Apr 6th, 11:30 AM

BioTools at UMassMed

David S. Lapointe
University of Massachusetts Medical School

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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.
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

Utilities
- PrettyPlot MSF files
- Translate Nucleic Acids

Links
- BioNetbook
- CoBRA (Biostatistics)
- HSLS Online
- BioGRID
- OregAnno
- PrimerBank
- Signaling Gateway
- Bioinformatics.Org
- GeneCards

Last updated: Friday February 27, 2009

Comments and Suggestions welcome.

Research Computing/Information Services @ UMass Medical School
55 Lake Avenue N, Worcester MA 01655
BioTools

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EMBOSS-WWW
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High Performance Computing
- UmassMed HPC Wiki

UMMS only
- BioTools Message Forum
- Statistics Message Forum
- TRANSFac [info]
- TRANSCompel [info]

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## ALIGNMENT CONSENSUS

<table>
<thead>
<tr>
<th>Program name</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>cons</td>
<td>Creates a consensus from multiple alignments</td>
</tr>
<tr>
<td>megamerger</td>
<td>Merge two large overlapping nucleic acid sequences</td>
</tr>
<tr>
<td>merger</td>
<td>Merge two overlapping nucleic acid sequences</td>
</tr>
</tbody>
</table>
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Comments and Suggestions welcome.
Primer3Plus
pick primers from a DNA sequence

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:
Browse
Upload File

Mark selected region: < > [ ] {}
Clear

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).

Save Sequence
Gateways to local resources

Lists

Wikis

Tools
<table>
<thead>
<tr>
<th>Date</th>
<th>Subject</th>
<th>Replies</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>2009-03-06 12:54:59</td>
<td>FW: Funding opportunities for construction/renovation and instrumentation</td>
<td></td>
<td>Lapointe, David</td>
</tr>
<tr>
<td>2009-03-05 12:40:33</td>
<td>FW: News on the ARRA Stimulus</td>
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<td>Lapointe, David</td>
</tr>
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<td>2009-02-25 09:43:43</td>
<td>Desktop Sequence Software</td>
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<tr>
<td>2009-02-15 09:53:30</td>
<td>Re: Ingenuity Software</td>
<td>3</td>
<td>Elizabeth Luna</td>
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<tr>
<td>2009-02-05 08:57:57</td>
<td>FW: [BioC] [JOB] National Cancer Institute, Bethesda, MD</td>
<td></td>
<td>Lapointe, David</td>
</tr>
<tr>
<td>2008-11-24 17:14:33</td>
<td>Mathworks Seminar Dec 3</td>
<td></td>
<td>Lapointe, David</td>
</tr>
<tr>
<td>2008-09-08 10:48:26</td>
<td>FW: [blast-announce] New BLAST 2 Sequences Interface</td>
<td></td>
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</tr>
<tr>
<td>2008-08-27 09:55:46</td>
<td>Ingenuity Software</td>
<td>1</td>
<td>Elizabeth Luna</td>
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<tr>
<td>2008-08-12 16:16:00</td>
<td>Mathworks Seminar</td>
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<td>Lapointe, David</td>
</tr>
<tr>
<td>2008-07-28 09:54:14</td>
<td>Simulation Tools/Software from Simbios</td>
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<tr>
<td>2008-07-22 09:23:50</td>
<td>FW: [blast-announce] Primer-BLAST now available - addendum</td>
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<td>Lapointe, David</td>
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<tr>
<td>2008-06-16 22:01:10</td>
<td>FW: RECOMB Regulatory Genomics, Systems Biology, and DREAM3 2008 announcement</td>
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<tr>
<td>2008-06-10 16:27:57</td>
<td>FW: NIH Notices and Funding Opportunities</td>
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<td>Lapointe, David</td>
</tr>
<tr>
<td>2008-06-05 12:16:30</td>
<td>FW: Reminder: Webinar Invitation - Advances in GPCR Research, June 17</td>
<td></td>
<td>Lapointe, David</td>
</tr>
</tbody>
</table>
## 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.

Enter PMIDS here (one pmid /line)

12036939
1769064
2501299

or upload file with PMIDS: 1 per line

Get Refs!  Reset

Last updated: Tuesday November 18, 2008
Comments and Suggestions welcome.
References

Download zipped references


Last updated: Thursday April 02, 2009
Comments and Suggestions welcome.
Links to External resources
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<table>
<thead>
<tr>
<th>Browse COBRA by Subject</th>
<th>Peer-Reviewed Journals</th>
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<tbody>
<tr>
<td>Categorical Data Analysis (71)</td>
<td>Statistical Applications in Genetics and Molecular Biology*</td>
</tr>
<tr>
<td>Clinical Epidemiology (55)</td>
<td>The International Journal of Biostatistics*</td>
</tr>
<tr>
<td>Clinical Trials (101)</td>
<td></td>
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<tr>
<td>Computation (120)</td>
<td></td>
</tr>
<tr>
<td>Computational Biology/Bioinformatics (218)</td>
<td></td>
</tr>
<tr>
<td>Design of Experiments and Sample Surveys (49)</td>
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<tr>
<td>Disease Modeling (89)</td>
<td></td>
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<tr>
<td>Epidemiology (187)</td>
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<tr>
<td>General Biostatistics (272)</td>
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<tr>
<td>Genetics (104)</td>
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<td>Health Services Research (33)</td>
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<td>Institutional and Historical (3)</td>
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<tr>
<td>Laboratory and Basic Science Research (19)</td>
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<tr>
<td>Longitudinal Data Analysis and Time Series (140)</td>
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<tr>
<td>Medical Specialties (27)</td>
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<td>Microarrays (198)</td>
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<td>Multivariate Analysis (132)</td>
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<tr>
<td>Statistical Models (372)</td>
<td></td>
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<tr>
<td>Statistical Theory and Methods (591)</td>
<td></td>
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<tr>
<td>Survival Analysis (269)</td>
<td></td>
</tr>
<tr>
<td>Vital and Health Statistics (11)</td>
<td></td>
</tr>
</tbody>
</table>

Paper counts as of 04/02/09
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

**Search the GeneCards Human Gene Database**

<table>
<thead>
<tr>
<th>Search by:</th>
<th>Keywords</th>
<th>Gene Symbol only</th>
<th>Symbol/alias</th>
<th>GC id</th>
<th>Symbol/External Id</th>
</tr>
</thead>
<tbody>
<tr>
<td>Examples:</td>
<td>tay sachs</td>
<td>ESR1</td>
<td>FRAXA</td>
<td>OC17M03*</td>
<td>3395</td>
</tr>
<tr>
<td></td>
<td>dimerization AND diabetes</td>
<td>wnt*</td>
<td></td>
<td>7431</td>
<td></td>
</tr>
<tr>
<td></td>
<td>neurodenerative OR scone</td>
<td></td>
<td></td>
<td>P12004</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>ENSG00000185515</td>
<td></td>
</tr>
</tbody>
</table>

**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.
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.
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.

### Protein-Protein Interactions

<table>
<thead>
<tr>
<th>Protein-Protein Interactions</th>
<th>Full Record</th>
<th>Availability</th>
<th>Standards</th>
</tr>
</thead>
<tbody>
<tr>
<td>3DID - 3D interacting domains</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>ABCdb - Archaea and Bacteria ABC transporter database</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>aFCS - Alliance for Cellular Signaling Molecule Pages Database</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>AllFase - Functional Associations of Proteins in Complete Genomes</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>aMAZE - Protein Function and Biochemical Pathways Project</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>ASEDb - Alanine Scanning Energetics Database</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>ASPD - Artificial Selected Proteins/Peptides Database</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>BID - Binding Interface Database</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>BIND - Biomolecular Interaction Network Database</td>
<td>Details</td>
<td>Free</td>
<td>PSI-MI</td>
</tr>
<tr>
<td>BioGRID - General Repository for Interaction Datasets</td>
<td>Details</td>
<td>Free</td>
<td>PSI-MI</td>
</tr>
<tr>
<td>BRITE - Biomolecular Relations in Information Transmission and Expression</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>CAIIP - Pathways of the hippocampal CAI neuron</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>Cancer Cell Map - The Cancer Cell Map</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>CellCircuits - CellCircuits</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>CPDB - CconsensusPathDB</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>CSP - Cytokine Signaling Pathway Database</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
<tr>
<td>CTB - Calmodulin Target Database</td>
<td>Details</td>
<td>Free</td>
<td></td>
</tr>
</tbody>
</table>
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!

Find workflows and Web services for bioinformatics

Pathways  Search

Creator
Name: Antoon Goderis
Member since: Nov 3, 2006

Contributors
José M.  Anonymous  Franck  Duncan  Paul Fish...
Stian Sid...  Alan R Wi...

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, www.biojava.org/docs,
taverna.sourceforge.net/index.php?doc=services.html,
bioweb.pasteur.fr/docs/EMBOSS

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

Last updated: Aug 14, 2007
Add this search engine to your Google homepage
Add this search engine to your blog or webpage
Create your own Custom Search Engine

©2008 Google - Google Home - About Google - Privacy Policy
Hmm, mostly journal articles. Let see Workflows only
Refine results for **Pathways**:

- 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/115
  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/725
  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
  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

Ok This looks better
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.

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..."
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..."
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..."
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..."
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)