

CACAO Training

BICH460

BICH461/661

Overview

- Pre-course survey
- What are we doing this semester?
- Big picture
- What is CACAO?
- Housekeeping

Overview of the semester

- Training
 - Today: Intro and training
 - Next week: More training: Practice papers
- Annotation
 - The rest of the semester: 5 rounds of finding papers, reading, doing annotation
 - Class time for meeting with your team and getting in-person help!
- Conclusion
 - Overview of what we did. Prizes?

Housekeeping

- Wiki accounts
 - Practice account: CACAOpractice
- Teams

Suggested papers

- Assignments for next week
 - Find some papers that appear relevant
 - Post to the talk page for the website

Big picture

- This class is about understanding how scientists
 - Infer the function of genes
 - Share knowledge with the larger community
- We will learn this by hands-on experience through CACAO
- **Warnings:**
 - This will be confusing at first. Stick with it!
 - Budget your time. This is not a class where you can cram at the end.

For those returning

- Changes:
 - Wiki software has been updated, so it will be buggy!
 - We will spend class time reviewing examples from previous annotation/challenge rounds

What is CACAO?

- **Community Assessment of Community Annotation with Ontologies (CACAO)**
 - Annotation of gene function
 - Competition
 - Within this class
 - Between TAMU and other schools (BTHO everyone!)
 - Rules next week

Annotation

- Annotation: a note that is made while reading any form of text
- For genome biology,
 - Nucleotide level: Where the genes are in the genome
 - Protein level: What their functions are

Annotation

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- For CACAO,
 - ~~Nucleotide level: Where the genes are in the genome~~
 - Protein level: What their functions are

Functional Annotation

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Why do functional annotation?

- Allow us to:
 - Infer the function of genes
 - Related by common descent
 - Related by similar expression patterns
 - Related by phylogenetic profiles
 - ...
- Allow us to:
 - Understand the capabilities of organisms' genomes
 - Understand patterns of gene expression
 - In different environments
 - In different tissues
 - In disease states
 - ...

Where do functional annotations come from?

Journal home > Archive > Letters to Nature > Abstract

Letters to Nature

Nature 425, 628–633 (9 October 2003) | doi: 10.1038/nature02030

Basal body dysfunction is a likely cause of pleiotropic Bardet–Biedl syndrome

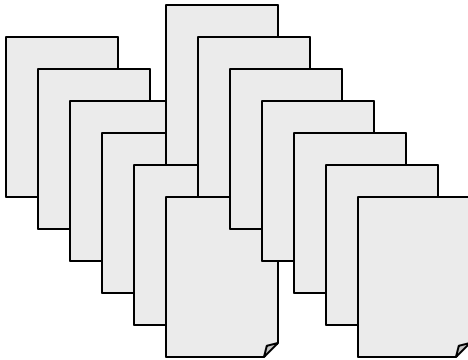
Stephen J. Ansley^{1,2}, Jose L. Badano^{1,2}, Oliver E. Blacque^{3,4}, Josephine Hill⁵, Bethan E. Hoskins^{1,6}, Carmen C. Leitch¹, Jun Chul Kim³, Alison J. Ross⁵, Erica R. Eichers⁵, Tanya M. Teslovich¹, Allan K. Mah³, Robert C. Johnson³, John C. Cavender⁷, Richard Alan Lewis^{2,6}, Michel R. Leroux³, Philip L. Beales⁵ and Nicholas Katsanis^{1,2}

Bardet–Biedl syndrome (BBS) is a genetically heterogeneous disorder characterized primarily by retinal dystrophy, obesity, polydactyly, renal malformations and learning disabilities. Although five BBS genes have been cloned^{1, 2, 3, 4, 5, 6}, the molecular basis of this syndrome remains elusive. Here we show that BBS is probably caused by a defect at the basal body of ciliated cells. We have cloned a new BBS gene, *BBS8*, which encodes a protein with a prokaryotic domain, *pilF*, involved in pilus formation and twitching motility. In one family, a homozygous null *BBS8* mutation leads to BBS with randomization of left–right body axis symmetry, a known defect of the nodal cilium. We have also found that *BBS8* localizes specifically to ciliated structures, such as the connecting cilium of the retina and columnar epithelial cells in the lung. In cells, *BBS8* localizes to centrosomes and basal bodies and interacts with PCMT1, a protein probably involved in cillogenesis. Finally, we demonstrate that all available *Caenorhabditis elegans* BBS homologues are expressed exclusively in ciliated neurons, and contain regulatory elements for RFX, a transcription factor that modulates the expression of genes associated with cillogenesis and intraflagellar transport.

• Top



Literature



Datasets

Biocurators
(rate limiting)

Database

Databases need help!

- >21 million peer-reviewed articles in PubMed
- Many millions of proteins recorded in UniProt

The screenshot displays the UniProtKB search interface. At the top, the UniProt logo and 'UniProtKB' are visible. Below this, there are navigation tabs for 'Search', 'Blast', 'Align', 'Retrieve', and 'ID Mapping *'. The 'Search' tab is active. In the search area, the 'Search in' dropdown is set to 'Protein Knowledgebase (UniProtKB)'. The 'Query' input field contains the text 'human'. To the right of the input field are buttons for 'Search', 'Advanced Search »', and 'Clear'. Below the search bar, a summary line reads '1 - 25 of 1,093,299 results for human in UniProtKB sorted by score descending'. Below this, there are links to 'Browse by taxonomy, keyword, gene ontology, enzyme class or pathway' and a filter option to 'Reduce sequence redundancy to 100%, 90% or 50%'. The 'Results' section is partially visible, showing a 'Customize' button and a filter option: 'Show only reviewed (45,159) UniProtKB/Swiss-Prot or unreviewed (1,048,140) entries'. The 'reviewed' and 'unreviewed' counts are highlighted with red boxes.

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What to annotate

- You can start with a paper
 - Find the proteins discussed
 - Start with a GO term
- You can start with a protein
 - Find papers about the protein
- Either way, don't get stuck on what you started with
 - Your first paper may not have **experiments** about function
 - Reading about your initial protein may lead you to better information about other proteins

Starting with a paper

- Need a scientific paper with experimental data
 - No review articles, no books, no textbooks, no wikipedia articles, no class notes...
 - BUT you should start with those!
 - DON'T start with a random PubMed search


Starting with a paper

- Need a scientific paper with experimental data
 - PubMed review?
 - You will need the PMID number

NCBI Resources ▾ How To ▾

PubMed.gov
US National Library of Medicine
National Institutes of Health

PubMed Hu AND McIntosh

 RSS [Save search](#) [Limits](#) [Advanced](#)

[Display Settings:](#) Summary, 20 per page, Sorted by Recently Added

[Send to:](#)

Results: 10

[GONUTS: the Gene Ontology Normal Usage Tracking System.](#)

1. Renfro DP, **McIntosh** BK, Venkatraman A, Siegele DA, **Hu** JC.

Nucleic Acids Res. 2012 Jan;40(1):D1262-9. Epub 2011 Nov 22.

PMID: 22110029

[Related citations](#)

22110029

Getting the full text

- The abstract is not enough
 - But may be enough to reject a paper!!!
- Some papers are open access
 - Pubmed Central
 - Journal sites
 - TAMU pays for lots of subscriptions
 - Access from off campus via <http://library.tamu.edu>
 - E-journals
 - Citation search takes PMIDs

Beware!

- Good science \neq good for annotation

Second Extracellular Loop of Human Glucagon-like Peptide-1 Receptor (GLP-1R) Differentially Regulates Orthosteric but Not Allosteric Agonist Binding and Function*^S

Received for publication, September 30, 2011, and in revised form, November 29, 2011 Published, JBC Papers in Press, December 6, 2011, DOI 10.1074/jbc.M111.309369

Cassandra Koole[‡], Denise Wootten[‡], John Simms[‡], Emilia E. Savage[‡], Laurence J. Miller[§], Arthur Christopoulos^{‡1}, and Patrick M. Sexton^{‡2}

From the [‡]Drug Discovery Biology, Monash Institute of Pharmaceutical Sciences and Department of Pharmacology, Monash University, Parkville, Victoria 3052, Australia and the [§]Department of Molecular Pharmacology and Experimental Therapeutics, Mayo Clinic, Scottsdale, Arizona 85259

Background: The ECL2 of the GLP-1R is critical for GLP-1 peptide-mediated selective signaling.

Results: Mutation of most ECL2 residues to alanine results in changes in binding and/or efficacy of oxyntomodulin and exendin-4 but not allosteric agonists.

Conclusion: ECL2 of the GLP-1R has ligand-specific as well as general effects on peptide agonist-mediated receptor activation.

Significance: This work provides insight into control of family B GPCR activation transition.

Beware!

- Good science \neq good for annotation

Robust design and optimization of retroaldol enzymes

Eric A. Althoff,^{1,2} Ling Wang,¹ Lin Jiang,^{1,3} Lars Giger,⁴ Jonathan K. Lassila,⁵ Zhizhi Wang,¹ Matthew Smith,¹ Sanjay Hari,¹ Peter Kast,⁴ Daniel Herschlag,⁵ Donald Hilvert,⁴ and David Baker^{1*}

¹Department of Biochemistry, University of Washington and HHMI, Seattle, Washington 98195

²Arzeda Corp., Seattle, Washington 98102

³Department of Biological Chemistry, UCLA, Los Angeles, California 90095

⁴Laboratory of Organic Chemistry, ETH Zurich, 8093 Zurich, Switzerland

⁵Department of Biochemistry, Stanford University, Stanford, California 94305

Beware!

- Good science \neq good for annotation

Cell Stem Cell

Short Article

Cell
PRESS

Vitamin C Enhances the Generation of Mouse and Human Induced Pluripotent Stem Cells

Miguel Angel Esteban,^{1,6} Tao Wang,^{1,6} Baoming Qin,^{1,6} Jiayin Yang,¹ Dajiang Qin,¹ Jinglei Cai,¹ Wen Li,¹ Zhihui Weng,¹ Jiekai Chen,¹ Su Ni,¹ Keshi Chen,¹ Yuan Li,¹ Xiaopeng Liu,¹ Jianyong Xu,¹ Shiqiang Zhang,¹ Feng Li,¹ Wenzhi He,¹ Krystyna Labuda,² Yancheng Song,³ Anja Peterbauer,⁴ Susanne Wolbank,² Heinz Redl,² Mei Zhong,⁵ Daozhang Cai,³ Lingwen Zeng,¹ and Duanqing Pei^{1,*}

¹Stem Cell and Cancer Biology Group, Key Laboratory of Regenerative Biology, South China Institute for Stem Cell Biology and Regenerative Medicine, Guangzhou Institutes of Biomedicine and Health, Chinese Academy of Sciences, Guangzhou 510663, China

²Ludwig Boltzmann Institute for Clinical and Experimental Traumatology, Austrian Cluster for Tissue Regeneration, Vienna 1200, Austria

Beware!

- Good science \neq good for annotation

10624 • The Journal of Neuroscience, August 11, 2010 • 30(32):10624–10638

Neurobiology of Disease

Excess Phosphoinositide 3-Kinase Subunit Synthesis and Activity as a Novel Therapeutic Target in Fragile X Syndrome

Christina Gross,¹ Mika Nakamoto,^{2*} Xiaodi Yao,^{1*} Chi-Bun Chan,³ So Y. Yim,¹ Keqiang Ye,³ Stephen T. Warren,^{2,4,5} and Gary J. Bassell^{1,6}

Departments of ¹Cell Biology, ²Human Genetics, ³Pathology and Laboratory Medicine, ⁴Biochemistry, ⁵Pediatrics, and ⁶Neurology, Emory University School of Medicine, Atlanta, Georgia 30322

Finding proteins

- Search UniProt for something interesting
- Look in UniProt for the protein(s) in the paper you are reading.

**No matter what, you will need to find the protein's accession on UniProt
(<http://uniprot.org>)**



**Use that accession to make a page for that protein on GONUTS
(<http://gowiki.tamu.edu>)**



Add your GO annotations to the protein's page on GONUTS

UniProt (<http://www.uniprot.org>)

- If you have a paper, look for an accession
- Otherwise, search by name/keyword

UniProt > UniProtKB Downloads · Contact · Documentation/Help

Search Blast Align Retrieve ID Mapping *

Search in **Query**
Protein Knowledgebase (UniProtKB)

1 - 25 of 2,360 results for **corynebacterium** AND **diphtheriae** in UniProtKB sorted by **score** descending

Browse by taxonomy, keyword, gene ontology, enzyme class or pathway | Reduce sequence redundancy to 100%, 90% or 50%

Page 1 of 95 | Next »

Results

• Show only [reviewed \(342\)](#) (UniProtKB/Swiss-Prot) or [unreviewed \(2,018\)](#) (UniProtKB/TrEMBL) entries

• Quote terms: "corynebacterium diphtheriae"

• Restrict term "corynebacterium" to [virus host \(9\)](#), [organism \(2,348\)](#), [taxonomy \(2,348\)](#)

• Restrict term "diphtheriae" to [virus host \(9\)](#), [organism \(2,340\)](#), [taxonomy \(2,340\)](#)

Entry	Entry name	Status	Protein names	Gene names	Organism	Length
<input type="checkbox"/> P33120	DTXR_CORDI	★	Diphtheria toxin repressor	dtxR DIP1414	Corynebacterium diphtheriae	226
<input type="checkbox"/> Q6NEC9	Y2346_CORDI	★	UPF0371 protein DIP2346	DIP2346	Corynebacterium diphtheriae	497
<input type="checkbox"/> P33119	GALE_CORDI	★	UDP-glucose 4-epimerase	galE DIP1415	Corynebacterium diphtheriae	328

Make sure you have the right protein

- Right species/strain
- Not a fragment
- Sometimes UniProt has multiple entries for the same protein
 - Gold star = SwissProt = reviewed
 - Blank star = TrEMBL = computational entry
- Sometimes the protein you want is not in UniProt
 - May want to find another paper/protein
- Ask for help
 - OK to email the UniProt help desk
 - check your reasoning with us!

Making a protein page in GONUTS

special page | page maker | translator

GONUTS is undergoing some *major* debugging for Pecan.
Please expect blank pages and some delays in updating.
[Email comments to Daniel.]

GoPageMaker

To create a new gene page, please select a database and enter a unique identifier such as an ID or an accession number. It may take a few minutes to gather data from the primary sources, please be patient.

UniProt Id/Acc Create

[edit]

The GONUTS gene page maker creates a gene page where you can add GO annotations for any gene that has a UniProt Identifier (ID/Entry or Accession) or a NCBI Identifier (GI Number, RefSeq Accession, GenPept Accession). The information generated by the GONUTS gene page maker is UniProt-centric. If NCBI identifiers are used to create a gene page, they are mapped to the

- GoPageMaker will:
 - Check if the page exists in GONUTS & take you there if it does.
 - Make a page if it does not exist in GONUTS already & pull all of the annotations from UniProt into a table that you can edit.
- Make as many protein pages as you would like!



navigation

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cacao

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page discussion edit history delete move protect watch

The Spring 2012 season of CACAO has started!

LAMBD:VLYS

Species (Taxon ID)	<i>Enterobacteria phage lambda (Bacteriophage lambda)</i> . ([1] E)
Gene Name(s)	S
Protein Name(s)	Holin gpS protein Lysis protein S Lysis inhibitor
External Links	
EMBL	J02459 M14035
PIR	H94164
RefSeq	NP_040644.1 YP_001551775.1
TCDB	1.E.2.1.1
GeneID	2703479 5740919
GenomeReviews	J02459_GR
ProtClustDB	CLSP2343227
GO	GO:0020002 GO:0016021 GO:0016998 GO:0019835
InterPro	IPR006481
Pfam	PF05106
TIGRFAMs	TIGR01554

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Annotations

Annotations

[edit]

Qualifier	GO ID	GO term name	Reference	Evidence Code	with/from	Aspect	Notes	Status
	GO:0016020	membrane	GO_REF:0000004	IEA: Inferred from Electronic Annotation	SP_KW:KW-0472	C	Seeded From UniProt	
	GO:0033644	host cell membrane	GO_REF:0000004	IEA: Inferred from Electronic Annotation	SP_KW:KW-1043	C	Seeded From UniProt	

[edit table](#)

[edit]

edit table

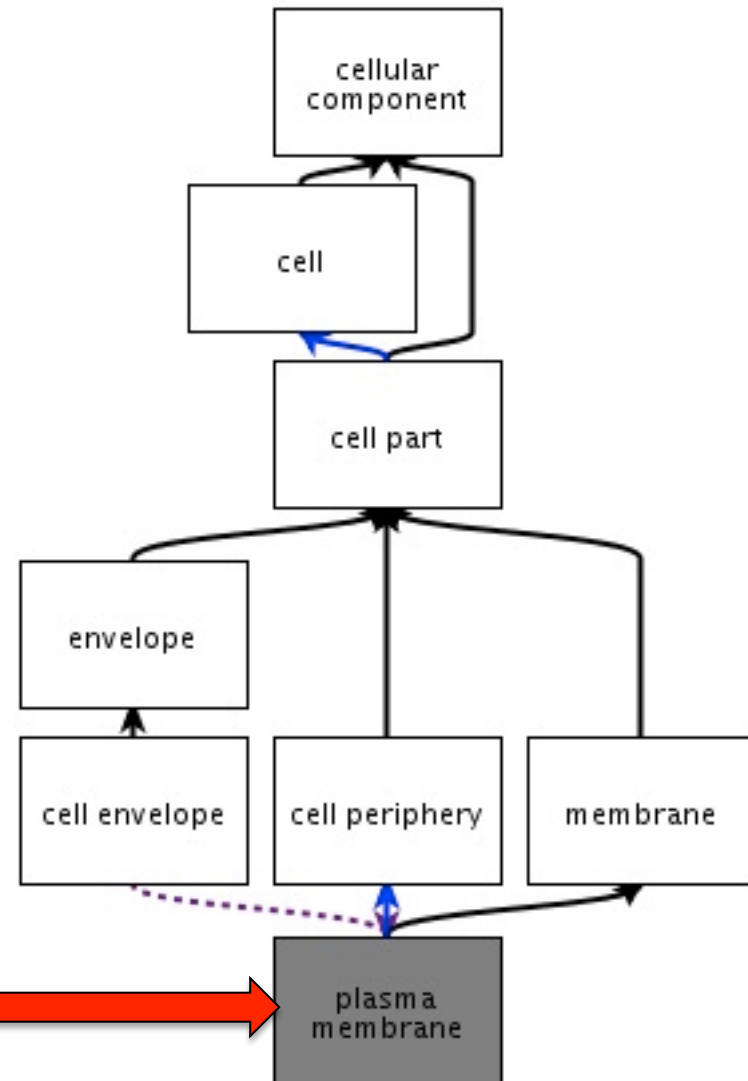
Notes

Functional Annotation

- Annotation: a note that is made while reading any form of text
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GO (Gene Ontology) Annotations

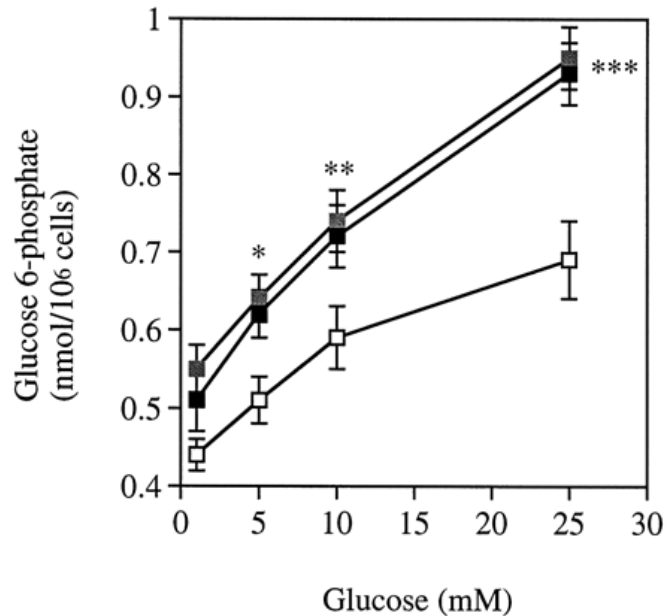
- 3 aspects (ontologies) :
 - Molecular Function
 - Biological Process
 - Cellular Component
- Controlled vocabulary
 - ID number for computers
 - Name and definition for humans
- Relationships



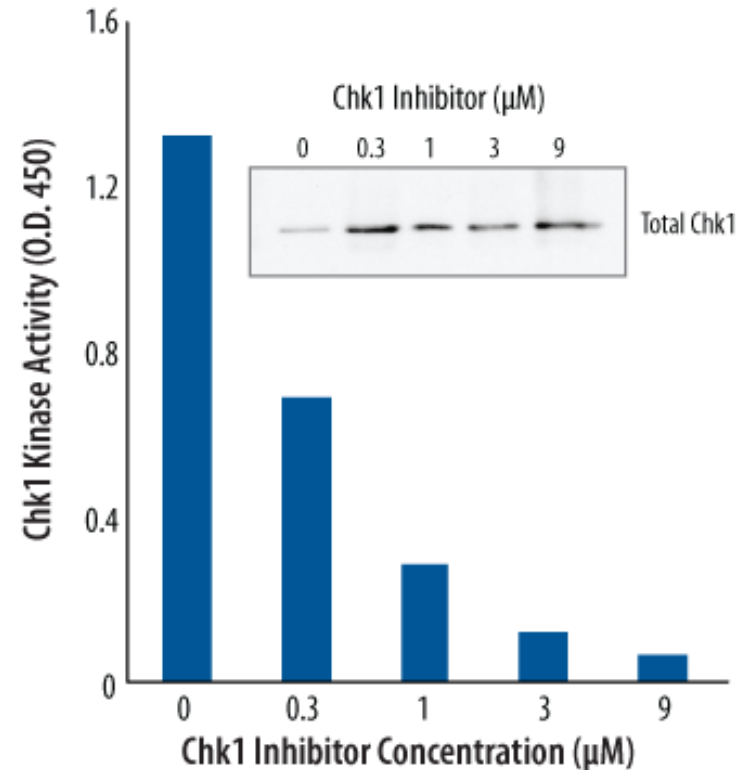
GO:0005886

Molecular Function

- activities or what a protein can do by itself



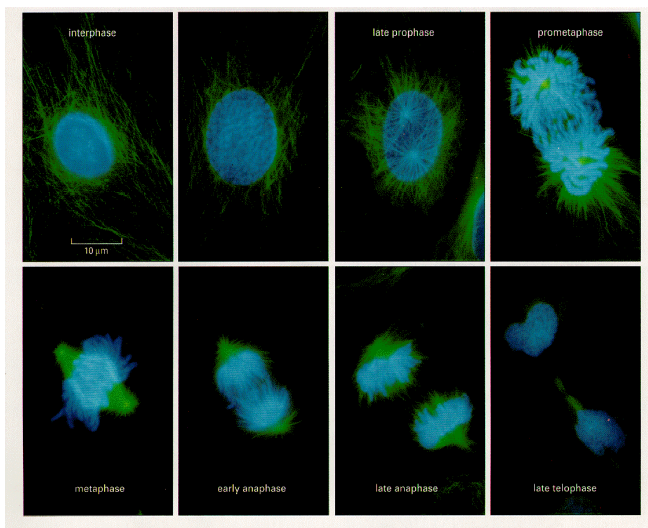
GO:0004347 hexokinase activity



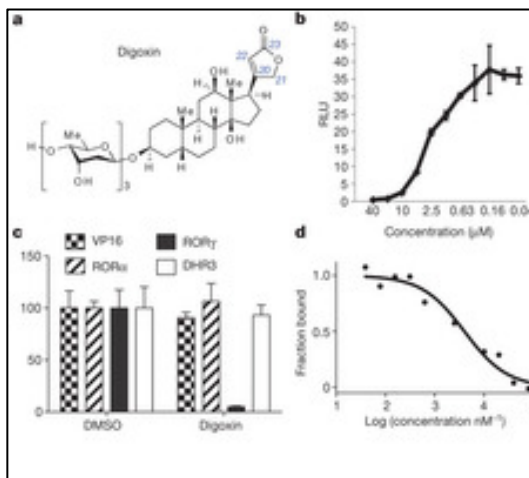
GO:0016301 Kinase activity

Biological Process

- a commonly recognized series of events
 - Including, but not just biochemical pathways



GO:0051301 cell division



GO:0006351 transcription, DNA dependent

Fig. 3. Multiple sand flea lesions at the fingertips



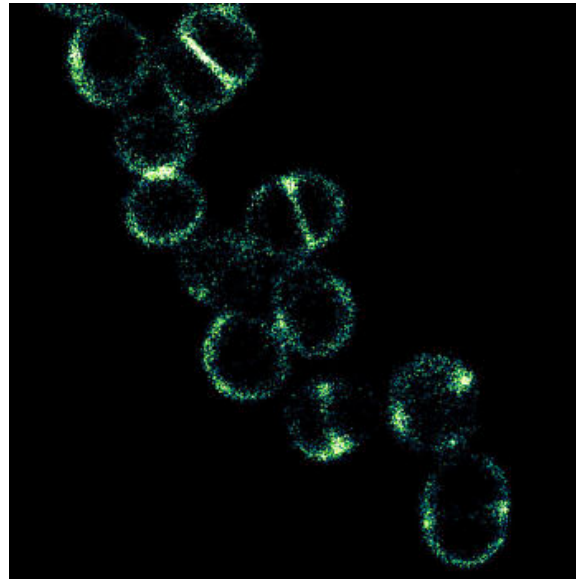
GO:0009405 pathogenesis

Cellular Component

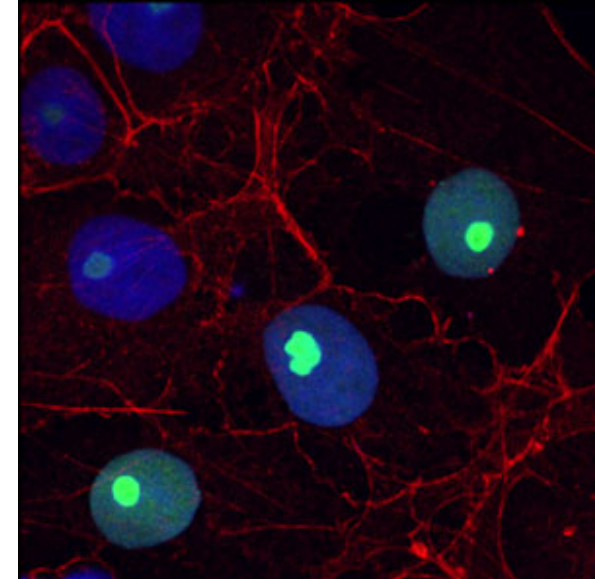
- where a gene product acts
 - Subcellular location
 - Multicomponent complex



GO:0005739
mitochondrion



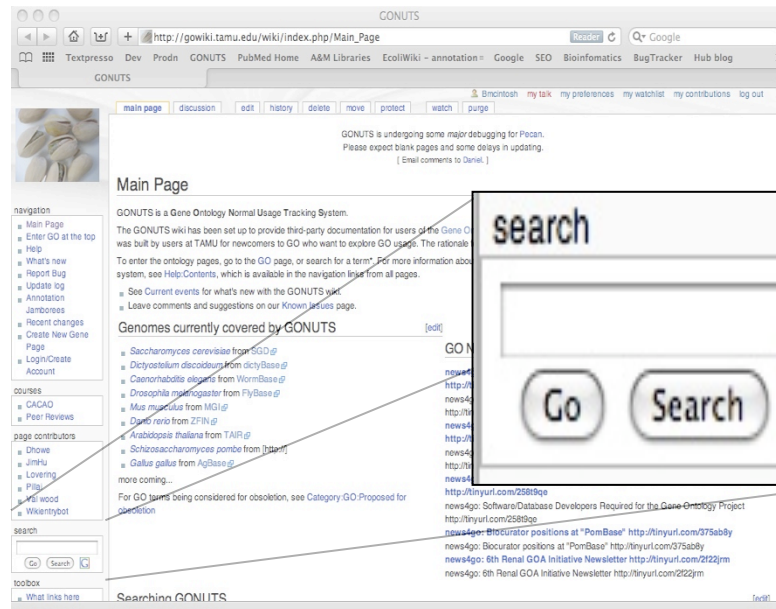
GO:0009274
peptidoglycan-based cell wall



GO:0005840
ribosome

Finding GO terms

- GONUTS: <http://gowiki.tamu.edu>
- QuickGO: <http://www.ebi.ac.uk/QuickGO>
- AmiGO: <http://amigo.geneontology.org>



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GONUTS is undergoing some *major* debugging for Pecan.
Please expect blank pages and some delays in updating.
[[Email comments to Daniel.](#)]

GO:0004713 ! protein tyrosine kinase activity

id: GO:0004713

name: protein tyrosine kinase activity

namespace: molecular_function

alt_id: GO:0004718

def: "Catalysis of the reaction: ATP + a protein tyrosine = ADP + protein tyrosine phosphate." [EC:2.7.10]

subset: gosubset_prok

synonym: "JAK" NARROW []

synonym: "Janus kinase activity" NARROW []

synonym: "protein-tyrosine kinase activity" EXACT []

xref: EC:2.7.10

xref: MetaCyc:EC-2.7.10

xref: Reactome:11065 "protein tyrosine kinase activity"

is_a: GO:0004672 ! protein kinase activity

[AmiGO](#)

Last version checked

date: 14:01:2011 17:26

saved-by: rfulger

auto-generated-by: OBO-Edit 2.0

Last updated

date: 08:10:2010 13:21

saved-by: dph

auto-generated-by: OBO-Edit 2.0

[Gene Ontology Home](#)

The contents of this box are automatically generated. You can help by adding information to the "Notes" [\[edit\]](#)

Usage Notes

[\[edit\]](#)

References

[\[edit\]](#)

See [Help:References](#) for how to manage references in GONUTS

Child Terms

This term has the following 4 child terms.

- [\[+\]](#) GO:0004714 - transmembrane receptor protein tyrosine kinase activity (13)
- [\[\]](#) GO:0004715 - non-membrane spanning protein tyrosine kinase activity
- [\[+\]](#) GO:0004716 - receptor signaling protein tyrosine kinase activity (1)
- [\[+\]](#) GO:0035400 - histone tyrosine kinase activity (1)

Pages in category "GO:0004713 ! protein tyrosine kinase activity"

The following 200 pages are in this category, out of 732 total.

Show articles starting with:

(previous 200) (next 200)

C

- CHICK:A0M8T9
- CHICK:A0SVH2
- CHICK:BTK

C cont.

- CHICK:Q90960
- CHICK:Q90961
- CHICK:Q90962

F cont.

- FB:Tk4
- FB:Tk6
- FB:tor



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Strategies

- Search for a keyword and browse the ontology for the right term
- Look at terms suggested by others for your protein
 - Computational with the IEA evidence code
 - Curators with TAS or IC
- Look at terms used for homologous proteins in model organisms

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Evidence Codes for CACAO

- Evidence codes describe the type of work or analysis done by the authors
 - IDA: Inferred from Direct Assay
 - IMP: Inferred from Mutant Phenotype
 - IGI: Inferred from Genetic Interaction
 - ISO: Inferred from Sequence Orthology
 - ISA: Inferred from Sequence Alignment
 - ISM: Inferred from Sequence Model
 - IGC: Inferred from Genomic Context
- Expert biocurators get to use others, but we restrict them for CACAO. If it's not one of these 7, your annotation is incorrect!!!
- http://gowiki.tamu.edu/wiki/index.php/evidence_codes

Evidence Codes for CACAO

- Picking the right evidence code is important
- Use the evidence code decision tree
- Use the evidence code guidelines at the GO consortium website:
 - <http://www.geneontology.org/GO.evidence.shtml>
- Discuss!

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4 REQUIRED parts of EVERY GO annotation

Qualifier	GO ID	GO term name	Reference	Evidence Code	with/from	Aspect	Notes	Status
	GO:0000183	chromatin silencing at rDNA	SGD_REF:0000182184 PMID:19737915 ^[3]	IMP: Inferred from Mutant Phenotype		P	From SGD	

GO

Reference

Evidence code

Notes (about evidence)

page discussion edit history delete move protect watch

The Spring 2012 season of CACAO has started!



LAMBD:VLYS

Species (Taxon ID)	<i>Enterobacteria phage lambda</i> (<i>Bacteriophage lambda</i>). ([1] E)
Gene Name(s)	S
Protein Name(s)	Holin gpS protein Lysis protein S Lysis inhibitor
External Links	
EMBL	J02459 M14035
PIR	H94164
RefSeq	NP_040644.1 YP_001551775.1
TCDB	1.E.2.1.1
GeneID	2703479 5740919
GenomeReviews	J02459_GR
ProtClustDB	CLSP2343227
GO	GO:0020002 GO:0016021 GO:0016998 GO:0019835
InterPro	IPR006481
Pfam	PF05106
TIGRFAMs	TIGR01554

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Annotations

Annotations

[\[edit\]](#)

Qualifier	GO ID	GO term name	Reference	Evidence Code	with/from	Aspect	Notes	Status
	GO:0016020 E	membrane	GO_REF:0000004 E	IEA: Inferred from Electronic Annotation	SP_KW:KW-0472 E	C	Seeded From UniProt	
	GO:0033644 E	host cell membrane	GO_REF:0000004 E	IEA: Inferred from Electronic Annotation	SP_KW:KW-1043 E	C	Seeded From UniProt	


[edit table](#)

[\[edit\]](#)

edit table

Notes

Entering/editing annotations



special page

The Spring 2012 s

TableEdit

LAMBD:VLYS

Qualifier	<input type="text"/>
GO ID	<input type="text"/>
GO term name	
Reference	<input type="text"/>
Evidence Code	<input type="text"/>
with/from	
Aspect	
Notes	<input type="text"/>
Status	Missing: GO ID, evidence, reference
<input type="text"/> Public <input type="button" value="Refresh"/> <input type="button" value="Save Row"/> <input type="button" value="Cancel"/>	

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journal clubs

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search

Public rows can be edited or deleted by any user who can edit

Private rows can be edited or deleted by their creator, or by admins

4 REQUIRED parts of EVERY GO annotation

Qualifier	GO ID	GO term name	Reference	Evidence Code	with/from	Aspect	Notes	Status
	GO:0000183	chromatin silencing at rDNA	SGD_REF:0000182184 PMID:19737915 ^[3]	IMP: Inferred from Mutant Phenotype		P	From SGD	

GO

Reference

Evidence code

Notes (about evidence)

2 other parts that may be required...

Qualifier



Qualifier	GO ID	GO term name	Reference	Evidence Code	with/from	Aspect	Notes	Status
contributes_to	GO:0004402	histone acetyltransferase activity	SGD_REF:S000074492 PMID:11773077 ^[10]	IDA: Inferred from Direct Assay		F	From SGD	
	GO:0004340	glucokinase activity	PMID:1097393 ^[1]	IGI: Inferred from Genetic Interaction	UniProtKB:P69797	F	table two: gpt glk mpt = no glucose activity	

With/From



Example paper

<http://www.ncbi.nlm.nih.gov/pubmed/8227000>

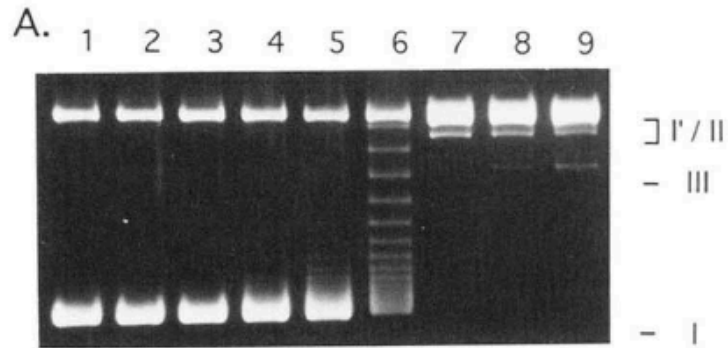
=

<http://www.jbc.org/content/268/32/24481.full.pdf>

What they did

- Finding the proteins
- Do these tell us about the function?
 - Figure 1: sequenced ParC and Part of ParE
 - Figure 2: SDS page of purified proteins
 - Figure 3: Relaxation and decatenation activities of TopoIV
 - ...

Figure 3



- Panel A: relaxation
- Panel B: decatenation
- What do these mean?

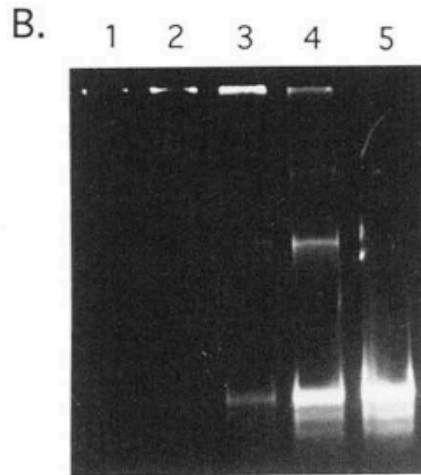
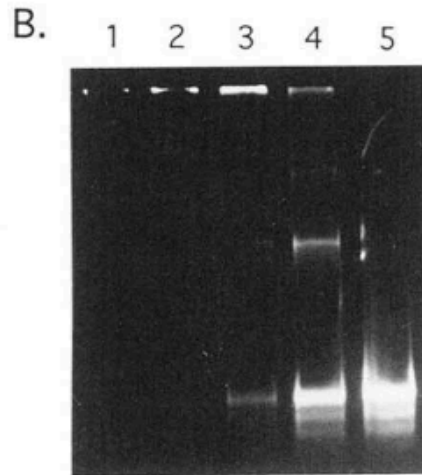
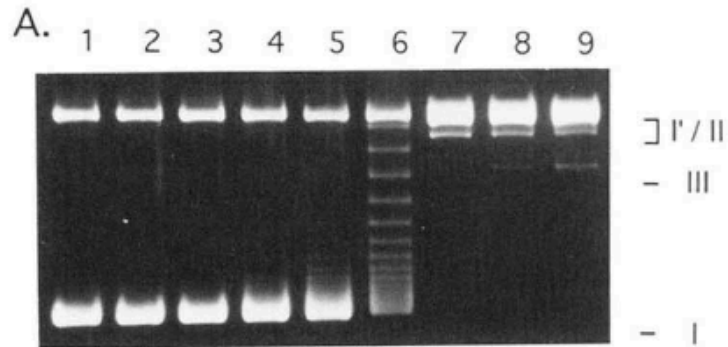
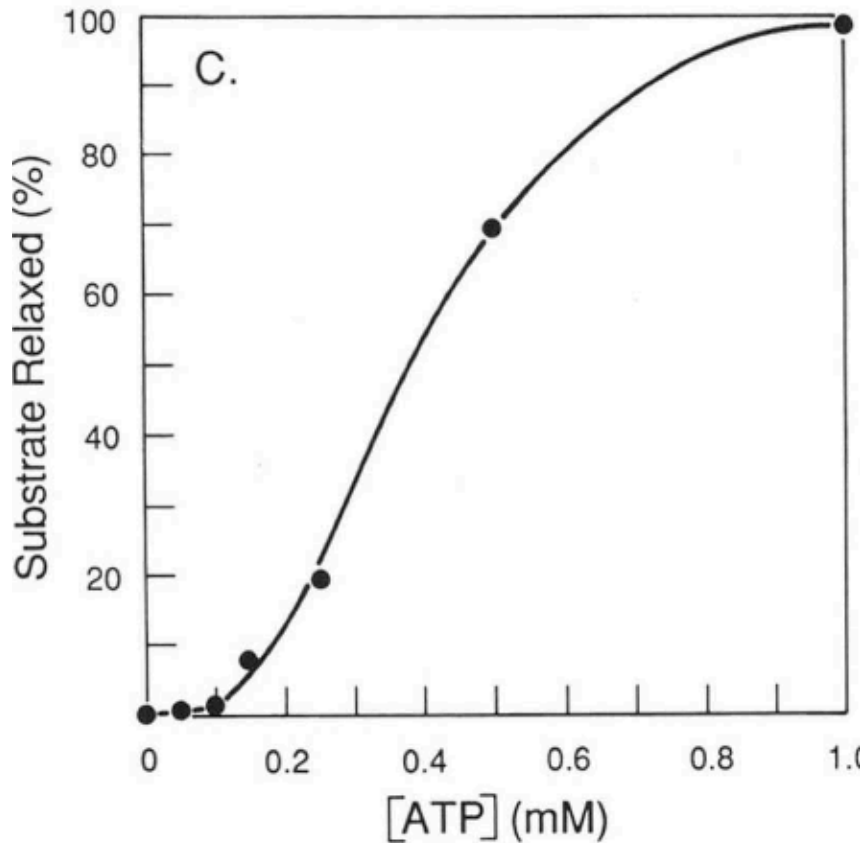


Figure 3



- Panel A: relaxation
- Panel B: decatenation
- What do these mean?
- Panel A shows GO: 0003916 ! DNA topoisomerase activity but does not show what kind
- Panel B shows GO: 0061505 ! DNA topoisomerase II activity

Figure 4



- Shows ATP dependence: [GO:0003918](https://www.ebi.ac.uk/GO/GO:0003918) ! DNA topoisomerase type II (ATP-hydrolyzing) activity