXP-IDA:3457190309:dreher, SHANZHE04:EV- EXP-IDA:3457190309:dreher, Nakagawara84:EV- EXP-IDA:3457190309:dreher
brassinosteroid biosynthesis i	6-deoxotyphasterol + 0 ₂ = typhasterol + H ₂ 0, 60-hydroxy-castasterone = castasterone + 2 H ⁴ , 6-deoxocastasterone + 0 ₂ + 2 H ⁴ = 60-hydroxy-castasterone + H ₂ 0, 6-deoxotyphasterol + 0 ₂ + 2 H ⁴ = 6-deoxocastasterone + H ₂ 0, 3-dehydro-6-deoxoteasterone + 2 H ⁴ = 6-deoxotyphasterol, 6-deoxoteasterone = 3-dehydro-6-deoxoteasterone + 2 H ⁴ , 6-deoxocathasterone + 0 ₂ + 2 H ⁴ = 6-deoxoteasterone + H ₂ 0, campestanol + NADPH + 0 ₂ + H ⁴ = 6-deoxocathasterone + NADP ⁴ + H ₂ 0, castasterone + NADPH + 0 ₂ + H ⁴ = brassinolide + NADP ⁴ + H ₂ 0, typhasterol + a reduced electron acceptor + 0 ₂ = castasterone + an oxidized electron acceptor + H ₂ 0, 3-dehydroteasterone + 2 H ⁴ + typhasterol, teasterone = 3-dehydroteasterone + 2 H ⁴ , cathasterone + a reduced electron acceptor + 0 ₂ = teasterone = 3-dehydroteasterone + 2 H ⁴ , cathasterone + a reduced electron acceptor + 0 ₂ = teasterone = 3-dehydroteasterone + H ₂ 0, 6-oxocampestanol + NADPH = 0 ₂ + H ⁴ = cathasterone + NADP ⁴ + H ₂ 0, (60)-hydroxycampestanol = 6-oxocampestanol + 2 H ⁴ , campestanol + a reduced electron acceptor + 0 ₂ = (60)-hydroxycampestanol + an oxidized electron acceptor + H ₂ 0, (50)-campestan-3-one + 2 H ⁴ = campestanol, campest-4-en-3-one +	curator09:EV- COMP-HINF:3444506243:adhl1

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Plant Metabolic Network goals

- Capture and organize published data
- Facilitate data analysis
- Make proteome-based metabolic pathway predictions for many plant species

PMN BLAST 2.2.8



Ontology-based search options



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!





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- Peifen Zhang (Director)
- Christophe Tissier
- Hartmut Foerster

Collaborators:

Sue Rhee

(PI)

- Peter Karp (SRI)
- Ron Caspi (SRI)
- Suzanne Paley (SRI)
- SRI Tech Team
- Lukas Mueller (SGN)
- Anuradha Pujar (SGN / SRI)
- Gramene, MedicCyc, ChlamyCyc

vledgements

National Science Foundation

CARNEGIE

Science

Current Tech Team Contributors:

ager)

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GIN

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- Damian Priamurskiy

- Caryn Johansen

- Purva Karia

Plant metabolic NETWORKING

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Booth 415: Plant Resources Outreach Tuesday, 10:10 – 10:25 AM Wednesday, 1:00 – 1:30 PM

Poster **P02029** : Monday: 5:30 – 7:30 PM