University of Massachusetts Medical School

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Apr 6th, 12:00 AM

BioTools at UMassMed

David S. Lapointe
University of Massachusetts Medical School

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Repository Citation

Biotools at UMassMed

David Lapointe, Ph.D.

Director Scientific Computing

University of Massachusetts Medical School

biotools.umassmed.edu

Bioinformatics has a large toolset
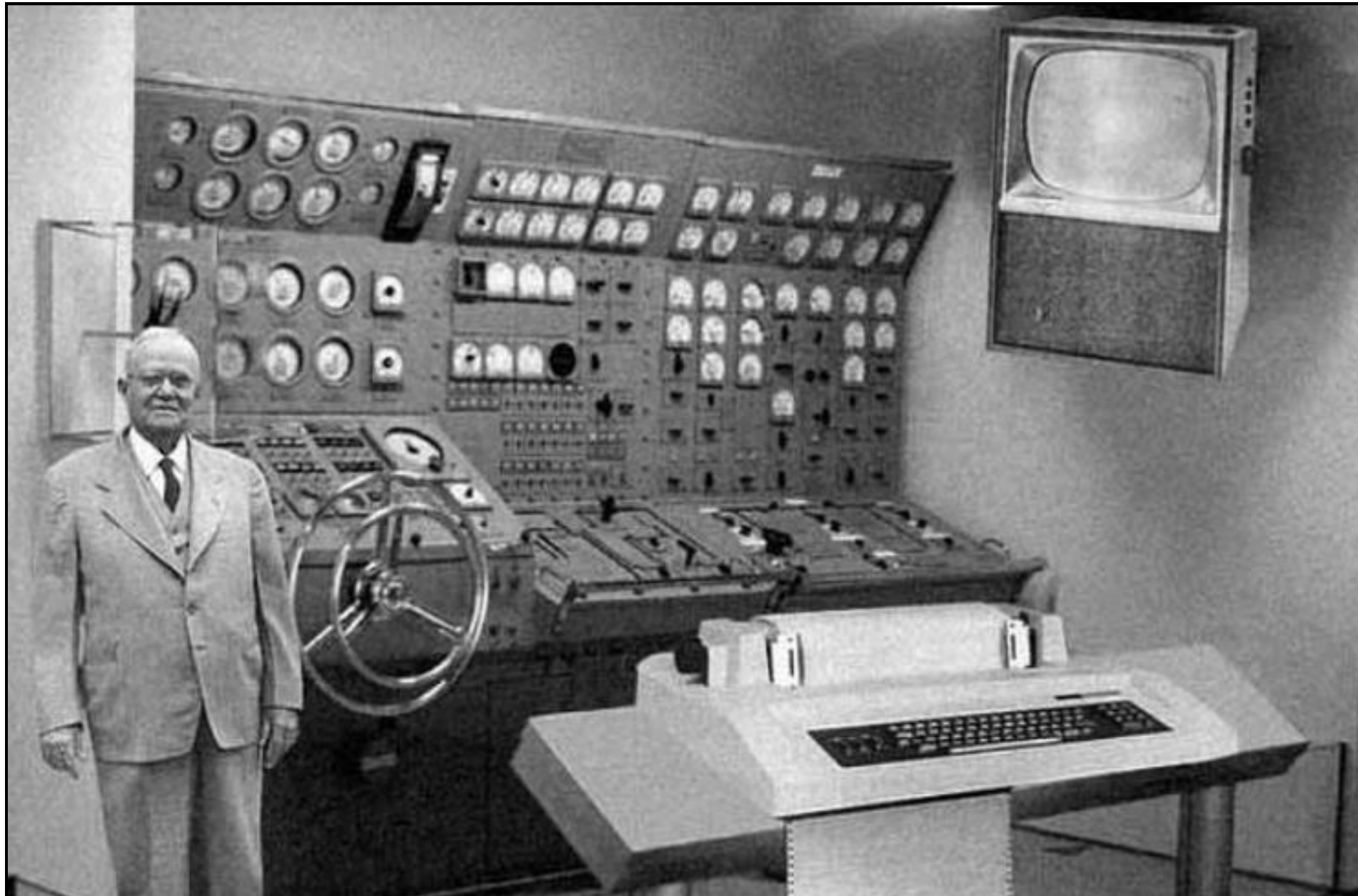
Bioinformatics?

- Bioinformatics covers a large territory

  – Sequence and Genome Analysis

  – Computational Biology

  – Databases

  – Visualization

  – Programming

- Informatics applied to Biology

Motivation

Biotools 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   **Home | News | Resources |**   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

Signal Sequence Cleavage Tool
Peptide/Protein Statistics
Garnier Secondary Structure
PRINTS protein motifs scan
MHC Motif Predictor New!

Utilities

PrettyPlot MSF files
Translate Nucleic Acids

Links

BioNetbook
CoBRA (Biostatistics)
HSLS Online
BioGRID New!
OregAnno New!
PrimerBank
Signaling Gateway
BioInformatics.Org
GeneCards

Last updated: Friday February 27, 2009
Comments and Suggestions welcome.

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55 Lake Avenue N, Worcester MA 01655

BioTools @ UMass Medical School

IS-Research Computing

Biotools Main

Thu, Apr 02   **Home | News | Resources | EMBOSS | Contact |**   17:42:42

BioTools

The BioTools site is a resource of tools for bioinformatics for the five schools of the UMass System. Some resources are licensed to the UMass Medical School and only usable at that site. Comments and Suggestions are welcome.

EMBOSS-WWW
    EmbossGUI
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    ClustalW Multiple Alignment
    Matrix2PNG
    WebLogo *New!*
    Guide to Unix

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Done

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Biotools Main

Thu, Apr 02   17:44:51

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Thu, Apr 02   Home | News | Resources | EMBOSS | Contact | Stats | Discuss   17:44:51

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BioTools @ UMass Medical School

Select a category to locate programs by function

Alignment Consensus	Nucleic Motifs
Alignment Differences	Nucleic Mutation
Alignment Dot Plots	Nucleic Primers
Alignment Global	Nucleic Profiles
Alignment Local	Nucleic Repeats
Alignment Multiple	Nucleic Restriction
Display	Nucleic Transcription
Edit	Nucleic Translation
Enzyme Kinetics	Phylogeny
Feature Tables	Protein 2D Structure
Nucleic 2D Structure	Protein Composition
Nucleic Codon Usage	Protein Motifs
Nucleic Composition	Protein Mutation
Nucleic CpG Islands	Protein Profiles
Nucleic Gene Finding	

ALIGNMENT CONSENSUS

Program name	Description
cons	Creates a consensus from multiple alignments
megamerger	Merge two large overlapping nucleic acid sequences
merger	Merge two overlapping nucleic acid sequences

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File   Edit   View   History   Bookmarks   Tools   Help

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.*   Pick Primers   Reset Form

| **Main** | **General Settings** | **Advanced Settings** | **Internal Oligo** | **Penalty Weights** | **Sequence Quality** |

Sequence Id:

Paste source sequence below   Or upload sequence file: Browse…   Upload File

Mark selected region: < >   [ ]   { }   Clear   Save Sequence

Excluded Regions: <   >

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).

Done

Gateways to local resources

Lists

Wikis

Tools

LYRIS ListManager

| Messages | Search | Conference | My Account | My Forums | All Forums | About |

Messages

create new message ▶

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

◀ previous | next ▶ | ◀ show less | show more ▶

page   discussion   view source   history

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 ✉.

search

| Go | Search |

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

Done

BioTools @ UMass Medical School

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Biotools ->MakeRefs

Thu, Apr 02   **Home | News | Resources | EMBOSS | Contact | Stats | Discuss**   17:55:38

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 Arts

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

[   ]   Browse..

Get Refs!   Reset

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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 45Ca2+ 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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Done

Links to External resources

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COBRA™

Collection of Biostatistics Research Archive
a bepress repository

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Medical Specialties (27)
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Statistical Models (372)
Statistical Theory and Methods (591)
Survival Analysis (269)
Vital and Health Statistics (11)

Paper counts as of 04/02/09

Peer-Reviewed Journals

Statistical Applications in Genetics and Molecular Biology*
The International Journal of Biostatistics*

Propose a journal

* guest registration

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Collection of Biostatistics Research Archive
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Duke University
Harvard University
Johns Hopkins University
Memorial Sloan-Kettering Cancer Center
University of California, San Francisco
University of California, Berkeley
University of Michigan School of Public Health
University of North Carolina at Chapel Hill
University of Pennsylvania
University of Texas, MD Anderson Cancer Center
University of Washington

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BETA
GeneALaCart
GeneCards Batch Queries

GeneDecks
Assorted Gene Sets

GeneNote
Gene Normal Tissue Expression

GeneAnnot
Microarray Gene Annotation

GeneLoc
Gene Location

GeneTide
Terra Incognita Discovery Endeavor

Version 2.40 (15 Feb 2009) New Features   NEW   **Batch queries via GeneALaCart**   Previous version at genecards.org
Add bookmark for the GeneCards Human Gene *Database:* BOOKMARK

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 Group--- ▼ Go GIFtS improved

Search the GeneCards Human Gene Database

[_____] Search 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

What's New
GeneCards Guide
  Getting Started
  About GeneCards
  Data Sources
  Citing This Resource
  Our Publications

GeneCards Gene Database statistics

Done

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

Home | BioPAX | cBio | MSKCC

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
[All ▼]
Availability
[All ▼]
Standards
[All ▼]
[Reset] [Search]

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

Hmm, mostly journal articles. Let see Workflows only

Refine results for **Pathways:**

No workflows   No local applications   Workflows only   WSDL only

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
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/2004/6/1/R2
by P Romero - 2004 - Cited by 80 - Related articles - All 13 versions
Labeled No workflows WSDL only

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
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
by I Vastrik - 2007 - Cited by 101 - Related articles - All 7 versions
Labeled No workflows WSDL only

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
by U Dogrusoz - 2006 - Cited by 19 - Related articles - All 8 versions
Labeled No workflows WSDL only

Ok This looks better

Refine results for **Pathways:**

No workflows   No local applications   **Workflows only**   WSDL only

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/688
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
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 searcg for **pathways** in the KEGG ...
www.myexperiment.org/workflows/726
Labeled Workflows only

myExperiment.org - Workflows - Mouse **Pathways** and Gene annotations **...**
The KEGG gene identifiers are then used to searcg for **pathways** in the KEGG **pathway** database. ....
Pathways and Gene annotations for Arabidopsis affy data ...
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
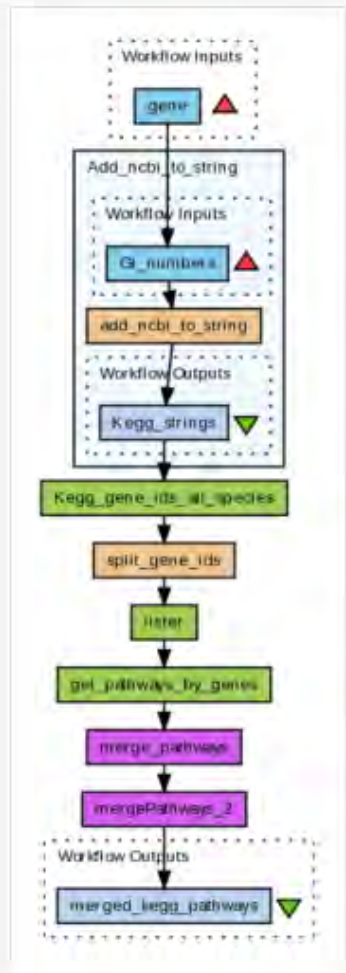Labeled Workflows only

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
Labeled Workflows only

Workflow Inputs
- gene ▲

Add_ncbi_to_string
  Workflow Inputs
  - Gi_numbers ▲
  - add_ncbi_to_string
  Workflow Outputs
  - Kegg_strings ▼

Kegg_gene_ids_all_species

split_gene_ids

lister

get_pathways_by_genes

merge_pathways

mergePathways_2

Workflow Outputs
- merged_kegg_pathways ▼

Download Scalable Diagram (SVG)

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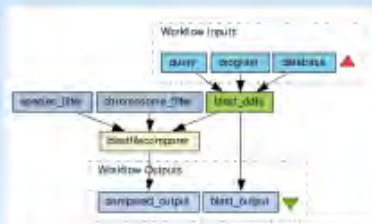
ⓘ **Credits** (0)
(People/Groups)
None

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

ⓘ **Tags** (8)

☐ **Original Uploader tags**

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

Log in to add Tags

ⓘ **Shared with Groups** (0)
None

ⓘ **Featured In Packs** (0)
None
Log in to add to one of your Packs

ⓘ **Ratings** (3)
Current:
4.7 / 5
(3 ratings)
Log in to rate and see breakdown of ratings

Popular Tags
25 tags
[All Tags]

AIDA | **benchmarks** | bio2rdf | BioAID | **bioinformatics** | BLAST | cdk-taverna | d-grid | data integration | demo | ebi | example | graph | gwes | gworkflowdl | kegg | localworker | microarray | mygrid | ondex | pathway | protein | taverna | text_mining | workflow pattern

www.myexperiment.org

www.biocatalogue.org

BioCatalogue
"The Life Science Web Services Registry"

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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

Scientist, 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 BioCatalogue project is co-developed by the University of Manchester and the EMBL-EBI.

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

Genomics (NCBI, Ensembl, UCSC,GMOD)

meets System Biology (KEGG,BIND,GO)