

Support for Phenotype Microarray Data in Pathway Tools

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PM display on All Growth Media Page

Plate ID: Biolog PM1 - Carbon Sources

No growth/respiration	Low growth/respiration	Growth/respiration	Inconsistent results	No data
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Conditions: wildtype at 37 °C (aerobic); 5 Datasets; Growth: 68; Low Growth: 2; No Growth: 20; Inconsistent results: 5.

A1 carbon negative control 	A2 L-Arabinose 	A3 N-Acetyl-D-Glucosamine 	A4 D-Saccharic acid 	A5 Succinic acid 	A6 D-Galactose 	A7 L-Aspartic acid 	A8 L-Proline 	A9 D-Alanine 	A10 D-Trehalose 	A11 D-Mannose 	A12 Dulcitol
B1 D-Serine 	B2 D-Sorbitol 	B3 Glycerol 	B4 L-Fucose 	B5 D-Glucuronic acid 	B6 D-Gluconic acid 	B7 DL-α-Glycerol Phosphate 	B8 D-Xylose 	B9 L-Lactic acid 	B10 Formic acid 	B11 D-Mannitol 	B12 L-Glutamic acid
C1 D-Glucose- 6- Phosphate 	C2 D-Galactonic acid- γ-Lactone 	C3 DL-Malic acid 	C4 D-Ribose 	C5 Tween 20 	C6 L-Rhamnose 	C7 D-Fructose 	C8 Acetic acid 	C9 α-D- Glucose 	C10 Maltose 	C11 D-Melibiose 	C12 Thymidine
D1 L-Asparagine 	D2 D-Aspartic acid 	D3 D-Glucosaminic acid 	D4 1,2-Propanediol 	D5 Tween 40 	D6 α-Ketoglutaric acid 	D7 α-Ketobutyric acid 	D8 α-Methyl-D- Galactoside 	D9 α-D- Lactose 	D10 Lactulose 	D11 Sucrose 	D12 Uridine
E1 L-Glutamine 	E2 M-Tartaric acid 	E3 D-Glucose- 1- Phosphate 	E4 D-Fructose- 6- Phosphate 	E5 Tween 80 	E6 α-Hydroxyglutaric acid-γ-Lactone 	E7 α- Hydroxybutyric acid 	E8 β-Methyl-D- Glucoside 	E9 Adonitol 	E10 Maltotriose 	E11 2- Deoxyadenosine 	E12 Adenosine
F1 Gly-Asp 	F2 Citric acid 	F3 M-Inositol 	F4 D-Threonine 	F5 Fumaric acid 	F6 Bromosuccinic acid 	F7 Propionic acid 	F8 Mucic acid 	F9 Glycolic acid 	F10 Glyoxylic acid 	F11 D-Cellobiose 	F12 Inosine
G1 Gly-Glu 	G2 Tricarballic acid 	G3 L-Serine 	G4 L-Threonine 	G5 L-Alanine 	G6 Ala-Gly 	G7 Acetoacetic acid 	G8 N-Acetyl-D- Mannosamine 	G9 Mono- Methylsuccinate 	G10 Methylpyruvate 	G11 D-Malic acid 	G12 L-Malic acid
H1 Gly-Pro 	H2 p-Hydroxyphenyl Acetic acid 	H3 m-Hydroxyphenyl Acetic acid 	H4 Tyramine 	H5 D-Psicose 	H6 L-Lyxose 	H7 Glucuronamide 	H8 Pyruvic acid 	H9 L-Galactonic acid- γ-Lactone 	H10 D-Galacturonic acid 	H11 Phenylethylamine 	H12 2- Aminoethanol

PM Growth Medium Representation

- **Plate ID, Well ID**
- **Constituents**
 - Concentration
 - Role: source of C, N, P or S
- **Base medium**
- **Name**
- **Abbreviated name (just the added compound for PM media)**
- **Citation, comment**
- **pH**
- **Osmolarity (computed from constituent concentrations)**

Growth Observation Representation

- **Growth media**
- **Growth status: growth, no-growth, or low-growth**
 - No support for capturing quantitative data
- **Citation, comment**
- **Experimental variables**
 - Aerobic/anaerobic
 - Temperature
 - Wildtype or knocked out genes

Conflicts

- **Conflicts occur when multiple observations for the same medium and conditions record different growth statuses**
 - We cannot detect conflicts when experiments use slightly different but equivalent media.
- **Conflict can be resolved by a curator**
 - This creates a new, privileged growth observation frame
 - Curator should record rationale with comment or citation
 - GUI will still show all primary observations

Growth Medium Display

 [Add to group](#)

[Escherichia coli K-12 substr. MG1655](#) Growth Medium: PMA carbon source test + pro


[See All Growth Media](#)


Superclasses: [Phenotype-Microarray-Media](#)

Plate Id: Biolog PM1 - Carbon Sources

Well Id: A8

Citations: [\[Bochner01\]](#)

Recipe Substances: 

Composition: 

Substances	Concentration	Role	Constituents	Concentration
ammonium chloride	5.0 mM	Source of N	chloride	136.10 mM
disodium phosphate	2.0 mM	Source of P	Na⁺	104.50 mM
ferric chloride	1.0 μM		triethanolamine	30.00 mM
L-proline		Source of C	ammonium	5.00 mM
MgCl₂	50.0 μM		phosphate	2.00 mM
potassium chloride	1.0 mM		K⁺	1.00 mM
sodium chloride	100.0 mM		sulfate	250.00 μM
sodium sulfate	250.00002 μM	Source of S	Mg²⁺	50.00 μM
triethanolamine HCl	30.0 mM		Fe³⁺	1.00 μM
			L-proline	[unknown]

Wildtype growth observations:

T (°C)	O ₂	Growth Observations	Consensus	Comment/Citations
37	Aerobic	Yes [Baumler11] No [AbuOun09] No [Bochner12] Yes [Mackie12] Low [Yoon12]	Yes*	[Frank64]
37	Anaerobic	Yes [Baumler11] No [Bochner12]	Indeterminate	Inconsistent Observations

*A curator has resolved the inconsistency.

References

[AbuOun09](#): AbuOun M, Suthers PF, Jones GI, Carter BR, Saunders MP, Maranas CD, Woodward MJ, Anjum MF (2009). "Genome scale reconstruction of a Salmonella metabolic model: comparison of similarity and differences with a commensal Escherichia coli strain." *J Biol Chem* 284(43):29480-8. PMID: 19690172

[Baumler11](#): Baumler DJ, Peplinski RG, Reed JL, Glasner JD, Perna NT (2011). "The evolution of metabolic networks of E. coli." *BMC Syst Biol* 5:182. PMID: 22044664

[Bochner01](#): Bochner BR, Gadzinski P, Panomitros E (2001). "Phenotype microarrays for high-throughput phenotypic testing and assay of gene function."

PM Data in EcoCyc

- 5 Aerobic Datasets (4 for plates 2-4)

	Carbon	Nitrogen	Phosphorus	Sulfur	Total
Total Wells	190	95	59	35	379
Observations	855	367	233	130	1585
Wells w/ conflicts	61	35	10	13	119
Resolved conflicts	53	10	6	5	74
Remaining unresolved	8	25	4	8	45
Remaining growth/no-growth conflicts	7	24	1	1	33

Other Growth Observations in EcoCyc

- **Low throughput data:**
 - Wildtype observations from literature for 23 media
 - Wildtype observations generated by our group for 21 media
- **High throughput gene knockout data**
 - 5 datasets
 - ◆ 2 on rich media
 - ◆ 2 on glucose media
 - ◆ 1 on glycerol media
 - 17,269 total knockout growth observations

Navigating to All Growth Media Page

Pathway Tools Metabolism and Phenotypes Workshop
Mar 4th-6th 2013

Home Search Tools Help

Genome Browser
Cellular Overview
Genome Overview
Regulatory Overview
Comparative Analysis
Summary Statistics
Dead-end Metabolites
Checkpoint Reactions
Groups
Reports

Escherichia coli, Strain K-12 substratum
Anamika Kothari¹, Suzanne Paley¹, M...
Beratta³, Alberto Santos-Zavaleta², Ve...
Universidad Nacional Autonoma de Mexic...
more information, see URL EcoCyc.org

U00096.2. Despite the involvement

Searching:
► [Escherichia coli K-12 substr. MG1655 change organism database](#)

Citations: [Keseler11]

	Total Genes	Protein Genes	RNA
Chromosome	4623	4420	
Genes without a physical map position:	2		

Pathways:	300
Enzymatic Reactions:	1577
Transport Reactions:	341
Polypeptides:	4517
Protein Complexes:	995
Enzymes:	1485
Transporters:	252
Compounds:	2363
Transcription Units:	4490
tRNAs:	89
Growth Media:	409

Pathway Tools Metabolism and Phenotypes Workshop
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Welcome,
Searching *Escherichia coli* K-12

Home Search Tools Help

Compounds
Genes/Proteins/RNAs
Reactions
Pathways
Growth Media
Advanced
Ontologies
Google this Site
BLAST
Search Full-text Articles

Searching:
► [Escherichia coli K-12 substr. MG1655 change organism database](#)

Media Search
Search Form All Growth Media for this Organism

Submit Query Clear Form

Note: Only... used in constructing the query. If multiple sea... must satisfy ALL of them. For more search options, see the [Advanced Search](#) page. For more details on how to the [Search Help](#) page.

Report Errors or Provide Feedback

Essentiality data for xylA knockouts: ?

Growth Medium	Growth?	T (°C)	O ₂	pH	Osm/L	Growth Observations
LB enriched	Yes	37	Aerobic	6.95		Yes [Gerdess03, Comment 1]
LB Lennox	Yes	37	Aerobic	7		Yes [Baba06, Comment 2]
M9 medium with 1% glycerol	Yes	37	Aerobic	7.2	0.35	Yes [Joyce06, Comment 3]
MOPS medium with 0.4% glucose	Yes	37	Aerobic	7.2	0.21	Yes [Feist07, Comment 4] Yes [Baba06, Comment 2]
PMA carbon source test + D-xylose	No	37	Aerobic			No [Bochner01]
PMA carbon source test + maltose	No	37	Aerobic			No [Bochner01]
PMA carbon source test + maltotriose	No	37	Aerobic			No [Bochner01]

Changing Display Conditions

- On All Growth Media page, can specify different set of conditions
- Colors in display tables will update accordingly

Tables are colored to show growth on wildtype at 37°C (aerobic)

Gene

Indiv

Condi

Aerobic

Knocked out gene (leave blank for wildtype):

Only show data that differs from wildtype

Show all data

Submit Cancel

	(Osm/L)	Available?
AB medium base	0.32	

Generating Heatmaps

Generate heatmap comparing growth on different nutrient sources for different knockouts or other experimental conditions:

Individual Growth Media

Conditions: wildtype at 37°C (a...)

Medium Name
AB medium base
AB medium with 0.2% glucose
AB medium with 0.4% acetate
ATCC medium 57
Bochner defined minimal medi...
Davis and Mingioli glucose mini...
Davis and Mingioli medium A
Davis and Mingioli Modified me...
E.coli minimal growth on acetat...
E.coli minimal growth on glucos...
LB enriched
LB Lennox
M58 medium
M63 medium base
M63 medium with 2% glucose
M63 medium with 2% glycerol

Comparison Parameters

This dialog allows you to generate a heatmap comparing recorded growth status (whether or not growth/respiration occurs) for different nutrient sources under different conditions.

Nutrient type: Carbon Sources
 Nitrogen Sources
 Phosphorus Sources
 Sulfur Sources

Conditions to compare (select at least one): Gene Knockouts
 Aerobic/Anaerobic

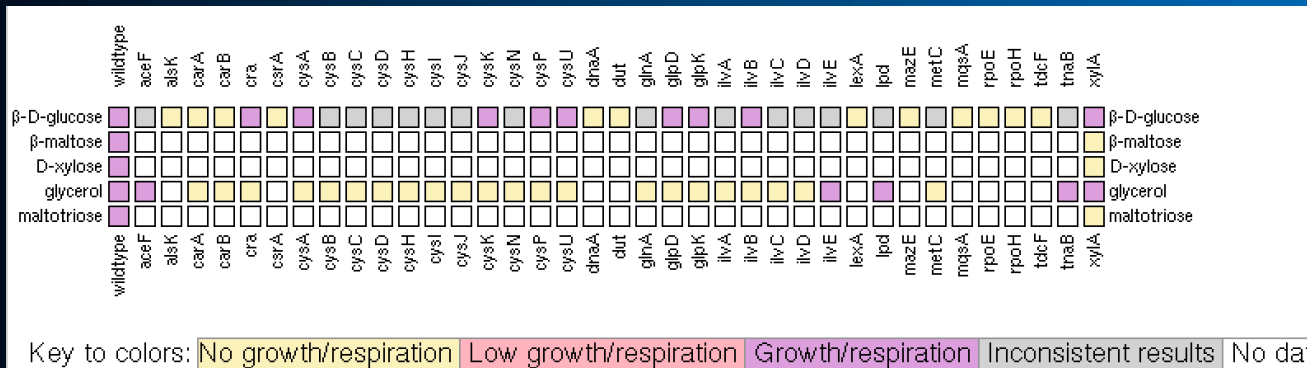
Genes to include: All knockouts with data different than wildtype
 Selected genes

696 genes selected

Growth Condition:

Exclude rows for nutrients that show no change?:

Exclude columns for which all data are same as wildtype?:



Importing PM Data

- **File->Import->Phenotype Microarray Data from Spreadsheet...**
- **Spreadsheet must be saved as tab-delimited text**
- **One file per PM plate**
- **Wells can be identified by either well ID or compound name/ID**
- **Data values in spreadsheet can be either quantitative or qualitative**
 - If quantitative, must specify cutoff values for no/low and low/normal growth
 - If qualitative, must specify what text values match normal/low/no growth

Importing PM Data

Phenotype Microarray Data Import

File: ?

Plate ID:

Media identified by: Well IDs Compound Names
Well ID column number: Sample Well IDs: "B2", "C7"

Data column contains: Text strings Numeric values
Data column number:

Note: column numbers start at 0.

Text string representing growth:

Text string representing low or weak growth:

Text string representing no growth:

Experimental conditions:

Knockout:

Growth Condition: Temperature (°C):

Citations:

Summary:

Importing PM Growth Media

- Can either use base media from EcoCyc (or other PGDB) or create your own.

Import PMA Growth Media

PGDB to import plate media from:

How to choose which media to use as base media:

- Copy plate base media from source database
- Select base media from current database

Note: if you wish to use different base media than those used in the source database, you must already have created those media in the current database. See the command File->Create->Growth Medium.

Create?	Plate ID from Source	Plate ID	Base Medium in Source	Base Medium
<input type="checkbox"/>	Biolog PM1 - Carbon Sources	<input type="text" value="Biolog PM1 - Carbon Sources"/>	Bochner defined minimal medium without carbon	<input type="text" value="Use Source Medium"/>
<input type="checkbox"/>	Biolog PM2 - Carbon Sources	<input type="text" value="Biolog PM2 - Carbon Sources"/>	Bochner defined minimal medium without carbon	<input type="text" value="Use Source Medium"/>
<input type="checkbox"/>	Biolog PM3 - Nitrogen Sources	<input type="text" value="Biolog PM3 - Nitrogen Source"/>	Bochner defined minimal medium without nitrogen	<input type="text" value="Use Source Medium"/>
<input type="checkbox"/>	Biolog PM4 - Phosphorus and Sulfur Sources	<input type="text" value="Biolog PM4 - Phosphorus and Sulfur Sources"/>	Bochner defined minimal medium without sulfur	<input type="text" value="Use Source Medium"/>
			Bochner defined minimal medium without phosphorous	<input type="text" value="Use Source Medium"/>