

Accessing information in plant metabolic pathway databases at the PMN, Gramene, and SGN



Part I: Contents, Search Strategies, and Data Sharing Opportunities

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Part II: Pathway Networks for Cereals

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Part III: Using the desktop version of the Pathway Tools software

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Part I overview

- **Introduction**
- **Data**
- **Search tools**
- **Data submissions**
- **Acknowledgments**
- **More examples**

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 databases

- Capture and organize published data
- Make metabolic predictions for “new” species
- Facilitate data analysis
- Focus on different aspects of metabolism
 - Pathways
 - KEGG
 - Reactome
 - **BioCyc / Pathway tools family**

BioCyc / Pathway Tools databases

- Multiple data providers:
 - SRI International
 - Plant Metabolic Network (PMN)
 - Gramene
 - Sol Genomics Network (SGN)
- One software package:
 - Pathway Tools
 - SRI International
 - Common set of data types
 - Common tools
 - Common display modes



Pathway tools pathways

PlantCyc Pathway: choline biosynthesis III

Enzyme View: All Organisms

Customize Diagram

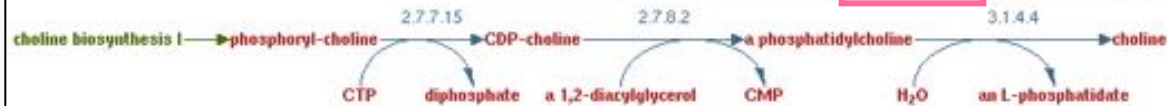
More Detail

Less Detail

Cross-Species Comparison

Download Genes

BioPAX format



PlantCyc

PlantCyc Enzyme: phosphatidyltransferase

Synonyms: aminoalcoholphosphotransferase

Species: [Arabidopsis thaliana](#) col

Gene: [AT3G25585](#)

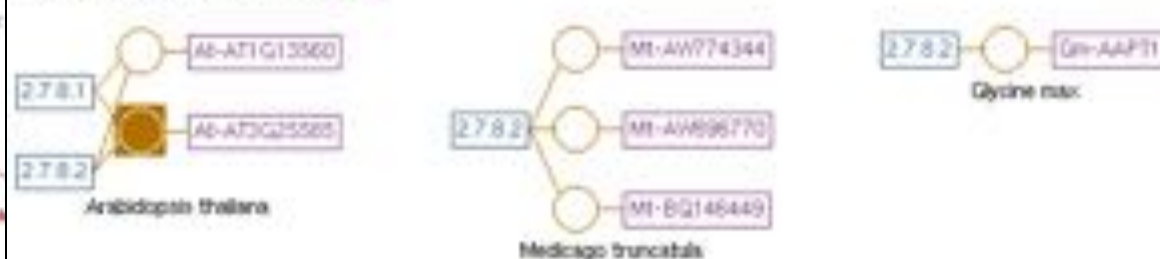
Sequence Length: 1145 AAs

Unification Links: [Entrez AAC61769](#), [Phytozome Plant Orthologs AT3G25585.1](#)

Gene-Reaction Schematic: ?



Upstream pathway



MultiFun Terms: [UNCLASSIFIED](#)

Enzymatic reaction of: cholinephosphotransferase (phosphatidyltransferase)

[1,2-diacylglycerol](#) + CDP-choline \rightleftharpoons [phosphatidylcholine](#) + 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](#), [phosphatidylcholine biosynthesis I](#), [phosphatidylcholine biosynthesis II](#)

Summary:

The enzyme is bifunctional that utilizes CDP-choline and CDP-ethanolamine in synthesizing phosphatidylcholine and phosphatidylethanolamine, respectively. Its cholinephosphotransferase activity is greater than its ethanolaminephosphotransferase activity.

Inhibitors (Unimech): [CMP](#) [[Gorde99](#)], [Ca²⁺](#) [[Gorde99](#)]

[Download Genes](#) [BioPAX format](#)



Evidence Codes

thway

Compound

Plant metabolic databases

PGDB	Plant	Source
AraCyc	Arabidopsis	Plant Metabolic Network
PoplarCyc	Poplar	Plant Metabolic Network
PlantCyc	PLANT KINGDOM	Plant Metabolic Network
RiceCyc	Rice	Gramene
SorghumCyc	Sorghum	Gramene
<i>MaizeCyc (beta)</i>	Sorghum	Gramene
<i>BrachyCyc (beta)</i>	<i>Brachypodium</i>	Gramene
LycCyc	Tomato	Sol Genomics Network
PotatoCyc	Potato	Sol Genomics Network
CapCyc	Pepper	Sol Genomics Network
NicotianaCyc	Tobacco	Sol Genomics Network
PetuniaCyc	Petunia	Sol Genomics Network
CoffeaCyc	Coffee	Sol Genomics Network
MedicCyc	Medicago	Noble Foundation

Data curation in databases

PGDB	Plant	Source	Status
AraCyc	Arabidopsis	Plant Metabolic Network	<u>extensive curation</u>
PoplarCyc	Poplar	Plant Metabolic Network	some curation
PlantCyc	PLANT KINGDOM	Plant Metabolic Network	mixed curation
RiceCyc **	Rice	Gramene	some curation
SorghumCyc	Sorghum	Gramene	all computational
MaizeCyc (beta)	Sorghum	Gramene	all computational
BrachyCyc (beta)	Brachypodium	Gramene	all computational
LycoCyc **	Tomato	Sol Genomics Network	some curation
PotatoCyc	Potato	Sol Genomics Network	all computational
CapCyc	Pepper	Sol Genomics Network	all computational
NicotianaCyc	Tobacco	Sol Genomics Network	all computational
PetuniaCyc	Petunia	Sol Genomics Network	all computational
CoffeaCyc	Coffee	Sol Genomics Network	all computational
MedicCyc **	Medicago	Noble Foundation	some curation

Database content statistics

□ Plant Metabolic Network

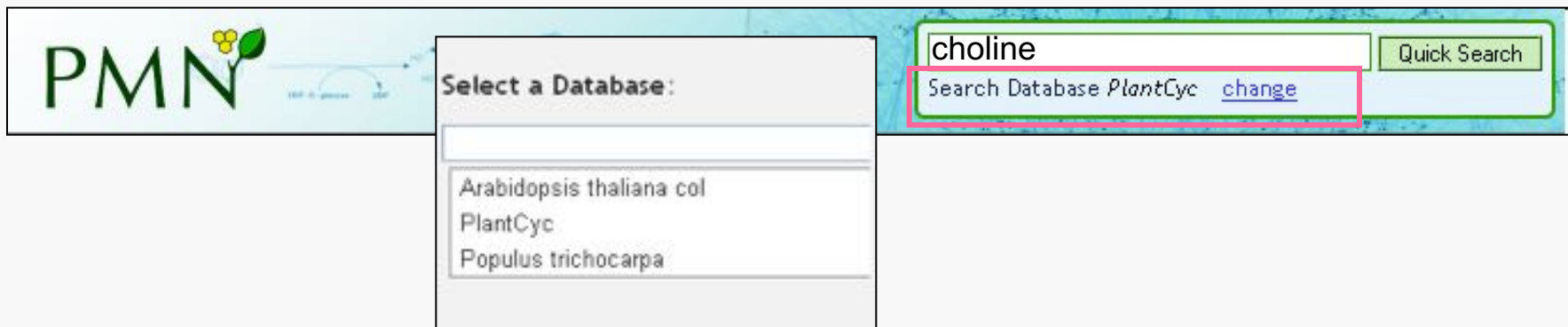
	PlantCyc 4.0	AraCyc 7.0	PoplarCyc 2.0
Pathways	685	369	288
Enzymes	11058	5506	3420
Reactions	2929	2418	1707
Compounds	2966	2719	1397
Organisms	343	1	1*

□ Gramene / SGN

	RiceCyc 3.0	LycoCyc 2.0	PetuniaCyc 2.1
Pathways	339	343	136
Enzymes	9315	5216	294
Reactions	2109	1793	758
Compounds	1592	1379	637
Organisms	1	1	1

Searching in plant metabolic databases

- Pathway Tools quick search bar



The screenshot shows the PMN Pathway Tools quick search bar. On the left is the PMN logo with a small plant icon and a metabolic pathway diagram. To its right is a 'Select a Database:' dropdown menu with a list of options: 'Arabidopsis thaliana col', 'PlantCyc', and 'Populus trichocarpa'. Further right is a search input field containing the text 'choline'. Below this field is a red-bordered box containing the text 'Search Database *PlantCyc* [change](#)'. To the right of the input field is a green 'Quick Search' button.

Quick search results

The query `choline` matched the following

Pathways

Pathway pages contain pathway, of chromo
genes, and of regu

- [choline biosynthesis I](#)
- [choline biosynthesis II](#)
- [choline biosynthesis III](#)
- [phosphatidylcholine biosynthesis I](#)
- [phosphatidylcholine biosynthesis II](#)
- [phosphatidylcholine biosynthesis III](#)
- [phosphatidylcholine biosynthesis IV](#)
- [supernatural pathway of phosphatidylcholine biosynthesis](#)
- [supernatural pathway of choline 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 \(pob\)](#)
- [choline kinase \(pob\)](#)
- [choline kinase \(pob\)](#)
- [choline kinase \(pob\)](#)
- [choline kinase \(pob\)](#)
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- [choline kinase \(pob\)](#)
- [choline kinase \(pob\)](#)
- [choline kinase \(pob\)](#)
- [CHOLINE MONOOXY](#)
- [choline monooxygenase](#)
- [choline monooxygenase](#)
- [choline monooxygenase](#)
- [expressed](#)
- [choline-phosphate](#)
- [AT2G32260](#)
- [choline-phosphate](#)
- [AT4G15130](#)
- [choline-phosphate](#)
- [LOC_Os02g07720.1](#)
- [cholinephosphate](#)

Compounds

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




- 16:0-18:1-PC (1-16)
- 16:0-18:2-PC (1-16)
- 16:0-18:3-PC (1-16)
- 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
- G-snagoylcholine
- Sn-3-glycerophosp
- a-1-acyl-2-lyso-gly
- a-1-alkyl-2-acetyl-s
- a-1-alkyl-sn-glycen
- a-1-lyso-2-acyl-sn-
- a-1-orynyl-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.

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

Specific search pages



Search Database *PlantCyc* [change](#)

About PMN

Search

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Databases Overview

Compounds

PlantCyc Compound Search

▼ Search for compound by name or ID

Enter a compound name, or a database identifier from this database or from an external database such as ChEBI, LIGAND, PubChem or CkS. This database may not contain mappings to all of these other databases. Partial names will generate a substring search on compound names only (not on database identifiers).
Examples: "tryptophan", "C00034"



▶ Search/Filter by ontology (inactive)

▶ Search/Filter by molecular weight (inactive)

▶ Search/Filter by chemical formula (partial or full) (inactive)

▶ Search by InChI string (inactive)

Specific search pages



Quick Search

PlantCyc Gene/Protein/RNA Search

▼ Search by gene name or database identifier

GENE

Enter a gene name, or a database identifier from this database or from an external database. The search results database contains links. Partial names will generate a substring search on gene names only (not on database identifiers).
Examples: "trpA", "trp", "b1234"

▼ Search by protein name, EC number, or database identifier

PROTEIN

Enter a protein name, or a database identifier from this database or from an external database. The search results database contains links. Partial names will generate a substring search on protein or RNA.

cytokinin oxidase - Zm mays		
cytokinin oxidase - Zm mays		
cytokinin oxidase - Zm mays		
cytokinin oxidase - Zm mays		
cytokinin oxidase - Zm mays	eight	(inactive)
cytokinin oxidase - Zm mays		(inactive)
cytokinin oxidase - Zm mays		(inactive)
cytokinin oxidase - Oryza sativa	ator, cofactor, substrate or ligand	(inactive)
Search/Filter by evidence code		(inactive)
Search/Filter by cell component		(inactive)
Search/Filter by organism		(inactive)
Search/Filter by publication		(inactive)

Specific search pages

DMANN

Quick Search

PlantCyc Gene/Protein/RNA Search

Submit Query Clear Form List of All Genes List of All Polypeptides List of All Protein Complexes List of All RNAs

Search by gene name or database identifier

Enter a gene name or database identifier. Examples: "trpA"

Search by product name

Enter a protein name or database identifier. Examples: "tryptophan synthase", "Phe"

Search/Filter by product name
Search/Filter by product name
Search/Filter by product name
Search/Filter by product name
Search/Filter by product name
Search/Filter by product name
Search/Filter by product name
Search/Filter by product name
Search/Filter by product name
Search/Filter by product name

PlantCyc Query Results

You searched for all gene products whose name contains the string "cytokinin oxidase", and that

Your query returned 2 results.

Gene Name ▲ ▼	Product Name ▲ ▼	Organism ▲ ▼	Evidence ▲ ▼
CKX1	cytokinin oxidase	Arabidopsis thaliana	Reaction enhanced in mutant
CKX1	cytokinin oxidase	Zea mays	Assay of 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.

Submit Query Clear Form List of All Genes List of All Proteins List of All RNAs



PlantCyc Pathway: ethylene biosynthesis from methionine

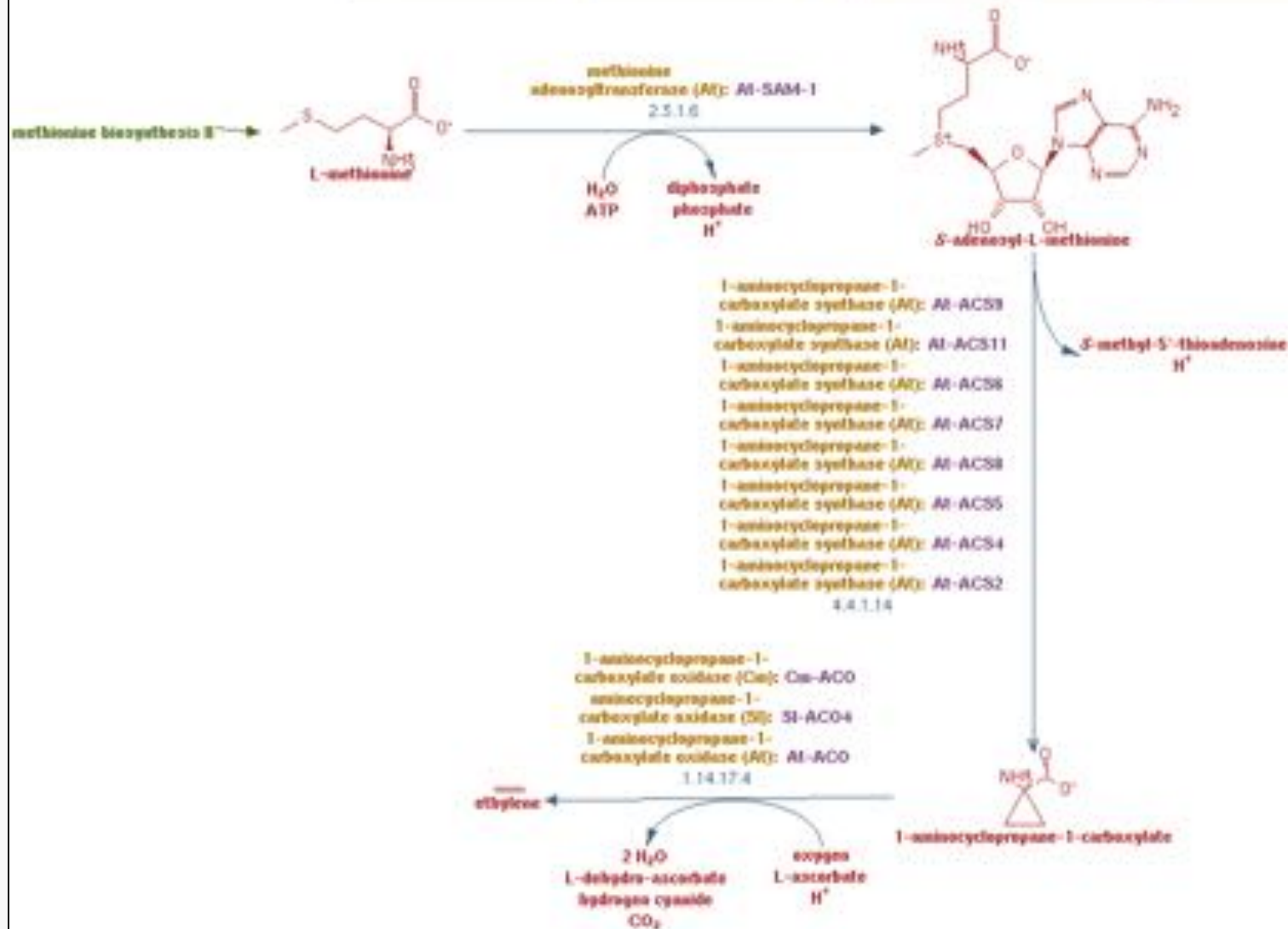
Enzyme View: All Organisms

Hide Predicted Enzymes

More Detail

Less Detail

Species Comparison



Searching by topic / keyword



Quick Search

About PMNSearchTools

Arabidopsis thaliana col superoxide radicals degradation
Jan 6, 2011... oxygen species (ROS) that are formed through metabolic processes and

Arabidopsis thaliana col Enzyme: abscisic acid glucose ester 8-glucosidase

Gene: BG1 Accession Number: AT1G52400 [AraCyc]

Synonyms: ABA-GE 8-glucosidase

Summary:

The BG1 glucosidase appears to play an important role in releasing free biologically active [\(+\)-abscisate](#) (ABA) from the inactive [abscisic acid glucose ester](#) (ABA-GE), particularly in response to dehydration stress. Consequently, mutant plants lacking BG1 have decreased levels of free [ABA](#) compared to wild type plants following a dehydration stress treatment. In addition, extracellular levels of ABA appear to be reduced in plants that lack BG1 [[Lee05b](#)].

Transcripts for this enzyme are up-regulated by conditions normally associated with increased ABA production, including NaCl and drought stress [[Lee05b](#)]. And, mutant plants lacking BG1 lose more water through transpiration, have defective stomatal closure in the dark, and are less tolerant of dehydration than comparable wild type plants [[Lee05b](#)].

Further analyses of the BG1 protein *in vitro* indicate that it does not act on zeatin glucose ester and that the glutamic acid at position 207 is important for its enzymatic activity toward [ABA-GE](#) [[Lee05b](#)]. In addition, BG1 homooligomerization, which happens in response to dehydration stress, appears to increase the enzymatic activity of the enzyme, and low molecular weight forms have a ~4-fold lower specific activity than high molecular weight forms. Based on the apparent molecular weight of 600 kDa of the major BG1 complex detected in dehydration-stressed plants, BG1 likely forms a homooligomer of 10 units [[Lee05b](#)].

The enzyme was originally shown to be glycosylated and targeted to the endoplasmic reticulum [[Lee05b](#)]. Later work indicated that the protein goes to a new organelle named the [ER body](#) [[Yamada09](#)]. Interestingly, [ABA-GE](#) is believed to accumulate in plant vacuoles and outside of the cell walls raising the question of how BG1 encounters the substrate within the cell [[Dietz00](#), [Lee05b](#)]. Currently, it is hypothesized that [ABA-GE](#) transporters may promote the release of this compound to the ER upon dehydration stress [[Lee05b](#)].

Citations: [[Katonoguch08](#)]


Locations: endoplasmic reticulum [[Lee05b](#)]

Map Position: [19,518,820 -> 19,521,880] (64.14 centisomes) on CHROMOSOME 1

Unification Links: [Phytozome Plant Orthologs:AT1G52400.1](#), [TAIR:AT1G52400](#), [UniProt:Q95E50](#)

Advanced searching in PMN databases

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



1. Enter your query here:

In database search for

2. Select fields to include in the query output:

Column 1
☒ Sort based on this column

3. Select query output format:

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

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 PlantCyc search for Compounds (2679 instances) add a condition

Where add a condition

and
or
or not
and not

Chemical-Formula

contains the substring

C30

is a substring of
does not contain the substring
is not a substring of
is equal to
is not equal to
is similar to (regular expression)
is not similar to (regular expression)
contains the substring (case-sensitive)
is a substring of (case-sensitive)
does not contain the substring (case-sensitive)
is not a substring of (case-sensitive)
is equal to (case-sensitive)
is not equal to (case-sensitive)

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 in Left-Side-Of
- Appears in Right-Side-Of
- Atomic-Weights
- Charge
- Chemical-Formula
- Citations
- Collection-Of
- Collectors-On-Prothelial-Groups-Of
- Comment
- Common-Name
- Component-Of
- Credits
- Data-Source
- EPIC-40
- Gibbs-6

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

and is greater than

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:

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

Column 1 <input checked="" type="radio"/> Sort based on this column NAME	Column 2 <input checked="" type="checkbox"/> <input type="radio"/> Sort based on this column Chemical-Formula	Column 3 <input checked="" type="checkbox"/> <input type="radio"/> Sort based on this column Appears-In-Right-Side-Of	Column 4 <input checked="" type="checkbox"/> <input type="radio"/> Sort based on this column Molecular-Weight	Column 5 <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)
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 + H₂O	897.68	(E)-cinnamoyl-CoA
(S)-2,3-epoxysqualene	C30H50O1	squalene + NADPH + O₂ = (S)-2,3-epoxysqualene + NADP⁺ + H₂O, O₂ + a reduced acceptor + squalene = (S)-2,3-epoxysqualene + H₂O + 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-ethylidenelophanol	C30H50O1	24-methylenelophanol + S-adenosyl-L-methionine = 24-ethylidenelophanol + S-adenosyl-L-homocysteine	426.724	24-ethylidenelophanol, (Z)-24-ethylidenelophanol, 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 + O₂ = 4,4-dimethyl-14α-formyl-5α-cholesta-8,24-dien-3β-ol + NADP⁺ + 2 H₂O	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 + O₂ = 4,4-dimethyl-14α-hydroxymethyl-5α-cholesta-8,24-dien-3β-ol + NADP⁺ + H₂O	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	913.629	4-coumaroyl-CoA, p-coumaroyl-CoA, 4-coumaroyl-CoA, coumaroyl-CoA, p-coumaroyl-CoA

Data and software downloads

- Install a local copy of the Pathway Tools software



Building better databases together

- To submit data, report an error, or ask a question . . .
 - Send an e-mail: curator@plantcyc.org
 - Use data submission “tools”



- **Meet with me individually at this conference**
 - **Plant Genome Database Outreach Consortium booth: # 427**
 - **Poster: C891**

Building better databases together

□ PMN future plans

- Develop a better enzyme annotation pipeline
- Predict plant metabolic pathways for many species with sequence data
- Solicit help from experts who work on different species for pathway validation
 - Remove mis-predictions
 - Add missed pathways

■ Potential candidates:

- wine grape
- cassava
- *Selaginella moellendorffii*
- moss
- eucalyptus
- sunflower
- apple
- cowpea
- ice plant
- papaya
- **YOUR FAVORITE SPECIES??**

Community gratitude

□ We



The screenshot shows the PMN website interface. The top navigation bar includes links for About PMN, Search, Tools, Downloads, Useful Sites, Submit Data, Help, and Feedback. The left sidebar contains a list of links: Project Overview, Documentation, Presentations, Statistics, Release Notes, Contact Info, News, PMN Staff, Collaborators, Contributors (highlighted with a red box), and Editorial Board. The main content area features a section titled 'Item of the Month' with a sub-header 'Recent Community Contributors'. The text in this section expresses gratitude to scientists who submit data and answer questions, listing contributors from the past few months. A list of contributors is provided, including Rob Ingle, Axel Tiessen, Stephen Tobe, Jacqueline Bede, Julian Hibbard, Alisdair R. Fernie, Carlos S. Andreo, Geoffrey Fucile, Alain Rahier, and Shannon M. Bell. Below this list, a message states: 'We hope that our complete list keeps growing with your help and expertise!'. At the bottom of the page, a list of contributors is shown, including Inad Ajawi, Jose Alonso, Richard Amasino, and Ian Baldwin.

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Project Overview
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Item of the Month

Recent Community Contributors

We are grateful to the scientists who submit their data directly to us and to those who answer the questions we send them, including the following contributors from the past few months:

- Rob Ingle
- Axel Tiessen
- Stephen Tobe
- Jacqueline Bede
- Julian Hibbard
- Alisdair R. Fernie
- Carlos S. Andreo
- Geoffrey Fucile
- Alain Rahier
- Shannon M. Bell

We hope that our complete list keeps growing with your help and expertise!

• Inad Ajawi - Michigan State University, USA
• Jose Alonso - North Carolina State University, USA
• Richard Amasino - University of Wisconsin, USA
• Ian Baldwin - Max Planck Institute for Chemical Ecology, Germany

Building better databases together



sol genomics network

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genomes

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Contact SGN

All fields are required.

Your name

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Subject

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sgn-feedback@solgenomics.net

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



**Sue Rhee
(PI)**

**Peifen Zhang
(Director)**

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
WHERE DISCOVERIES BEGIN

CARNEGIE
INSTITUTION FOR
SCIENCE

Advanced searching in PMN databases

□ Other queries

- Identify all of the “glycosyltransferase” enzymes associated with no more than two reactions in AraCyc
 - List their:
 - name
 - subcellular localization
 - reactions catalyzed
- Find all of the biochemical pathways 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

1. Enter your query here:

Query database <i>Regula, trichocarpa</i> for Pathways (323 instances)		<input type="button" value="let's call them Z1"/>	<input type="button" value="remove condition"/>
where the number of objects of <input type="button" value="Reaction-List (323 values)"/> is greater than or equal to <input type="text" value="5"/> <input type="button" value="Switch to variable entry"/>			
and <input type="button" value="for some object ..."/> in <input type="button" value="Reaction-List (323 values)"/> of type <input type="button" value="Generalized-Reactions (let's call them Z2)"/>			
we have for some object ... in <input type="button" value="Z2"/> <input type="button" value="Enzymatic-Reaction (1134 values)"/> of type <input type="button" value="Enzymatic-Reactions (let's call them Z3)"/>			
we have for some object ... in <input type="button" value="Z3"/> <input type="button" value="Reaction (6138 values)"/> of type <input type="button" value="Reactions (let's call them Z4)"/>			
we have for some object ... in <input type="button" value="Z4"/> <input type="button" value="Left"/> of type <input type="button" value="Chemicals"/> (let's call them Z5)			
we have <input type="button" value="Z5"/> <input type="button" value="Name"/> is equal to <input type="text" value="NADPH"/> <input type="button" value="Switch to variable entry"/>			
<input type="button" value="add a condition"/>			
or <input type="button" value="for some object ..."/> in <input type="button" value="Z4"/> <input type="button" value="Right"/> of type <input type="button" value="Chemicals"/> (let's call them Z6)			
we have <input type="button" value="Z6"/> <input type="button" value="Name"/> contains the substring <input type="text" value="NADPH"/> <input type="button" value="Switch to variable entry"/>			
<input type="button" value="add a condition"/>			
<input type="button" value="add a condition"/>			
<input type="button" value="add a condition"/>			
<input type="button" value="add a condition"/>			

Advanced Query Results

Your query in BioVelo is `html-sort-ascending([(Z1^NAME, Z1^REACTION-LIST, Z1^CITATIONS) : Z1<POPULAR^Pathways, 12 := [Z2 : Z2 <- Z1^REACTION-LIST, (0 < #[Z3 : Z3 <- Z2^ENZYMATIC-REACTION, (0 < #[Z4 : Z4 <- Z3^REACTION, ((0 < #[Z5 : Z5 <- Z4^LEFT, ("NADPH" inststringc1 Z5^NAME))) : (0 < #[Z6 : Z6 <- Z4^RIGHT, ("NADPH" inststringc1 Z6^NAME))])])]), ((#Z1^REACTION-LIST) >= 5) & (0 < #12)],1)` (click the query to edit it in the Free Form Advanced Query Page)

This query resulted in a single table of 29 rows.

NAME ▲ ▼	Reaction-List ▲ ▼	Citations ▲ ▼
arginine biosynthesis ii (acetyl cycle)	$2 \text{ ATP} + \text{L-glutamine} + \text{bicarbonate} + \text{H}_2\text{O} = \text{L-glutamate} + 2 \text{ ADP} + \text{phosphate} + \text{carbamoyl-phosphate} + 4 \text{ H}^+$, $\text{L-glutamate} + \text{acetyl-CoA} = \text{N-acetyl-L-glutamate} + \text{coenzyme A} + \text{H}^+$, $\text{L-glutamate} + \text{N-acetyl-L-ornithine} =$ $\text{N-acetyl-L-glutamate} + \text{L-ornithine}$, $\text{N-acetyl-L-glutamate} + \text{ATP} = \text{N-acetylglutamyl-phosphate} + \text{ADP} + \text{H}^+$, $\text{N-acetyl-L-glutamate 5-semialdehyde} + \text{NADP}^+ + \text{phosphate} = \text{N-acetylglutamyl-phosphate} + \text{NADPH} + \text{H}^+$, $\text{N-acetyl-L-ornithine} + 2\text{-ketoglutarate} = \text{N-acetyl-L-glutamate 5-semialdehyde} + \text{L-glutamate}$, $\text{L-ornithine} +$ $\text{carbamoyl-phosphate} = \text{citrulline} + \text{phosphate} + \text{H}^+$, $\text{L-arginino-succinate} = \text{L-arginine} + \text{fumarate}$, $\text{L-aspartate} + \text{citrulline} + \text{ATP} = \text{L-arginino-succinate} + \text{diphosphate} + \text{AMP} + 2 \text{ H}^+$	curator09:EV- COWP-HMF:3452886714;pellenz
ascorbate glutathione cycle	$\text{L-ascorbate} + \text{O}_2 + 5 \text{ H}^+ = \text{monodehydroascorbate} + 2 \text{ H}_2\text{O}$, $2 \text{ monodehydroascorbate} \rightarrow \text{L-ascorbate} +$ $\text{L-dehydro-ascorbate} + 3 \text{ H}^+$, $2 \text{ monodehydroascorbate} + \text{NADPH} = 2 \text{ L-ascorbate} + \text{NADP}^+ + 3 \text{ H}^+$, 2 $\text{L-ascorbate} + \text{H}_2\text{O}_2 + 4 \text{ H}^+ = 2 \text{ monodehydroascorbate} + 2 \text{ H}_2\text{O}$, $2 \text{ glutathione} + \text{NADP}^+ = \text{glutathione disulfide}$ $+ \text{NADPH} + \text{H}^+$, $\text{L-dehydro-ascorbate} + 2 \text{ glutathione} = \text{glutathione disulfide} + \text{L-ascorbate} + \text{H}^+$	17899442:EV- EXP-IDA:3457189877:dreher, EDJOL001:EV- EXP-IDA:3457190309:dreher, SHANZH004:EV- EXP-IDA:3457190309:dreher, Nakagawara84:EV- EXP-IDA:3457190309:dreher
brassinosteroid biosynthesis i	$6\text{-deoxotyphasterol} + \text{O}_2 = \text{typhasterol} + \text{H}_2\text{O}$, $6\alpha\text{-hydroxy-castasterone} = \text{castasterone} + 2 \text{ H}^+$, $6\text{-deoxocastasterone} + \text{O}_2 + 2 \text{ H}^+ = 6\alpha\text{-hydroxy-castasterone} + \text{H}_2\text{O}$, $6\text{-deoxotyphasterol} + \text{O}_2 + 2 \text{ H}^+ =$ $6\text{-deoxocastasterone} + \text{H}_2\text{O}$, $3\text{-dehydro-6-deoxoteasterone} + 2 \text{ H}^+ = 6\text{-deoxotyphasterol}$, $6\text{-deoxoteasterone} =$ $3\text{-dehydro-6-deoxoteasterone} + 2 \text{ H}^+$, $6\text{-deoxocathasterone} + \text{O}_2 + 2 \text{ H}^+ = 6\text{-deoxoteasterone} + \text{H}_2\text{O}$, $\text{campestanol} + \text{NADPH} + \text{O}_2 + \text{H}^+ = 6\text{-deoxocathasterone} + \text{NADP}^+ + \text{H}_2\text{O}$, $\text{castasterone} + \text{NADPH} + \text{O}_2 + \text{H}^+ =$ $\text{brassinolide} + \text{NADP}^+ + \text{H}_2\text{O}$, $\text{typhasterol} + \text{a reduced electron acceptor} + \text{O}_2 = \text{castasterone} + \text{an oxidized}$ $\text{electron acceptor} + \text{H}_2\text{O}$, $3\text{-dehydroteasterone} + 2 \text{ H}^+ = \text{typhasterol}$, $\text{teasterone} = 3\text{-dehydroteasterone} + 2$ H^+ , $\text{cathasterone} + \text{a reduced electron acceptor} + \text{O}_2 = \text{teasterone} + \text{an oxidized electron acceptor} + \text{H}_2\text{O}$, $6\text{-oxocampestanol} + \text{NADPH} + \text{O}_2 + \text{H}^+ = \text{cathasterone} + \text{NADP}^+ + \text{H}_2\text{O}$, $[(6\alpha)\text{-hydroxycampestanol}] =$ $6\text{-oxocampestanol} + 2 \text{ H}^+$, $\text{campestanol} + \text{a reduced electron acceptor} + \text{O}_2 = [(6\alpha)\text{-hydroxycampestanol}] + \text{an}$ $\text{oxidized electron acceptor} + \text{H}_2\text{O}$, $[(5\alpha)\text{-campestan-3-one}] + 2 \text{ H}^+ = \text{campestanol}$, $\text{campest-4-en-3-one} +$	curator09:EV- COWP-HMF:3444506243:achi1