

Biotoools at UMassMed

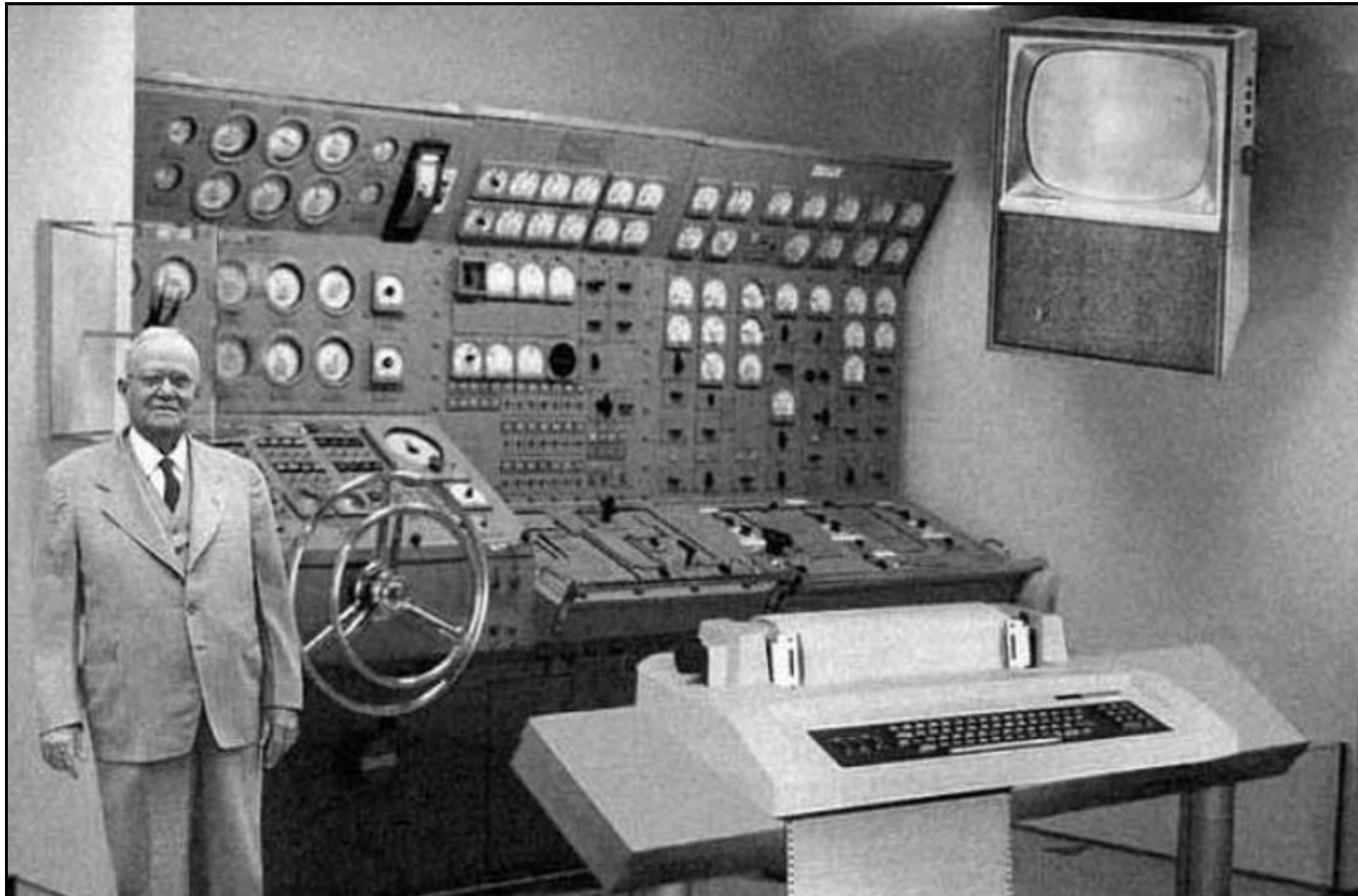
David Lapointe, Ph.D.

Director Scientific Computing

University of Massachusetts Medical School

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 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](#)
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- [PRINTS protein motifs scan](#)
- [MHC Motif Predictor **New!**](#)

Utilities

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- [CoBRA \(Biostatistics\)](#)
- [HSLs Online](#)
- [BioGRID **New!**](#)
- [OregAnno **New!**](#)
- [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 Main

Thu, Apr 02

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17:42:42

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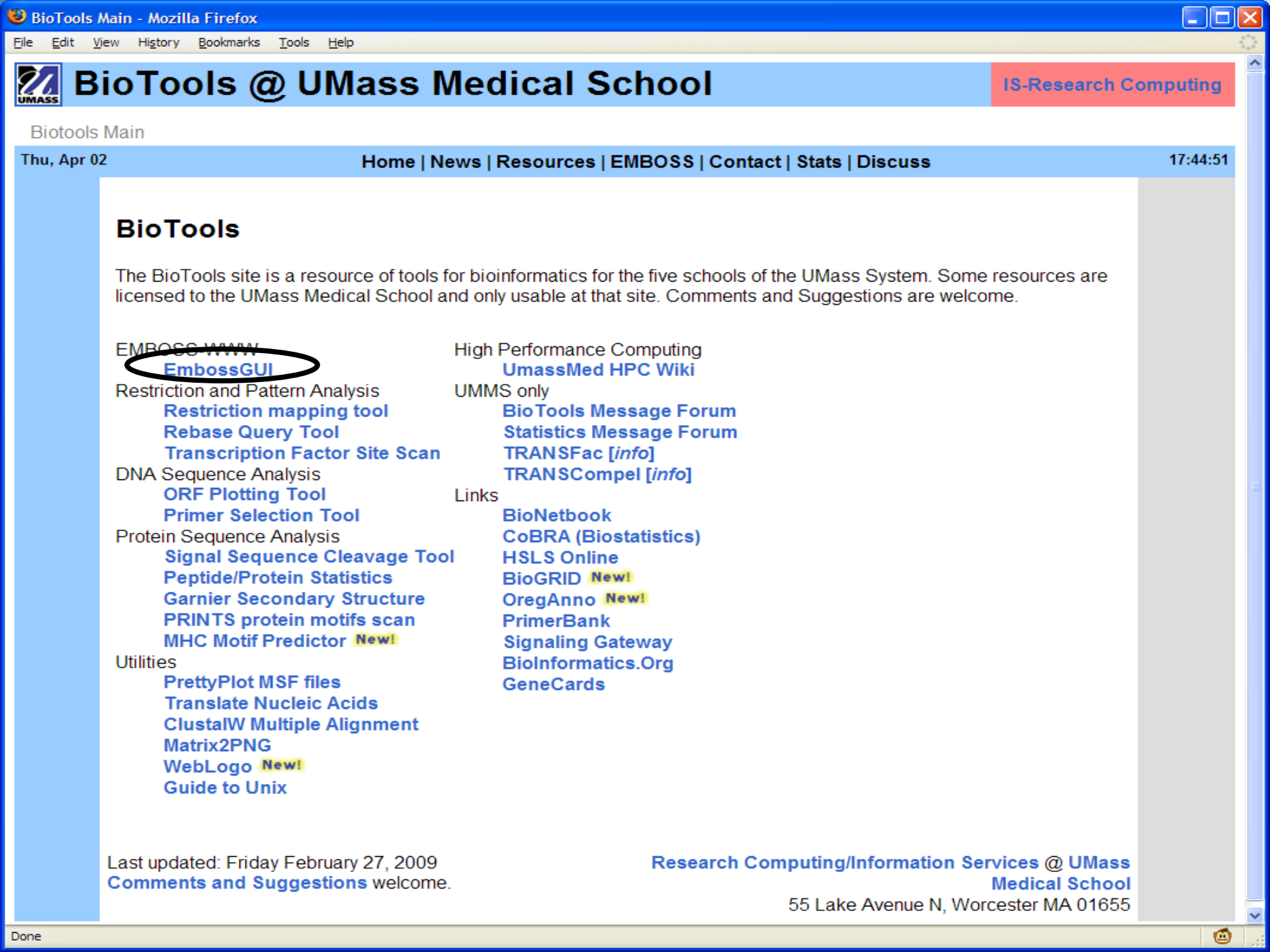
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Biotoools->EMBOSS ->All programs by group

Sun, Apr 05

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20:03:55

Select a category to locate programs by function

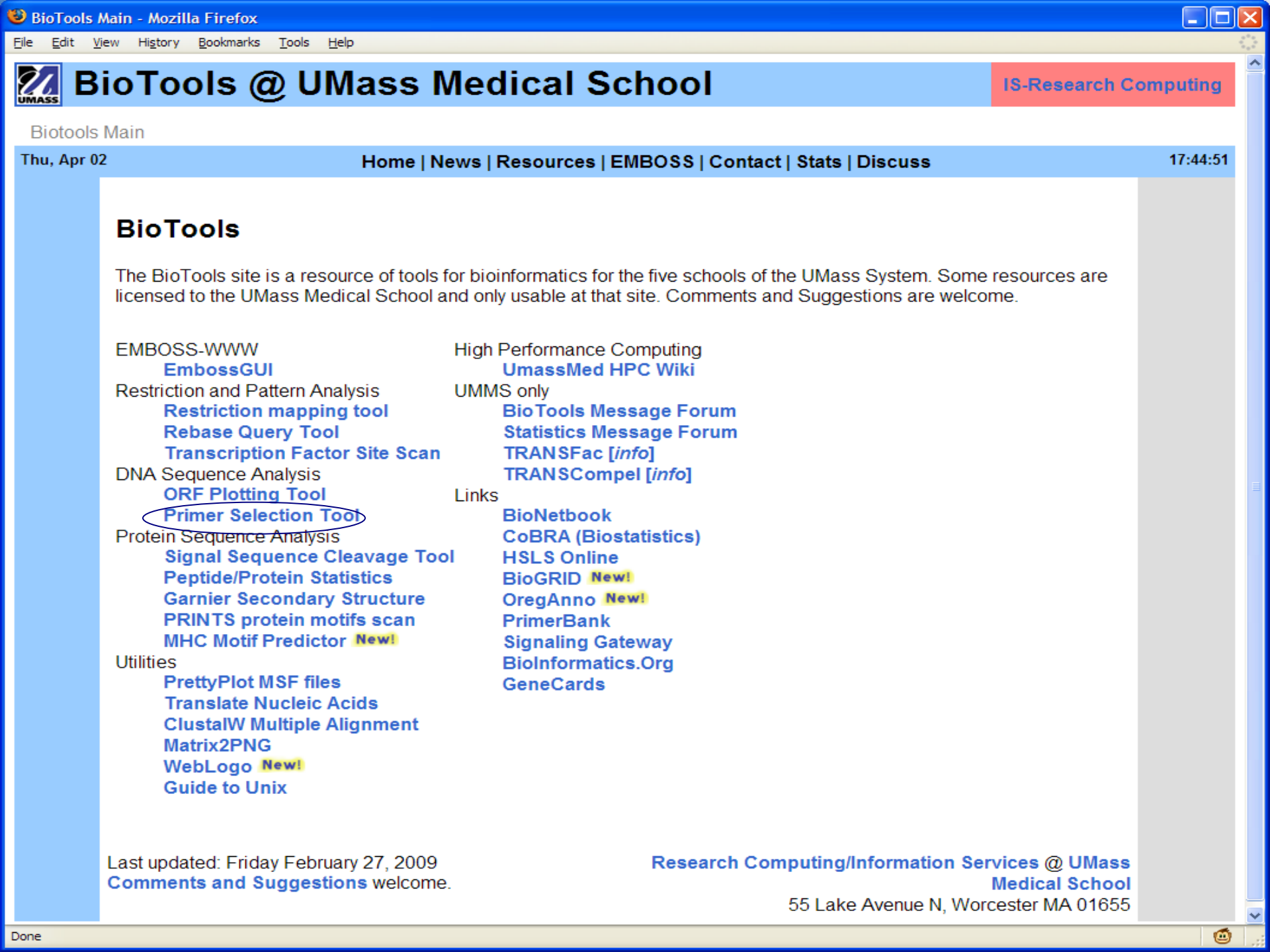
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[Alignment Differences](#)
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[Nucleic 2D Structure](#)
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[Nucleic CpG Islands](#)
[Nucleic Gene Finding](#)

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[Nucleic Profiles](#)
[Nucleic Repeats](#)
[Nucleic Restriction](#)
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[Nucleic Translation](#)
[Phylogeny](#)
[Protein 2D Structure](#)
[Protein Composition](#)
[Protein Motifs](#)
[Protein Mutation](#)
[Protein Profiles](#)

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





Biotools Main

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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.*

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).

Gateways to local resources

Lists

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LYRIS ListManager

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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	

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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.

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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

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- [HPCC](#)
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Using Clusters

- [Queues](#)
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This page was last modified on 3 March 2009, at 14:51.

This page has been accessed 585 times.

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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 Article
 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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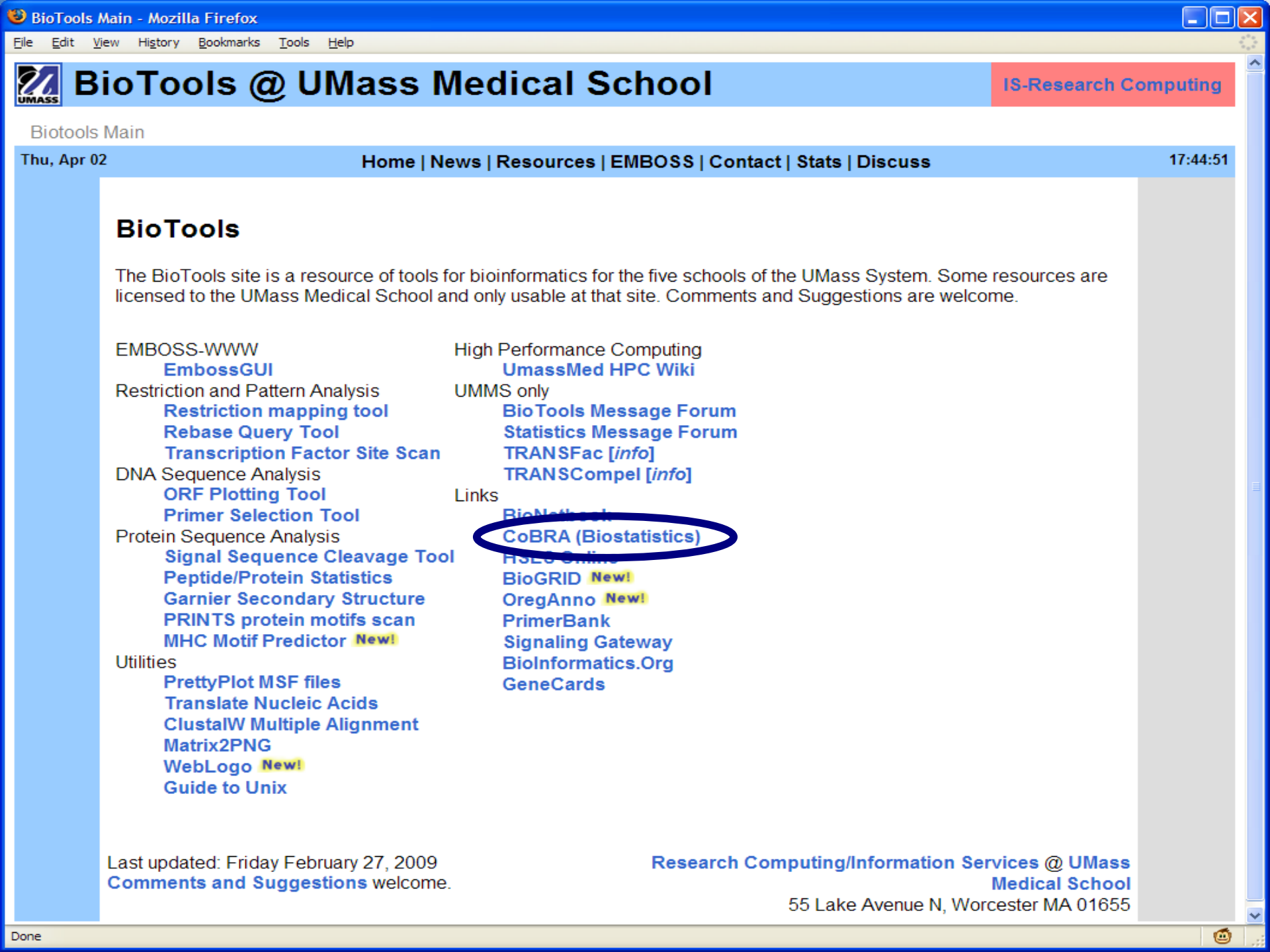
- [van der Meijden Caroline M J, Lapointe David S, Luong Mai X, Peric-Hupkes Daniel, Cho Brian, Stein Janet L, van Wijnen Andre J, Stein Gary S Gene profiling of cell cycle progression through S-phase reveals sequential expression of genes required for DNA replication and nucleosome assembly Cancer Res. 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.](#)

Last updated: Thursday April 02, 2009
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Links to External resources



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Collection of Biostatistics Research Archive

a bepress repository

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Paper counts as of 04/02/09

Peer-Reviewed Journals

[Statistical Applications in Genetics and Molecular Biology*](#)
[The International Journal of Biostatistics*](#)

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Browse COBRA by Institution

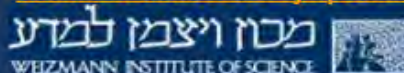
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Version 2.40 (15 Feb 2009) **New Features**



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

GeneCards Gene Database statistics

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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

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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

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Detailed Pathguide resource statistics now available

Pathguide Published
Please cite the [Pathguide Publication](#)

Protein-Protein Interactions

Database Name (Order: alphabetically) [by web popularity](#)

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!



david.lapointe@gmail.com | [My 4](#)

Find workflows and Web services for bioinformatics

Creator



Name: Antoon Goderis
Member since: Nov 3, 2006

Contributors [\[Volunteer to contribute\]](#)



José M. ...



Anonymous



Franck



Duncan



Paul Fish..



Stian Sol...



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

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Hmm, mostly journal articles. Let see Workflows only

Refine results for **Pathways**:

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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

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

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

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

Results 1 - 10 for Pathwa

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/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

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

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

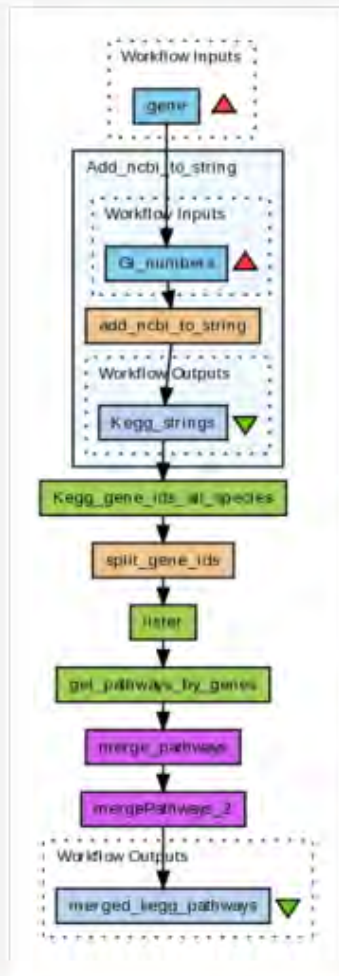
Labeled Workflows only

[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



[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.

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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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None

Featured In Packs (0)

None

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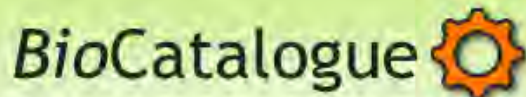
Remember me: ☐

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



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

Genomics (NCBI, Ensembl, UCSC,GMOD)

meets System Biology (KEGG,BIND,GO)