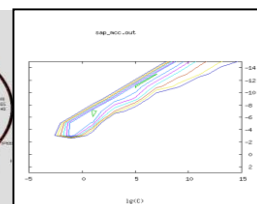
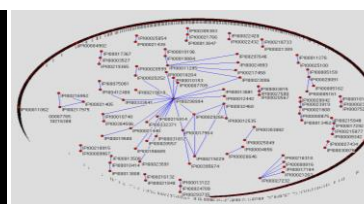
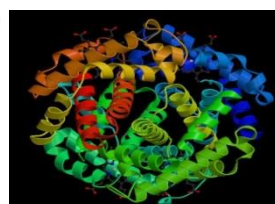
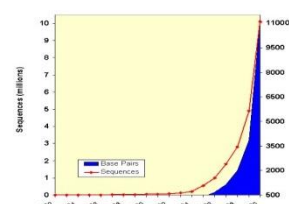
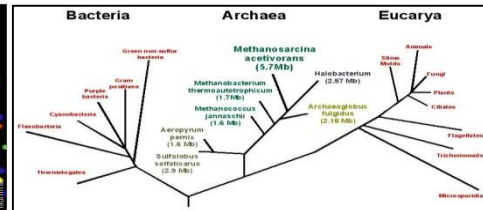


北京大学生物信息学中心 魏丽萍

Liping Wei, Ph.D.

Center for Bioinformatics, Peking University

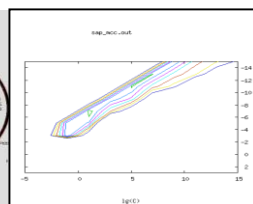
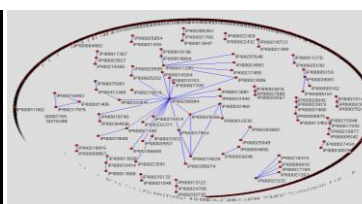
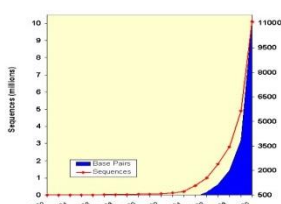





北京大学生物信息学中心 魏丽萍

Liping Wei, Ph.D.




Center for Bioinformatics, Peking University



PDB (<http://www.rcsb.org/>)




An Information Portal to Biological Macromolecular Structures

As of **Tuesday Nov 26, 2013 at 4 PM PST** there are **95839** Structures | [PDB Statistics](#) |    

Search
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Everything Author Macromolecule Sequence Ligand ?

 e.g., PDB ID, molecule name, author



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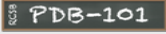
All Deposit Services



Biological Macromolecular Resource

Full Description

Learn: Featured Molecules

Structural View of Biology



 **Protein Synthesis** 



Molecule of the Month
SNARE Proteins
Small membrane-enclosed vesicles are used like cargo trucks to deliver proteins and other molecules inside and outside of cells. When these vesicles reach their proper destination, they fuse with a membrane and deliver their cargo. For instance, vesicles are used inside cells to transport digestive enzymes from the Golgi to their final location in lysosomes. They are also used to deliver molecules out of the cell: for example, neurotransmitters are released from vesicles that fuse with the cell membrane at nerve synapses. The 2013 Nobel Prize was awarded to three researchers who have revealed the central molecular machinery for this process of vesicle fusion.

Full Article



Protein Structure Initiative Featured System
Methylation of Arginine
The function of many proteins is tuned and regulated after they are synthesized by modification of key amino acids. These modifications change the chemistry of the amino acid, creating a distinctive mark that can be used as a signal or to customize interactions with other molecules. Phosphate groups, for instance, can change a serine or tyrosine into a strongly polar group, which is widely used in signaling cascades. Methyl groups, on the other hand, mask polar lysines and arginines, blocking their ability to form hydrogen bonds.

Full Article | **Archive** | **PSI Structural Biology Knowledgebase**


Explore Archive

Organism

Taxonomy


New Features Hide

Latest release: September 2013




Protein Symmetry and Stoichiometry

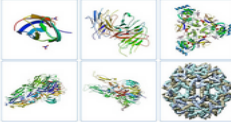
Visualize, browse & search symmetry / stoichiometry

Website Release Archive: 

RCSB PDB News Hide

Weekly |  Quarterly | Yearly

2013-11-26
Browse Membrane Transport Proteins



PDB statistics (December 2013)

Exp.Method	Proteins	Nucleic Acids	Protein/NA Complexes	Other	Total
X-RAY	79083	1496	4125	4	84708
NMR	8937	1054	197	7	10195
ELECTRON MICROSCOPY	489	51	162	0	702
HYBRID	53	3	2	1	59
other	152	4	6	13	175
Total	88714	2608	4492	25	95839

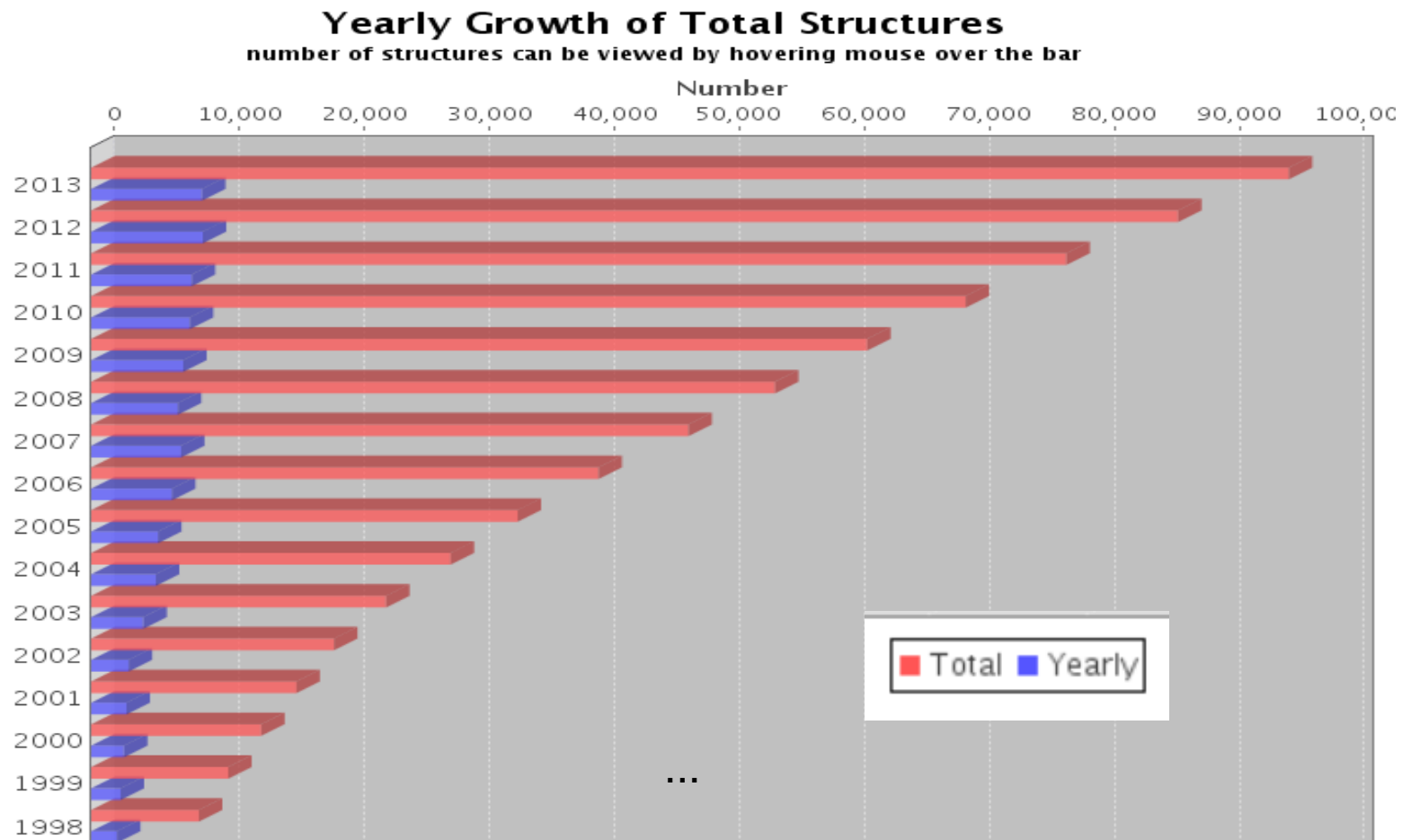





Image collected from <http://www.rcsb.org/pdb/statistics/contentGrowthChart.do?content=total&seqid=100>

Copyright © Peking University on December 1st, 2013 (UTC+0800)

SWISS-MODEL Workspace

(http://swissmodel.expasy.org/workspace/index.php?func=modelling_simple1&userid=USERID&token=TOKEN)



SWISS-MODEL Workspace

ModellingToolsRepositoryDocumentation

[myWorkspace] [login]

SwissModel Automatic Modelling Mode ?

Email:
Project Title:

Provide a protein sequence or a UniProt AC Code: ?

Submit Modelling Request

Advanced options:

Use a specific template: ?
or
Template file: ?

PDB-ID: Chain:

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SWISS-MODEL Repository

(<http://swissmodel.expasy.org/repository/?pid=smr01&zid=async>)



BIOZENTRUM
Universität Basel
The Center for Molecular Life Sciences



SWISS-MODEL Repository

[Modelling](#)[Tools](#)[Repository](#)[Documentation](#)

[\[Repository Query \]](#) [\[Full Text Query \]](#)

Welcome to the SWISS-MODEL Repository

The SWISS-MODEL Repository is a database of annotated three-dimensional comparative protein structure models generated by the fully automated homology-modelling pipeline SWISS-MODEL.

Example Queries:

[\[P23298\]](#) [\[GLDA_ECOLI\]](#) [\[IPI00743503\]](#) [\[NP_416402\]](#) [\[GI:28872740\]](#) [\[ENTREZ:54401\]](#) [\[Sequence\]](#)

List of “model organisms” regularly updated in Repository

The proteomes of the following organisms are regularly updated in SWISS-MODEL Repository. A reference proteome is the complete proteome of a representative, well-studied model organism or an organism of interest for biomedical research. **Reference proteomes** are retrieved from the UniProt database.

Organism	Taxonomy	Number of models
Human	Homo Sapiens	144435
Mouse	Mus musculus	129327
Caenorhabditis elegans	C. elegans	49205
Escherichia coli (strain K12)	E.coli K12	6814
Mouse-ear cress	A. thaliana	85066
Fruit Fly	D. melanogaster	53483
Bakers Yeast	S. cerevisiae	11199
Caulobacter crescentus	C. crescentus	6394
Mycobacterium tuberculosis	M. tuberculosis	7913
Pseudomonas aeruginosa	P. aeruginosa	9964
Staphylococcus aureus	S. aureus	3755
Plasmodium falciparum	P. falciparum	8109

Statistics based on UniProt release [2013_11](#)

I-TASSER (<http://zhanglab.ccmb.med.umich.edu/I-TASSER/>)



Zhang Lab

M UNIVERSITY OF MICHIGAN

Home

Research

Services

Publications

People

Teaching

Job Opening

Laboratory

Online Services

- I-TASSER
- QUARK
- LOMETS
- COACH
- COFACTOR
- MUSTER
- SEGMENT
- FG-MD
- ModRefiner
- REMO
- SPRING
- COTH



I-TASSER ONLINE

Protein Structure & Function Predictions

(The server completed predictions for 160966 proteins submitted by 41734 users from 113 countries)

(The template library was updated on 2013/12/06)

I-TASSER server is an on-line platform for protein structure and function predictions. 3D models are built based on multiple-threading alignments by LOMETS and iterative template fragment assembly simulations; function insights are derived by matching the 3D models with BioLiP protein function database. I-TASSER (as 'Zhang-Server') was ranked as the No 1 server for protein structure prediction in recent CASP7, CASP8, CASP9, and CASP10 experiments. It was also ranked as the best for function prediction in CASP9. The server is in active development with the goal to provide the most accurate structural and function predictions using state-of-the-art algorithms. The server is only for non-commercial use. Please report any problems and questions at I-TASSER message board and some members will study and answer the questions asap. ([>> More about the server ...](#))

[Download I-TASSER Standalone Package \(Version 2.1\)](#)

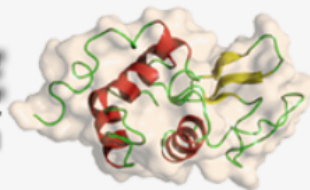
[\[Queue\]](#) [\[Forum\]](#) [\[Download\]](#) [\[Example\]](#) [\[Search\]](#) [\[Registration\]](#) [\[About\]](#) [\[Statistics\]](#) [\[Remove\]](#) [\[Potential\]](#) [\[Decoys\]](#) [\[News\]](#)

QUARK (<http://zhanglab.ccmb.med.umich.edu/QUARK/>)



QUARK ONLINE

Ab Initio Protein Structure Prediction



QUARK is a computer algorithm for ab initio protein folding and protein structure prediction, which aims to construct the correct protein 3D model from amino acid sequence only. QUARK models are built from small fragments (1-20 residues long) by replica-exchange Monte Carlo simulation under the guide of an atomic-level knowledge-based force field. QUARK was ranked as the No 1 server in Free-modeling (FM) in [CASP9](#) and [CASP10](#) experiments. Since no global template information is used in QUARK simulation, the server is suitable for proteins which are considered without homologous templates.

Go to [Job Q24927](#) to view an example of QUARK output. The description of predicted feature files can be seen in [readme.txt](#). Questions about the QUARK server can be posted at the [Service System Discussion Board](#).

Cut and paste your sequence (in [FASTA format](#), less than 200 AA. Please submit bigger proteins to [I-TASSER Server](#)):

Or upload the sequence from your local computer:

 浏览...

Email: (mandatory, where results will be sent to. Only academic email accounts are acceptable.)

ID: (optional, your given name of the protein)

Optional: You can assign additional distance restraints for modeling (example is in [distrestraint.txt](#); format is described in [readme.txt](#)).

Protein Model Portal (<http://www.proteinmodelportal.org/>)

☐ ModWeb ↗

Server Policy:

☐ By checking this box, I assert that I am part of an academic institution (not a government research lab such as NIH) and I agree with the [Modeller license](#).

☐ I have a MODELLER access key:

☐ M4T ↗

Server Policy:

☐ I am a non-profit/academic user and this server will be used solely for educational purposes or for basic research.

☐ SWISS-MODEL ↗

Server Policy:

Usage of SWISS-MODEL Server and Workspace are free of charge.

☐ I-TASSER ↗

Server Policy:

Usage of I-TASSER is free of charge.
However, there is a limitation of one job per email address and only academic email addresses are allowed.

☐ HHpred ↗

Server Policy:

Usage of HHpred is free of charge for academic use.

☐ Phyre2 ↗

Server Policy:

Usage of Phyre2 is restricted to academic users.

CASP (<http://www.predictioncenter.org/>)



Protein Structure Prediction Center



Menu

- [Home](#)
- [FORCASP Forum](#)
- [PC Login](#)
- [PC Registration](#)
- ▼ [CASP Experiments](#)
- ▼ [CASP ROLL](#)
 - [Home](#)
 - [My CASP ROLL profile](#)
- ▼ [Targets](#)
 - [Target List](#)
 - [Target Submission](#)
- [CASP11 \(2014\)](#)
- [CASP10 \(2012\)](#)
- [CASP9 \(2010\)](#)
- [CASP8 \(2008\)](#)
- [CASP7 \(2006\)](#)
- [CASP6 \(2004\)](#)
- [CASP5 \(2002\)](#)
- [CASP4 \(2000\)](#)
- [CASP3 \(1998\)](#)

Welcome to the Protein Structure Prediction Center!

Our goal is to help advance the methods of identifying protein structure from sequence. The Center has been organized to provide the means of objective testing of these methods via the process of blind prediction. The Critical Assessment of protein Structure Prediction (CASP) experiments aim at establishing the current state of the art in protein structure prediction, identifying what progress has been made, and highlighting where future effort may be most productively focused.

There have been ten previous CASP experiments. The eleventh experiment will start in May 2014. Description of these experiments and the full data (targets, predictions, interactive tables with numerical evaluation results, dynamic graphs and prediction visualization tools) can be accessed following the links:

[CASP1 \(1994\)](#) | [CASP2 \(1996\)](#) | [CASP3 \(1998\)](#) | [CASP4 \(2000\)](#) | [CASP5 \(2002\)](#) | [CASP6 \(2004\)](#) | [CASP7 \(2006\)](#) | [CASP8 \(2008\)](#) | [CASP9 \(2010\)](#) | [CASP10 \(2012\)](#) | [CASP11 \(2014\)](#)

Raw data for the experiments held so far are archived and stored in our [data archive](#).

In November 2011 we have opened a new rolling CASP experiment for all-year-round testing of ab initio modeling methods:

[CASP ROLL](#)

Details of the experiments have been published in a scientific journal *Proteins: Structure, Function and Bioinformatics*. [CASP proceedings](#) include papers describing the structure and conduct of the experiments, the numerical evaluation measures, reports from the assessment teams highlighting state of the art in different prediction categories, methods from some of the most successful prediction teams, and progress in various aspects of the modeling.

Prediction methods are assessed on the basis of the analysis of a large number of blind predictions of protein structure. Summary of numerical evaluation of the methods tested in the latest CASP experiment can be found [on this web page](#). The main numerical measures used in evaluations are described in the papers [\[1\]](#), [\[2\]](#). The latter paper also contains explanations of data handling procedures and guidelines for navigating the data presented on this website.

Message Board

Resuming CASP ROLL

[Dear CASPers, Best regards for all of you in the New Year! Hoping that you had good rest after the CASP10 experiment and meeting, we are resuming CASP ROLL with two new targets later this week. ...](#)

Predictors meeting in Gaeta

[Dear CASP10 Participants, On the last day of the Meeting we will have our regular Predictors get-together. In advance, I would like to ask you to send in any comments regarding the CASP process in ...](#)

Release of CASP10 results

[Dear CASP10 Predictors, We have released results of the CASP10 and CASP ROLL experiments. You can check now interactive results tables](#)

CASP10: Top servers for template-based modeling

035s	Zhang Server
114s	QUARK
108s	PMS
370s	HHpred-thread
122s	RaptorX-ZY
330s	BAKER-ROSETTASERVER
430s	HHpredA
223s	HHPredAO
486s	RaptorX
424s	MULTICOM-NOVEL

CASP10: Top servers for free modeling

			Target																		
Group name	Group ID	#Top Hits	T0651-D0	T0653-D1	T0658-D1	T0663-D0	T0666-D1	T0684-D2	T0690-D0	T0693-D1	T0695-D1	T0713-D0	T0719-D6	T0726-D3	T0734-D1	T0735-D2	T0737-D1	T0739-D1	T0739-D2	T0740-D1	T0741-D1
keasar	315	4																			
QUARK	114 s	3																			
Pcons	267	3																			
Zhang-Server	035 s	2																			
Zhang_Ab_Initio	45	2																			
TASSER	79	2																			
Pcomb	130	2																			
TsaiLab	201	2																			
ProQ2	388	2																			
Mufold2	405	2																			
PconsQ	428	2																			
CNIO	475	2																			

- Group name and ID in blue are **servers**.

- Target name in gray are their best models from one of the servers.

best model

submitted model

no submission

modENCODE (<http://www.modencode.org/>)



The National Human Genome Research Institute
model organism **ENC**yclopedia Of DNA Elements



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“The modENCODE Project will try to identify all of the sequence-based functional elements in the *Caenorhabditis elegans* and *Drosophila melanogaster* genomes.”

modMine

Release #32

amazon

Instance

Dataset

FTP

Upload your list of fly genes and view an expression score heatmap.



[Networks](#)



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The entire modENCODE data set available for analysis in the Amazon compute cloud.

Find, view and download datasets in bulk.

Download released data using the traditional FTP interface.

Choose an organism below to see GBrowse, Dataset Search links:



C. elegans



C. brenneri



C. briggsae



C. japonica



C. remanei



D. melanogaster



D. ananassae



D. mojavensis



D. pseudoobscura



D. simulans



D. virilis



D. yakuba

Rfam (<http://rfam.sanger.ac.uk>)



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Please note: this site relies heavily on the use of javascript. Without a javascript-enabled browser, this site will not function correctly. Please enable javascript and reload the page, or switch to a different browser.

Rfam 11.0 (August 2012, 2208 families)

The Rfam database is a collection of RNA families, each represented by **multiple sequence alignments**, **consensus secondary structures** and **covariance models (CMs)**. [More...](#)

QUICK LINKS

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YOU CAN FIND DATA IN RFAM IN VARIOUS WAYS...

Analyze your RNA sequence for Rfam matches

View Rfam family annotation and alignments

View Rfam clan details

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Fetch families or sequences by NCBI taxonomy

Enter any type of accession or ID to jump to the page for a Rfam family, sequence or genome

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Citing Rfam

If you find Rfam useful, please consider [citing](#) the references that describe this work:

Rfam 11.0: 10 years of RNA families. S.W. Burge, J. Daub, R. Eberhardt, J. Tate, L. Barquist, E.P. Nawrocki, S.R. Eddy, P.P. Gardner, A. Bateman.

Nucleic Acids Research (2012) doi: 10.1093/nar/gks1005

Mirrors

The following are official Rfam [mirror](#) sites:

[WTSI, UK](#)

[JFRC, USA](#)

Screenshot made at <http://rfam.sanger.ac.uk/> on December 1st, 2013 (UTC+0800)

PlantTFDB (<http://planttfdb.cbi.pku.edu.cn/>)



Plant Transcription Factor Database

v3.0

Center for Bioinformatics, Peking University, China

Previous versions: v1.0 v2.0

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Search (eg: LFY)

Browse by Species

[open all](#) | [close all](#)


Taxonomic Group (83 species) (G)-species with genome sequence

- ☐ Chlorophyta (10 species)
- ☐ Bryophyta (1 species)
- ☐ Lycopodiophyta (1 species)
- ☐ Coniferopsida (4 species)
- ☐ Basal Magnoliophyta (1 species)
- ☐ Monocot (17 species)
- ☐ Eudicot (49 species)

Browse by Family

AP2 (1776)	ARF (1914)	ARR-B (914)	B3 (4051)	BBR-BPC (492)	BES1 (651)
----------------------------	----------------------------	-----------------------------	---------------------------	-------------------------------	----------------------------

SOAPdenovo (<http://soap.genomics.org.cn/soapdenovo.html>)

**Short Oligonucleotide
Analysis Package**

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SOAPdenovo

[Introduction](#) [System requirements](#) [Download](#) [Installation](#) [Command Line Options](#) [FAQ](#)

Feedback:
soap@genomics.org.cn

Introduction

SOAPdenovo is a novel short-read assembly method that can build a de novo draft assembly for the human-sized genomes. The program is specially designed to assemble Illumina GA short reads. It creates new opportunities for building reference sequences and carrying out accurate analyses of unexplored genomes in a cost effective way. Now the new version is available. SOAPdenovo2, which has the advantage of a new algorithm design that reduces memory consumption in graph construction, resolves more repeat regions in contig assembly, increases coverage and length in scaffold construction, improves gap closing, and optimizes for large genome.

System requirements

SOAPdenovo aims for large plant and animal genomes, although it also works well on bacteria and fungi genomes. It runs on 64-bit Linux system with a minimum of 5G physical memory. For big genomes like human, about 150 GB memory would be required.

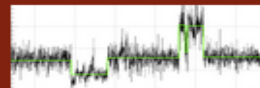
Download

The executable program and source code are now available on SourceForge:

CNVnator (<http://sv.gersteinlab.org/cnvnator/>)

Genome Structural Variations

portal for genome SV research in the [Gerstein Lab](#)



Structural Variations (SVs) and Copy Number Variations (CNVs) are a major source of genomic variation. However, compared to SNPs, accurate detection, genotyping and understanding of CNVs is lagging behind due to much greater analytical challenges related to SV/CNV detection and analysis. In our lab we analyse SVs/CNVs using high-throughput sequencing and different analytical approaches. Related tools, databases and publications are listed below.

TOOLS

PAPERS

vcf2diploid	personal genome constructor, it can be used to construct a personal diploid genome sequence by including personal variants into reference genome.	2011
CNVnator	a tool for CNV discovery and genotyping from depth of read mapping.	2011a, 2011b
AGE	a tools that implements an algorithm for optimal alignment of sequences with SVs.	2011
BreakSeq	a pipeline for annotation, classification and analysis of SVs at single nucleotide resolution.	2010
PEMer	a computational and simulation framework for discovering SVs by paired-end read mapping.	2009, 2007

DATABASES AND DATASETS

PAPERS

BreakSeq	The database contains information about breakpoints of SVs at single nucleotide level. The information has been gathered from literature.	2010
Break-DB	The database contains information about SVs and associated breakpoints detected by PEMer .	2009

WEB SUPPLEMENTS

Supplement to	Nucleotide-resolution analysis of structural variants using BreakSeq and a breakpoint library. Nat Biotechnol. 2010 Jan;28(1):47-55. Epub 2009 Dec 27.
Supplement to	Paired-End Mapping Reveals Extensive Structural Variation in the Human Genome. Science. 2007 Oct 19;318(5849):420-6. Epub 2007 Sep 27.

PAPERS


[Click here](#) for a complete list of SV-related papers published in our group. Individual references to some of these have also been provided above.

©2011 Mark Gerstein.

Screenshot made at <http://sv.gersteinlab.org/> (upper figure) on December 1st, 2013 (UTC+0800)

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Bioconductor (<http://bioconductor.org/>)



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OPEN SOURCE SOFTWARE FOR BIOINFORMATICS

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About Bioconductor

Bioconductor provides tools for the analysis and comprehension of high-throughput genomic data. Bioconductor uses the R statistical programming language, and is open source and open development. It has two releases each year, [749 software packages](#), and an active user community. Bioconductor is also available as an [Amazon Machine Image \(AMI\)](#).

Use Bioconductor for...

- ➔ **Microarrays**
Import Affymetrix, Illumina, Nimblegen, Agilent, and other platforms. Perform quality assessment, normalization, differential expression, clustering, classification, gene set enrichment, genetical genomics and other workflows for expression, exon, copy number, SNP, methylation and other assays. Access GEO, ArrayExpress, Biomart, UCSC, and other community resources.
- ➔ **High Throughput Assays**
Import, transform, edit, analyze and visualize flow cytometric, mass spec, HTqPCR, cell-based, and other assays.
- ➔ **Recent Courses**
Explore material from recent courses, including [BioC2013](#), [useR! 2013](#), [CSAMA 2013](#), [Intermediate R / Bioconductor for High Throughput Sequence Analysis](#).
- ➔ **Variants**
Read and write VCF files. Identify structural location of variants and compute amino acid coding changes for non-synonymous variants. Use SIFT and PolyPhen database packages to predict consequence of amino acid coding changes.

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30 July - 01 August 2014 — Boston, USA

[Bioconductor European Developers' Workshop](#)
09 - 10 December 2013 — Cambridge, UK

[Next Generation Data Analysis](#)
12 - 16 December 2013 — Riverside, CA, USA

[Summer Bioinformatics Course](#)

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BioPerl (<http://bioperl.org/>)



BioPerl

Main Links

Main Page

Getting Started

Downloads

Installation

Recent changes

Random page

documentation

Quick Start

FAQ

HOWTOs

API Docs

Scrapbook

Tutorials

Deobfuscator

Browse Modules

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News

Mailing lists

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Main Page

Welcome to BioPerl, a community effort to produce Perl code which is useful in biology.

For more background on the BioPerl project please see the [History of BioPerl](#).

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Installation	Documentation	Support
<ul style="list-style-type: none">LinuxWindowsMac OSXUbuntu ServerFreeBSDFedora	<ul style="list-style-type: none">API Docs and BioPerl docs HOWTOScrapbookThe (in)famous Deobfuscator 	<ul style="list-style-type: none">FAQIRC : #bioperl Webchat Mailing listsSearch mail list archives BioPerl Media options
Developers	How Do I...?	BioPerl-related Distributions
<ul style="list-style-type: none">Using GitAdvanced BioPerlThe SeqIO ModulesFeatures and Annotations in BioPerlWriting BioPerl TestsBioPerl Best PracticesBrowse the Core ModulesBugs	<ul style="list-style-type: none">...install BioPerl?...find a nice, readable BioPerl overview?...get help?...learn Perl?...read a sequence file?...parse a BLAST/FASTA search?...get genomic sequences and coordinates?...query GenBank sequence/annotations?...contribute code to BioPerl?...submit a bug report?...see open BioPerl bugs? 	<ul style="list-style-type: none">CoreBioSQL adaptors (BioPerl-DB)BioPerl-Run wrappersNetwork analysis (BioPerl-Network)Bio::Graphics BioPerl-PedigreeGbrowse

- BioPerl v.1.6.910 released
- Travis-CI for Testing
- BioPerl-DB, BioPerl-Run, BioPerl-Network 1.6.9 released
- BioPerl 1.6.9 released
- OBF and Google Summer of Code 2011
- Introduction of OpenID logins for OBF wikis
- OBF Redmine server now available
- BioPerl has moved to GitHub
- OIBIF Google Summer of Code Accepted Students
- OIBIF in Google Summer of Code

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Screenshot made at http://bioperl.org/wiki/Main_Page on December 1st, 2013 (UTC+0800)

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Biopython

Introduction

Biopython is a set of freely available tools for biological computation written in [Python](#) by an international team of developers.

It is a distributed collaborative effort to develop Python libraries and applications which address the needs of current and future work in bioinformatics. The source code is made available under the [Biopython License](#), which is extremely liberal and compatible with almost every license in the world. We work along with the [Open Bioinformatics Foundation](#), who generously host our website, bug tracker, and mailing lists.

This wiki will help you download and install Biopython, and start using the libraries and tools.

Get Started

- [Download Biopython](#)
- [Installation help](#) (PDF)

Get help

- [Tutorial](#) (PDF)
- [Documentation on this wiki](#)
- [Cookbook \(working examples\)](#)
- [Discuss and ask questions](#)

Contribute

- [What's being worked on](#)
- [Developing on Github](#)
- [Google Summer of Code](#)
- [Report bugs](#) (older issues)

- [Biopython 1.63 beta released](#)
- [Biopython 1.62 released](#)
- [Biopython 1.61 released](#)
- [Travis-CI for Testing](#)
- [Biopython 1.60 released](#)
- [Students selected for GSoC](#)
- [Cross-links in GenomeDiagram](#)
- [Biopython 1.59 released](#)
- [Chromosome Diagrams in Biopython](#)
- [Biopython 1.58 released](#)

See also our [news page](#), and [twitter](#).

The latest release is [Biopython 1.62](#), released on 28 August 2013. A beta version of 1.63 is also available.

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Navigation

[Main Page](#)
[Downloads](#)
[Mailing lists](#)
[Documentation](#)
[Cookbook](#)
[News](#)
[Source Code](#)
[New issue tracker](#)
[Old issue tracker](#)
[Buildbot Tests](#)
[Participants](#)
[Script Central](#)
[Recent changes](#)
[Random page](#)

Toolbox

[What links here](#)
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[Special pages](#)
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