

Bioinformatics Tools	Version	Description
AutoDock	4.2	AutoDock is a suite of automated docking tools. It is designed to predict how small molecules, such as substrates or drug candidates, bind to a receptor of known 3D structure.
AutoDock Vina	1.1.1	AutoDock Vina is a new open-source program for drug discovery, molecular docking and virtual screening, offering multi-core capability, high performance and enhanced accuracy and ease of use.
Avogadro	1.0.0	An advanced molecular editor designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas, which offers flexible rendering and a powerful plugin architecture.
NCBI-Blast	2.2.23+	The NCBI Basic Local Alignment Search Tool (BLAST) finds regions of local similarity between sequences. The program compares nucleotide or protein sequences to sequence databases and calculates the statistical significance of matches. BLAST can be used to infer functional and evolutionary relationships between sequences as well as help identify members of gene families.
Chemtool	1.6.12	Chemtool is a program for drawing organic molecules easily and store them in a variety of output formats including as a X bitmap, Xfig, SVG or EPS file. It runs under the X Window System using the GTK widget set.
ClustalX	2.0	ClustalX is a windows interface for the ClustalW multiple sequence alignment program. It provides an integrated environment for performing multiple sequence and profile alignments and analyzing the results. The sequence alignment is displayed in a window on the screen. A versatile coloring scheme has been incorporated allowing you to highlight conserved features in the alignment. The pull-down menus at the top of the window allow you to select all the options required for traditional multiple sequence and profile alignment.
EMBOSS	6.1.0	EMBOSS is a new, free Open Source software analysis package specially developed for the needs of the molecular biology (e.g. EMBnet) user community. The software automatically copes with data in a variety of formats and even allows transparent retrieval of sequence data from the web. Also, as extensive libraries are provided with the package, it is a platform to allow other scientists to develop and release software in true open source spirit. EMBOSS also integrates a range of currently available packages and tools for sequence analysis into a seamless whole.
Glimmer	3.02	Glimmer is a system for finding genes in microbial DNA, especially the genomes of bacteria, archaea, and viruses. Glimmer (Gene Locator and Interpolated Markov ModelER) uses interpolated Markov models (IMMs) to identify the coding regions and distinguish them from noncoding DNA.

GROMACS	4.0.7	GROMACS is a versatile and extremely well optimized package to perform molecular dynamics computer simulations and subsequent trajectory analysis. It is developed for biomolecules like proteins, but the extremely high performance means it is used also in several other fields like polymer chemistry and solid state physics.
GROMACS - Open MPI	1.4.3	Open MPI is an open source, freely available implementation of both the MPI-1 and MPI-2 standards, combining technologies and resources from several other projects (FT-MPI, LA-MPI, LAM/MPI, and PACX-MPI) in order to build the best MPI library available. A completely new MPI-2 compliant implementation, Open MPI offers advantages for system and software vendors, application developers, and computer science researchers.
HMMER	2.3.2	Profile hidden Markov models (profile HMMs) can be used to do sensitive database searching using statistical descriptions of a sequence family's consensus. HMMER is a freely distributable implementation of profile HMM software for protein sequence analysis.
InPACdb	1.0	InPACdb is a database of known anticancer compounds from plants of Indian origin
Jackal	1.5	Jackal is a collection of programs designed for the modeling and analysis of protein structures. Its core program is a versatile homology modeling package nest.
Jmol	11.8.26	Jmol is a free, open source molecule viewer for students, educators, and researchers in chemistry and biochemistry.
Mgltools *	1.5.4	MGL tools for Autodock
MODELLER *#	9v8	MODELLER is used for homology or comparative modeling of protein three-dimensional structures. The user provides an alignment of a sequence to be modeled with known related structures and MODELLER automatically calculates a model containing all non-hydrogen atoms. MODELLER implements comparative protein structure modeling by satisfaction of spatial restraints and can perform many additional tasks, including de novo modeling of loops in protein structures, optimization of various models of protein structure with respect to a flexibly defined objective function, multiple alignment of protein sequences and/or structures, clustering, searching of sequence databases, comparison of protein structures, etc.
NCBI genome workbench	2.1.1	NCBI Genome Workbench is an integrated application for viewing and analyzing sequence data. With Genome Workbench, you can view data in publically available sequence databases at NCBI, and mix this data with your own private data. Genome Workbench can display sequence data in many ways, including

		graphical sequence views, various alignment views, phylogenetic tree views, and tabular views of data. It can also align your private data to data in public databases, display your data in the context of public data, and retrieve BLAST results.
Open Babel	2.2.3	Babel is composed of two major parts: <ul style="list-style-type: none"> * tools to build and work with get text message catalogs * a Python interface to the CLDR (Common Locale Data Repository), providing access to various locale display names, localized number and date formatting, etc.
PatchDock	2.0	PatchDock is an algorithm for molecular docking. The input is two molecules of any type: proteins, DNA, peptides, drugs. The output is a list of potential complexes sorted by shape complementarity criteria.
PHYLIP	3.6b	The PHYLIP programs in this EMBASSY package are ported from release 3.572.
PyMol	1.2	PyMol is a molecular graphics system with an embedded Python interpreter designed for real-time visualization and rapid generation of high-quality molecular graphics images and animations. It is fully extensible and available free to everyone via the "Python" license. Although a newcomer to the field, PyMOL can already be used to generate stunning images and animations with ease. It can also perform many other valuable tasks (such as editing PDB files) to assist you in your research.
PyRx	0.7	PyRx A virtual screening add-on which uses AutoDock
Python Molecular Viewing*	1.5.4	Python-based Molecular Viewing Environment (PMV) is a general purpose viewer that can be integrated into any computational chemistry package available in Python.
R-Bioconductor	2.11.1	Bioconductor is a free, open source and open development software project for the analysis and comprehension of genomic data generated by wet lab experiments in molecular biology.
Raccoon	1.0	Raccoon, a virtual screening add-on which uses AutoDock
Seaview Multiple Sequence Alignment	4.0	SeaView is a graphical multiple sequence alignment editor developed by Manolo Gouy. SeaView is able to read and write various alignment formats (NEXUS,SF, CLUSTAL, FASTA, PHYLIP, MASE). It allows to manually edit the alignment, and also to run DOT-PLOT or CLUSTALW/MUSCLE programs to locally improve the alignment.
Swiss-PdbViewer	4.0.1	Swiss-PdbViewer (aka DeepView) is a visualization tool that provides a user friendly interface allowing to analyze several proteins at the same time.

Unipro UGENE	1.7.2	Unipro UGENE is a cross-platform visual environment for DNA and protein sequence analysis. UGENE integrates the most important bioinformatics computational algorithms and provides an easy-to-use GUI for performing complex analysis of the genomic data. One of the main features of UGENE is a designer for custom bioinformatics workflows.
Visual Molecular Dynamics (VMD)*	1.8.7	VMD is a molecular modelling and visualization computer program. VMD is primarily developed as a tool for viewing and analyzing the results of molecular dynamics simulations, but it also includes tools for working with volumetric data, sequence data, and arbitrary graphics objects.

GUI enabled Tools		
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Compilers		
C	4.4.4	The gcc package contains the GNU Compiler Collection version 4.4. You'll need this package in order to compile C code.
C++	4.4.4	This package adds C++ support to the GNU Compiler Collection. It includes support for most of the current C++ specification, including templates and exception handling.
Java	4.4.4	This package adds support for compiling Java(tm) programs and bytecode into native code.

Perl	5.10.0	Perl is a high-level programming language with roots in C, sed, awk and shell scripting. Perl is good at handling processes and files, and is especially good at handling text. Perl's hallmarks are practicality and efficiency. While it is used to do a lot of different things, Perl's most common applications are system administration utilities and web programming. A large proportion of the CGI scripts on the web are written in Perl. You need the perl package installed on your system so that your system can handle Perl scripts.
Python	2.6.2	Python is an interpreted, interactive, object-oriented programming language often compared to Tcl, Perl, Scheme or Java. Python includes modules, classes, exceptions, very high level dynamic data types and dynamic typing. A Python support interfaces to many system calls and libraries, as well as to various windowing systems (X11, Motif, Tk, Mac and MFC).
Bioperl	1.6.12	BioPerl is a toolkit of Perl modules useful in building bioinformatics solutions in Perl. It is built in an object-oriented manner so that many modules depend on each other to achieve a task.
Biopython	1.54	A set of freely available Python tools for computational molecular biology.

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