

# eScholarship@UMassChan

## BioTools at UMassMed

Item Type	Presentation
Authors	Lapointe, David S.
DOI	<a href="https://doi.org/10.13028/s0bp-9q31">10.13028/s0bp-9q31</a>
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# Biotoools at UMassMed

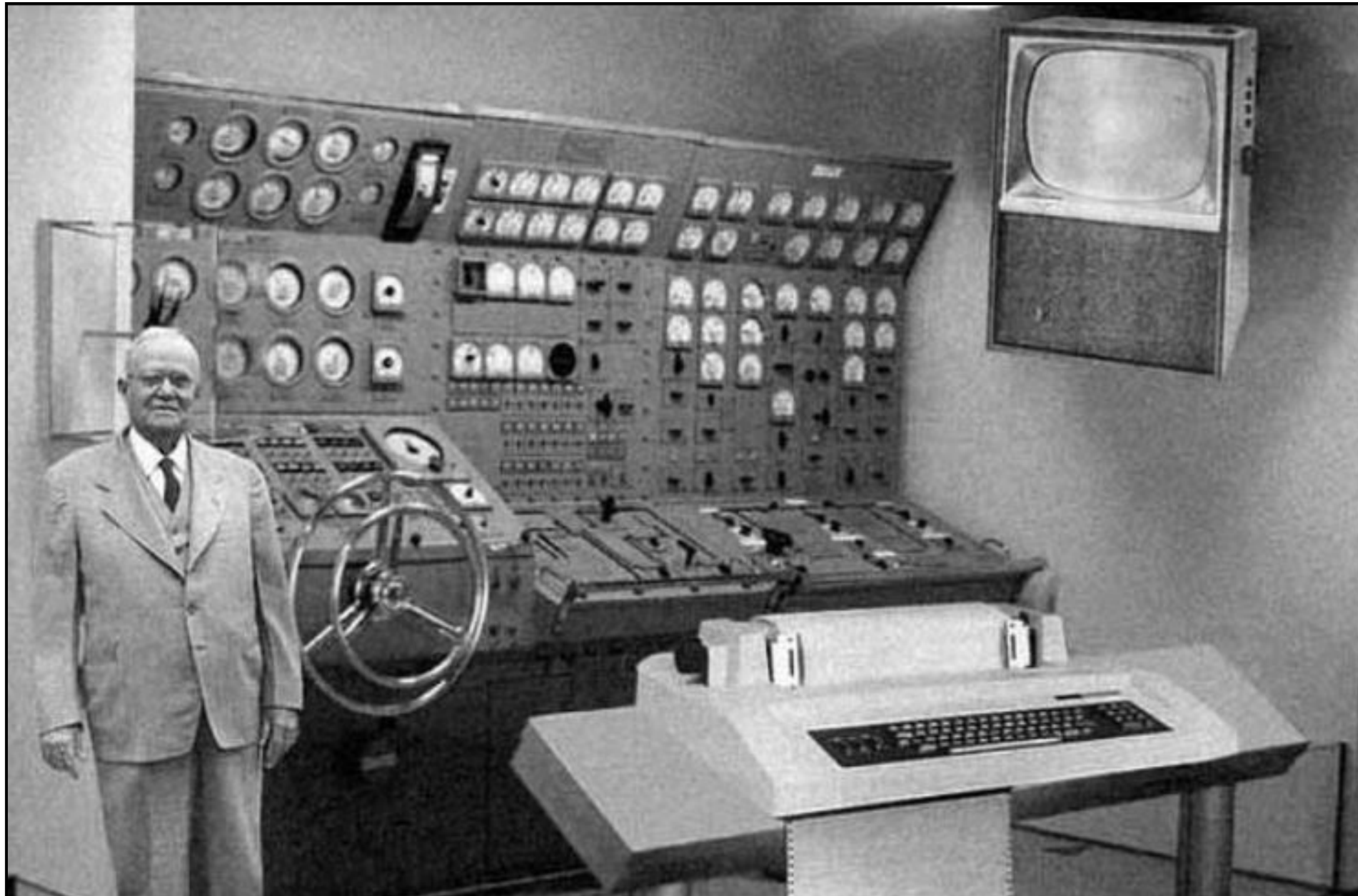
David Lapointe, Ph.D.

Director Scientific Computing

University of Massachusetts Medical School

[biotoools.umassmed.edu](http://biotoools.umassmed.edu)

# Bioinformatics has a large toolset



# Bioinformatics?

- Bioinformatics covers a large territory
  - Sequence and Genome Analysis
  - Computational Biology
  - Databases
  - Visualization
  - Programming
- Informatics applied to Biology

# Motivation

Biotoools started 2001

First as a resource for the Bioinformatics Course

Later expanded access to UMass system,  
Worcester Colleges, and global.

Last month, 12000 visits from 73 countries.



# BioTools @ UMass Medical School

IS-Research Computing

Biotools Main

Thu, Apr 02

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17:39:48

Welcome to the Biotools site at the University of Massachusetts Medical School.

## Restriction and Pattern Analysis

[Restriction mapping tool](#)[Rebase Query Tool](#)[Transcription Factor Site Scan](#)

## DNA Sequence Analysis

[ORF Plotting Tool](#)[Primer Selection Tool](#)

## Protein Sequence Analysis

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## BioTools

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  - [MHC Motif Predictor New!](#)

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### Utilities

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- [ClustalW Multiple Alignment](#)
- [Matrix2PNG](#)
- [WebLogo New!](#)
- [Guide to Unix](#)

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Biotools->EMBOSS ->All programs by group

Sun, Apr 05

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20:03:55

## Select a category to locate programs by function

[Alignment Consensus](#)  
[Alignment Differences](#)  
[Alignment Dot Plots](#)  
[Alignment Global](#)  
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[Nucleic CpG Islands](#)  
[Nucleic Gene Finding](#)

[Nucleic Motifs](#)  
[Nucleic Mutation](#)  
[Nucleic Primers](#)  
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[Phylogeny](#)  
[Protein 2D Structure](#)  
[Protein Composition](#)  
[Protein Motifs](#)  
[Protein Mutation](#)  
[Protein Profiles](#)

## ALIGNMENT CONSENSUS

Program name	Description
<a href="#">cons</a>	Creates a consensus from multiple alignments
<a href="#">megamerger</a>	Merge two large overlapping nucleic acid sequences
<a href="#">merger</a>	Merge two overlapping nucleic acid sequences





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# Primer3Plus

pick primers from a DNA sequence

[Primer3Manager](#)[Help](#)[About](#)[Source Code](#)**Task:** Detection *Select primer pairs to detect the given template sequence. Optionally targets and included/excluded regions can be specified.***Main****General Settings****Advanced Settings****Internal Oligo****Penalty Weights****Sequence Quality**[Sequence Id:](#) [Paste source sequence below](#)

Or upload sequence file:

Mark selected region:

[Excluded Regions:](#)

&lt;

&gt;

[Targets:](#)

[

]

[Included Region:](#)

{

}

 Pick left primer  
or use left primer below. Pick hybridization probe  
(internal oligo) or use oligo below. Pick right primer or use right primer  
below (5'→3' on opposite strand).

# Gateways to local resources

Lists

Wikis

Tools

## Messages

[create new message](#)

Date	Subject	Replies	Author	
2009-03-06 12:54:59	<a href="#">FW: Funding opportunities for construction/renovation and instrumentation</a>	0	<a href="#">Lapointe, David</a>	
2009-03-05 12:40:33	<a href="#">FW: News on the ARRA Stimulus</a>	0	<a href="#">Lapointe, David</a>	
2009-02-25 09:43:43	<a href="#">Desktop Sequence Software</a>	2	<a href="#">Lapointe, David</a>	
2009-02-19 13:18:39	<a href="#">FW: Leveraging Data Pipelining for On-the-Fly Data Integration of Multiple Experiments</a>	0	<a href="#">Kittler, Ellen Ph. D.</a>	
2009-02-15 09:53:30	<a href="#">Re: Ingenuity Software</a>	5	<a href="#">Elizabeth Luna</a>	
2009-02-05 08:57:57	<a href="#">FW: [BioC] [JOB] National Cancer Institute, Bethesda, MD</a>	0	<a href="#">Lapointe, David</a>	
2008-12-30 10:35:42	<a href="#">FW: NHGRI Planning Process- White Papers Available for Review and Comments</a>	0	<a href="#">Lapointe, David</a>	
2008-11-24 17:14:33	<a href="#">Mathworks Seminar Dec 3</a>	0	<a href="#">Lapointe, David</a>	
2008-09-08 10:48:26	<a href="#">FW: [blast-announce] New BLAST 2 Sequences Interface</a>	0	<a href="#">Lapointe, David</a>	
2008-08-27 09:55:46	<a href="#">Ingenuity Software</a>	1	<a href="#">Elizabeth Luna</a>	
2008-08-12 16:16:00	<a href="#">Mathworks Seminar</a>	0	<a href="#">Lapointe, David</a>	
2008-07-28 09:54:14	<a href="#">Simulation Tools/Software from Simbios</a>	0	<a href="#">Lapointe, David</a>	
2008-07-22 09:23:50	<a href="#">FW: [blast-announce] Primer-BLAST now available - addendum</a>	0	<a href="#">Lapointe, David</a>	
2008-07-21 11:36:31	<a href="#">FW: [Gene-announce] Enhancements to Entrez Gene</a>	0	<a href="#">Lapointe, David</a>	
2008-06-16 22:01:10	<a href="#">FW: RECOMB Regulatory Genomics, Systems Biology, and DREAM3 2008 announcement</a>	0	<a href="#">Lapointe, David</a>	
2008-06-16 21:59:13	<a href="#">FW: [Genbank-bb] GenBank Release 166.0 Now Available</a>	0	<a href="#">Lapointe, David</a>	
2008-06-10 16:27:57	<a href="#">FW: NIH Notices and Funding Opportunities</a>	0	<a href="#">Lapointe, David</a>	
2008-06-06 14:35:20	<a href="#">FW: [Gene-announce] Entrez Gene removes links to GDB</a>	0	<a href="#">Lapointe, David</a>	
2008-06-05 12:16:30	<a href="#">FW: Reminder: Webinar Invitation - Advances in GPCR Research, June 17</a>	0	<a href="#">Lapointe, David</a>	
2008-06-02 13:32:18	<a href="#">FW: [Bioclusters] NBCR Summer Institute 2008 -- Cyberinfrastructure for Biomedicine</a>	0	<a href="#">Lapointe, David</a>	

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## Main Page

# High Performance Computing at UMassMed

The High Performance Wiki is maintained by [Academic and Research Computing Services](#) at the University of Massachusetts Medical School. If you would like to participate in this wiki contact us.

### navigation

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- [Community portal](#)
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### search

### toolbox

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## What is HPC?

High Performance Computing refers to the use of supercomputers and computer clusters to solve computationally intensive problems applied generally to scientific research.

In the biomedical arena, high performance computing is used to solve problems of

- [Medical Physics](#)
- [Protein Structure](#)
- [Molecular Dynamics](#)
- [Comparative Genomics](#)
- [Computational Biology](#)

to name a few.

## Topics

### Overview

- [Binar](#)
- [HPCC](#)
- [Getting Access](#)
- [Resources](#)
- [UNIX Related QA](#)


### Using Clusters

- [Queues](#)
- [Software](#)



## PMID Lookup to HTML

Here's where to locate the pmid for a publication on PubMed.  
Just use the number on the form or create a **text** file of pmids to upload.

- 5: [Legorel RS, Hardin MP, Ter-Ghazaryan D](#) Related Art  
 Organization and operation of the marine ornamental fish and invertebrate export fishery in Puerto Rico.  
Rev Biol Trop. 2005 May;53 Suppl 1:145-53.  
PMID: 17465154 [PubMed - in process]

### Enter PMIDS here ( one pmid /line)

```
12036939
1769064
2501299
```

### or upload file with PMIDS: 1 per line

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## References

### Download zipped references

- [van der Meijden Caroline M J, Lapointe David S, Luong Mai X, Peric-Hupkes Daniel, Cho Brian, Stein Janet L, van Wijnen Andre J, Stein Gary S Gene profiling of cell cycle progression through S-phase reveals sequential expression of genes required for DNA replication and nucleosome assembly Cancer Res. 2002 Jun 1;62\(11\):3233-43.](#)
- [Lapointe D S, Olson M S Compartmental analysis of  \$^{45}\text{Ca}^{2+}\$  efflux in perfused rat liver: effects of hormonal stimulation Cell Calcium. 1991 Nov;12\(10\):743-53.](#)
- [Lapointe D S, Olson M S Platelet-activating factor-stimulated hepatic glycogenolysis is not mediated through cyclooxygenase-derived metabolites of arachidonic acid J Biol Chem. 1989 Jul 25;264\(21\):12130-3.](#)

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# Links to External resources



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# Collection of Biostatistics Research Archive

a bepress repository

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[Survival Analysis \(269\)](#)  
[Vital and Health Statistics \(11\)](#)

Paper counts as of 04/02/09

## Peer-Reviewed Journals

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[The International Journal of Biostatistics\\*](#)

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\* guest registration

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Decade of GeneCards Symposium



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Version 2.40 (15 Feb 2009) **New Features**

Batch queries via [GeneALaCart](#)

[Previous version at genecards.org](#)

Add bookmark for the [GeneCards Human Gene Database](#):



GeneCards® is a searchable, integrated database of human genes that provides concise genomic, proteomic, transcriptomic, genetic and functional information on all known and predicted human genes. Information featured in GeneCards includes orthologies, disease relationships, mutations and SNPs, gene expression, gene function, pathways, protein-protein interactions, related drugs & compounds and direct links to cutting edge research reagents and tools such as antibodies, recombinant proteins, clones, expression assays and RNAi reagents.



SAMPLE GENE: [CASP3](#)

[GeneCards Guide](#)

[Getting Started](#)

[Statistics](#)

[[Gene Index](#)] [[Disease genes](#)] [[Hot genes](#)] Random Gene From:   [GIFtS](#) **improved**



### Search the GeneCards Human Gene Database

[Advanced Gene Search](#)

Search by:  Keywords  Gene Symbol only  Symbol/alias  GC id  Symbol/External id

Examples: [tay sachs](#) [ESR1](#) [FRAXA](#) [GC17M03\\*](#) [3395](#)  
[dimerization AND diabetes](#) [wnt\\*](#) [7431](#)  
[neurodegenerative OR senile](#) [P12004](#)  
[ENSG00000185515](#)

Options:  Show microcards only  Show minicards also (slower)  
 Sort microcards alphabetically (faster)  Sort microcards by relevance

[More search examples](#)

*The GeneCards search is case insensitive*



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GeneCards Gene Database statistics

# Next Up

Provide links to local resources

- Faculty developed applications

- Portal to data storage

Develop applications for Web 3.0

# Web 3.0?

## Where is this going?

The web is a great vehicle for distributing information, creating resources.

The web, however, is human readable It is difficult to harvest information from websites.

Resource creators are moving to semantic web along with web service models to allow machine harvest of information.

Example

http://www.pathguide.org

# Pathguide the pathway resource list

## Navigation

- Protein-Protein Interactions
- Metabolic Pathways
- Signaling Pathways
- Pathway Diagrams
- Transcription Factors / Gene Regulatory Networks
- Protein-Compound Interactions
- Genetic Interaction Networks
- Protein Sequence Focused
- Other

## Search

Organisms

Availability

Standards

## Statistics

Analyze Pathguide

## Contact

Comments, Questions, Suggestions are Always Welcome!

## Complete Listing of All Pathguide Resources

Pathguide contains information about **291** biological pathway resources. Click on a link to go to the resource home page or 'Details' for a description page. Databases that are free and those supporting BioPAX, CellML, PSI-MI or SBML standards are respectively indicated.

If you know of a pathway resource that is not listed here, or have other questions or comments, please [send us an e-mail](#).

### News

were added

---

#### Get the Stats



Detailed Pathguide resource statistics now available

---

#### Pathguide Published

Please cite the [Pathguide Publication](#)

## Protein-Protein Interactions

Database Name (Order: alphabetically   <a href="#">by web popularity</a> )	Full Record	Availability	Standards
3DID - 3D interacting domains	<a href="#">Details</a>	Free	
ABCdb - Archaea and Bacteria ABC transporter database	<a href="#">Details</a>	Free	
AfCS - Alliance for Cellular Signaling Molecule Pages Database	<a href="#">Details</a>	Free	
AllFuse - Functional Associations of Proteins in Complete Genomes	<a href="#">Details</a>	X	
aMAZE - Protein Function and Biochemical Pathways Project	<a href="#">Details</a>	Free	
ASEdb - Alanine Scanning Energetics Database	<a href="#">Details</a>	Free	
ASPD - Artificial Selected Proteins/Peptides Database	<a href="#">Details</a>	Free	
BID - Binding Interface Database	<a href="#">Details</a>	X	
BIND - Biomolecular Interaction Network Database	<a href="#">Details</a>	Free	<a href="#">PSI-MI</a>
BioGRID - General Repository for Interaction Datasets	<a href="#">Details</a>		<a href="#">PSI-MI</a>
BRITE - Biomolecular Relations in Information Transmission and Expression	<a href="#">Details</a>	Free	
CA1Neuron - Pathways of the hippocampal CA1 neuron	<a href="#">Details</a>	Free	
Cancer Cell Map - The Cancer Cell Map	<a href="#">Details</a>	Free	<a href="#">BioPAX</a>
CellCircuits - CellCircuits	<a href="#">Details</a>	Free	
CPDB - ConsensusPathDB	<a href="#">Details</a>		<a href="#">BioPAX</a>
CSP - Cytokine Signaling Pathway Database	<a href="#">Details</a>	X	
CTDB - Calmodulin Target Database	<a href="#">Details</a>	Free	

So a researcher might come to me or you and ask

I have 200 Entrez gene Ids.

What pathways do these genes belong to?

What resource would you direct them toward?

There is always Google!

david.lapointe@gmail.com | [My](#)



## Find workflows and Web services for bioinformatics

### Creator



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### Search engine details

Find Web services and workflows for bioinformatics applications, compatible with the open source Taverna workflow editor; <http://www.mygrid.org.uk/taverna>

searches 136 sites, including:

<http://www.mygrid.org.uk/wiki/Mygrid/BiologicalWebServices>,  
[workflows.mygrid.org.uk](http://workflows.mygrid.org.uk), [www.biojava.org/docs/](http://www.biojava.org/docs/),  
[taverna.sourceforge.net/index.php?doc=services.html](http://taverna.sourceforge.net/index.php?doc=services.html),  
[bioweb.pasteur.fr/docs/EMBOSS/](http://bioweb.pasteur.fr/docs/EMBOSS/)

Keywords: biology, bioinformatics, web services, workflows, Taverna, myGrid, registry, myExperiment

Last updated: Aug 14, 2007

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Hmm, mostly journal articles. Let see Workflows only

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Refine results for **Pathways**:

[No workflows](#)

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[BioMed Central | Full text | Systems biology for identifying liver ...](#)

Mar 10, 2009 ... The objective of this paper is to describe systems biology methods for identifying **pathways** involved in liver toxicity induced by free fatty ...

[www.biomedcentral.com/1753-6561/3/S2/S2](http://www.biomedcentral.com/1753-6561/3/S2/S2)

by Z Li - 2009

Labeled [No workflows](#) [WSDL only](#)

[Genome Biology | Full text | Computational prediction of human ...](#)

PathoLogic predicts the metabolic **pathways** of the organism, providing new ... Current knowledge of human nutrition based on metabolic **pathways** is derived ...

[genomebiology.com/2004/5/1/R2](http://genomebiology.com/2004/5/1/R2)

by P Romero - 2004 - [Cited by 80](#) - [Related articles](#) - [All 13 versions](#)

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[Bioinformatics—from genes to pathways - Nature Methods](#)

Combined with the right computational tools, genomic data can uncover unknown **pathways** to cellular processes. Because few researchers have the resources to ...

[www.nature.com/nmeth/journal/v1/n2/full/nmeth1104-169.html](http://www.nature.com/nmeth/journal/v1/n2/full/nmeth1104-169.html)

by L Bonetta - 2004 - [Cited by 12](#) - [Related articles](#)

Labeled [WSDL only](#) [No workflows](#)

[Genome Biology | Full text | Reactome: a knowledgebase of ...](#)

Reactome: a knowledge base of biologic **pathways** and processes .... **Pathways** can be part of larger **pathways**. Reactome represents glycolysis and ...

[genomebiology.com/2007/8/3/r39](http://genomebiology.com/2007/8/3/r39)

by I Vastrik - 2007 - [Cited by 101](#) - [Related articles](#) - [All 7 versions](#)

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[PATIKAwEB: a Web interface for analyzing biological pathways ...](#)

Summary: PATIKAwEB provides a Web interface for retrieving and analyzing biological **pathways** in the PATIKA database, which contains data integrated from ...

[bioinformatics.oxfordjournals.org/cgi/content/abstract/22/3/374](http://bioinformatics.oxfordjournals.org/cgi/content/abstract/22/3/374)

by U Dogrusoz - 2006 - [Cited by 19](#) - [Related articles](#) - [All 8 versions](#)

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# Ok This looks better

## Refine results for **Pathways**:

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**Workflows only**

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### [myExperiment.org - Workflows - omim and \*\*pathways\*\* \(Katy ...](#)

Mar 3, 2009 ... Title: omim and **pathways**. Type: Taverna 1 ... **pathways**, KeggGenestoPathways: pathway\_by\_genes, pathwayDescriptions, KeggGenestoPathways: ...

[www.myexperiment.org/workflows/588](http://www.myexperiment.org/workflows/588)

Labeled Workflows only

### [myExperiment - Workflows - Entrez Gene to KEGG \*\*Pathway\*\* \(Paul ...](#)

These gene ids are then cross-referenced to KEGG gene ids. Each KEGG gene id is then sent to the KEGG **pathway** database and its relevant **pathways** returned. ...

[www.myexperiment.org/workflows/15](http://www.myexperiment.org/workflows/15)

Labeled Workflows only

### [myExperiment.org - Workflows - \*\*Pathways\*\* and Gene annotations for ...](#)

Workflow Entry: **Pathways** and Gene annotations for Arabidopsis affy data ... The KEGG gene identifiers are then used to search for **pathways** in the KEGG ...

[www.myexperiment.org/workflows/726](http://www.myexperiment.org/workflows/726)

Labeled Workflows only

### [myExperiment.org - Workflows - Mouse \*\*Pathways\*\* and Gene annotations ...](#)

The KEGG gene identifiers are then used to search for **pathways** in the KEGG **pathway** database. .... **Pathways** and Gene annotations for Arabidopsis affy data ...

[www.myexperiment.org/workflows/16](http://www.myexperiment.org/workflows/16)

Labeled Workflows only

### [myExperiment.org - Workflows - Mapping microarray data onto ...](#)

Nov 22, 2007 ... This workflow maps microarray data onto metabolic **pathway** diagrams represented as SBML models drawn using Cell Designer. ...

[www.myexperiment.org/workflows/79](http://www.myexperiment.org/workflows/79)

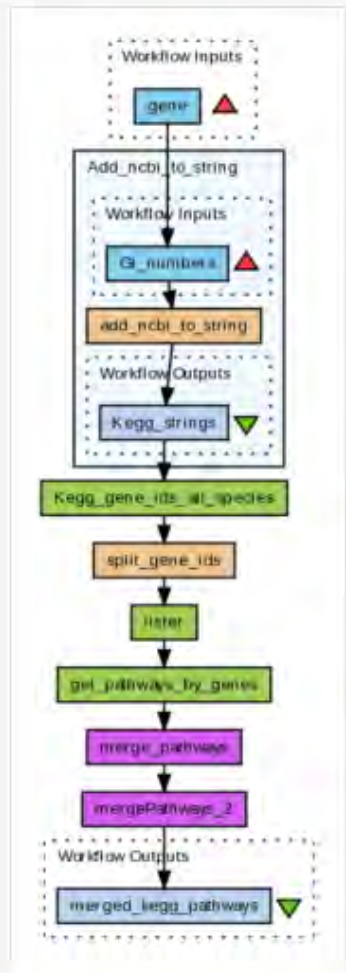
Labeled Workflows only

### [myExperiment - Workflows - KEGG \*\*pathways\*\* common to both QTL and ...](#)

This workflow takes in two lists of KEGG **pathway** ids. These are designed to come from **pathways** found from genes in a QTL (Quantitative Trait Loci) region. ...

[www.myexperiment.org/workflows/13](http://www.myexperiment.org/workflows/13)

Labeled Workflows only



[Download Scalable Diagram \(SVG\)](#)

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**Credits (0)**  
(People/Groups)  
None

**Attributions (0)**  
(Workflows/Files)  
None

**Tags (8)**

Original Uploader tags

entrez | genotype | kegg | pathway | pathway-driven | pathways | phenotype | shim

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**Shared with Groups (0)**  
None

**Featured In Packs (0)**  
None

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**Ratings (3)**

Current:  
**4.7 / 5**  
(3 ratings)

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**Description**

This workflow takes in Entrez gene ids then adds the string "ncbi-geneid:" to the start of each gene id. These gene ids are then cross-referenced to KEGG gene ids. Each KEGG gene id is then sent to the KEGG pathway database and its relevant pathways returned.



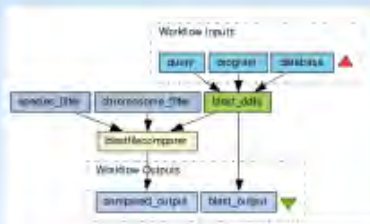
myExperiment makes it really easy to **find, use and share** scientific workflows and other files, and to build communities.

All

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- [The BioCatalogue Project](#)
- [myExperiment Publications](#)

## Register

### or Login:

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(eg: name.myopenid.com)

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myExperiment has over 1500 users, 130 groups, 560 workflows, 150 files and 40 packs

## BioCatalogue

"The Life Science Web Services Registry"

### BioCatalogue: providing a curated catalogue of Life Science Web Services.




BioCatalogue will provide a **single registration point** for Web Service providers and a **single search site** for scientists and developers.

BioCatalogue will also act as a place where the **community** can **find contacts** and **meet** the experts and maintainers of these services.

The BioCatalogue team is currently working with the Embrace team to **merge their registries**. In the meantime, if you are keen to register your web services, please use the [EMBRACE Registry](#), the contents of which will be merged with BioCatalogue in due course.

The BioCatalogue team is currently working on its **first release**, the pilot BioCatalogue, which has been released for testing to our [biocatalogue-friends mailing list](#).

More information about the pilot and current BioCatalogue activities can be found on the [BioCatalogue public wiki](#) .

"Web Services are hard to find..."

#### SEARCH

**Scientists, tool developers, bioinformaticians** will be able to find the right Web Service they were looking for, thanks to an **easy and powerful search interface** harvesting the information made available by the Web Services providers and the BioCatalogue community.

"My Web Services are not visible..."

#### REGISTER

**Service providers** will be able to **easily register** their Web Services in the BioCatalogue, making them **instantly available** to the scientific community as well as the tool developers.

"Web Services are poorly described..."

#### ANNOTATE

**Expert curators** will provide oversight, monitor the catalogue and provide **high quality annotations** for services. The wider **community** will also participate to this effort using **social networking** for recommending, tagging, commenting and rating the services.

"Web Services are volatile..."

#### MONITOR

Web Services are **volatile**. They change their location, capability and interaction or become **outdated**. BioCatalogue will allow agents to **monitor** the Web Services and **automatically** add information to the catalogue.

The end result is that we are approaching  
eScience (EU)/cyberinfrastructure(USA)

Genomics (NCBI, Ensembl, UCSC,GMOD)

meets System Biology (KEGG,BIND,GO)