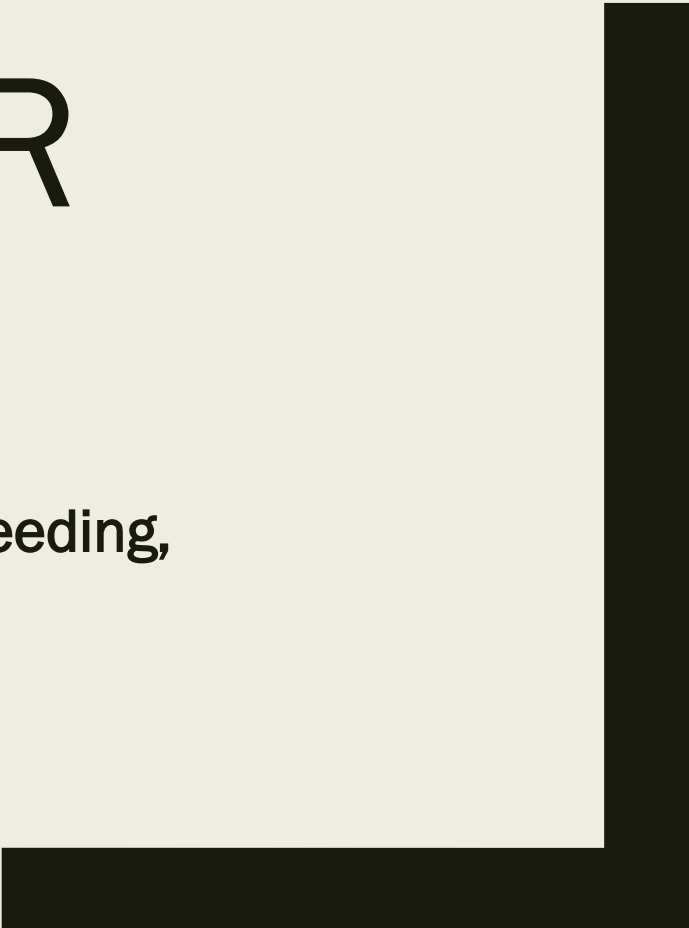




MOLECULAR DOCKING

Bioinformatics approaches in animal breeding,
Summer School, Zagreb, 2025



Molecular Docking with AutoDock Vina

Download softwares:

- Pearl: <https://padre.perlide.org/download.html>
- MGL Tools: <https://ccsb.scripps.edu/mgltools/downloads/>
- OpenBabel GUI: <https://github.com/openbabel/openbabel/releases>
- AutoDock Vina: <https://bioinfo2025.splet.arnes.si/things-to-do-before-summer-school/>
 - *.zip file on the official website of summer school*
- ChimeraX: <https://www.cgl.ucsf.edu/chimerax/download.html>

Pearl

<https://padre.perlide.org/download.html>



Download Padre, the Perl IDE

Ready made packages of Padre for Windows, Linux and Mac OS X.

[Home](#) [Screenshots](#) [Documentation](#) [Support / Contact us](#) [Get Involved](#) [People](#) [About](#)   

Mobiplus

 **prenesite svojo vsebino** [DOWNLOAD >](#)

Windows



Download **DWIM Perl 5.14.2.1 (v7)**.

Released on 12 Feb 2012, the DWIM Perl for Windows package contains

- Strawberry Perl 5.14.2.1
- Padre 0.94
- Padre::Plugin::PerlCritic,
- Padre::Plugin::PerlTidy
- Moose
- DBD::mysql, DBD::Pg, DBD::SQLite
- DBD::ODBC
- DBIx::Class
- Try::Tiny
- Dancer
- Plack
- Task::Kensho (partially)
- Spreadsheet reader and writer modules
- Win32::GUI::Test
- Template::Toolkit
- ... a lot more CPAN modules ...
- see [DWIM Perl for Windows](#) for further details.

Download from here:

- [dwimperl-5.14.2.1-v7-32bit.exe](#)

Download size: 47 Mb. After installation it takes up 300 MB.

Linux



[Ubuntu 10.10](#)

```
sudo apt-get install padre
wget http://www.eekboek.nl/repo/ubuntu_10.10/libwx-perl_0.9702-1_i386.deb
sudo dpkg --install libwx-perl_0.9702-1_i386.deb
```

[Ubuntu 9.10 till 10.04](#)

```
sudo apt-get install padre
```

[Fedora 11 and later](#)

```
yum install perl-Padre
```

[Mandriva 2009.0 and later](#)

```
urpmi perl-Padre
```

[Debian 6.0 \(squeeze\)](#)

```
aptitude install padre
```

[Other Linux and *BSD](#)

For installation on other Linux distributions and *BSD, please look at the [detailed installation instructions](#).

MGL Tools

<https://ccsb.scripps.edu/mgltools/downloads/>

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MGLTools

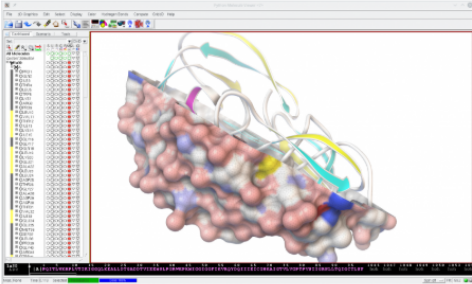
Patched Versions for 1.5.7 and 1.5.6



Oct 29 2022

- Supersedes latest stable for version 1.5.6 and 1.5.7
- Dynamic determination of installation folder at runtime, allowing an installation tree to be moved and still work
- Python interpreter in bin folder of installation is now called MGLPython<\$PyVersion> to avoid interference with system python
- pythonsh and other scripts in bin folder of installation set PYTHONPATH to avoid importing packages from user site-packages such as ~/local/lib/pythonX.Y/site-packages




Nov 2 2022

- Bug fix in BRIX parser of the Volume package, in calculation of grid spacing variables



platform	installer
 1.5.7	mgltools_Linux-x86_64_1.5.7.tar.gz Patch 1 (Linux 64 tarball installer 125Mb)
 1.5.6	mgltools_x86_64Linux2_1.5.6.tar.gz Patch 1 (Linux 64 tarball installer 68Mb)

Version 1.5.7

platform	installer
	mgltools_win32_1.5.7_Setup.exe (80Mb)
	mgltools-1.5.7-MacOS-X-Install.dmg (GUI installer 91Mb)
	mgltools_1.5.7_MacOS-X.tar.gz (tarball installer 85Mb)

```

AutoDockTools-1.5.7

C:\Users\atansek>set BABEL_DATADIR=C:\Program Files (x86)\MGLTools-1.5.7\OpenBabel-2.3.2\data

C:\Users\atansek>set path=C:\Program Files (x86)\MGLTools-1.5.7\OpenBabel-2.3.2;C:\Windows\system32;C:\Windows;C:\Windows\System32\Wbem;C:\Windows\System32\WindowsPowerShell\v1.0\;C:\Windows\System32\OpenSSH\;C:\Program Files\MEGA11;C:\Program Files\Pandoc\;C:\Program Files\Microsoft VS Code\bin;C:\Dwimper1\perl\bin;C:\Dwimper1\perl\site\bin;C:\Dwimper1\c\bin;;C:\Program Files (x86)\MGLTools-1.5.7;C:\Program Files\OpenBabel-3.1.1;C:\Program Files\MySQL\MySQL Shell 8.0\bin\;C:\Users\atansek\AppData\Local\Microsoft\WindowsApps

C:\Users\atansek>"C:\Program Files (x86)\MGLTools-1.5.7\python.exe" "C:\Program Files (x86)\MGLTools-1.5.7\lib\site-packages\AutoDockTools\bin\runAdt.py"
Run ADT from C:\Program Files (x86)\MGLTools-1.5.7\lib\site-packages\AutoDockTools
MSMSLIB 1.4.4 started on Local PC
Copyright M.F. Sanner (March 2000)
Compilation flags

```

74 AutoDockTools

File 3D Graphics Edit Select Display Color Hydrogen Bonds Compute Grid3D Help

ADT4.2 Ligand Flexible Residues Grid Docking Run Analyze

Dashboard Scenario Tools

Sel.: CMD

	S	L	B	C	RMS	L	CI
All Molecules	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Current Selection	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>

Mod.: None Time: 1.061 Selected: 0 Atom(s) Done 100% Spin off FR: 333.3

OpenBabel GUI

<https://github.com/openbabel/openbabel/releases>

openbabel / openbabelPublic

SponsorNotificationsFork 442Star 1.2k

<> CodeIssues 650Pull requests 52ActionsProjectsWikiSecurityInsights

ReleasesTags

Find a release

May 8, 2020

ghutchis

openbabel-3-...cbd4db4

Compare

Open Babel 3.1.1Latest

This version primarily reflects fixes for packaging on Linux and FreeBSD relative to 3.1.0. No features or significant bug fixes were involved.

Assets5

openbabel-3.1.1-source.tar.bz2	26.5 MB	May 8, 2020
OpenBabel-3.1.1-x64.exe	36.9 MB	May 17, 2020
OpenBabel-3.1.1.exe	35.8 MB	May 17, 2020
Source code (zip)		May 8, 2020
Source code (tar.gz)		May 8, 2020

3441633

47 people reacted

---- INPUT FORMAT ----

sdf -- MDL MOL format

☐ Use this format for all input files (ignore file extensions)

C:\Users\atansek\Downloads\

☐ Input below (ignore input file)

CONVERT

---- OUTPUT FORMAT ----

pdbqt -- AutoDock



Output file

☐ Output below only (no ou Start import at molecule # specified End import at molecule # specified☐ Continue with next object after error, if possible☐ Compress the output with gzip☐ Decompress the input with gzip☐ Attempt to translate keywords☐ Delete hydrogens (make implicit)☐ Add hydrogens (make explicit) Add hydrogens appropriate for this pH☐ Convert dative bonds e.g. [N+](O-)=O to -N(=O)=O☐ Make dative bonds e.g. [N+](O-)=O from -N(=O)=O☐ Remove all but the largest contiguous fragment☐ Center Coordinates☐ Combine mols in first file with others by name

Convert only if match SMARTS or mols in file:

Filter: convert only when tests are true:

 Add properties from descriptors Delete properties in list

Append properties or descriptors in list to title:

☐ Join all input molecules into a single output molecule☐ Output disconnected fragments separately add or replace a property (SDF) Add or replace molecule title Append text to title☐ Output multiple conformers separately☐ Append output index to title Additional file output☐ Append input filename to title

AutoDock Vina

- Download from official summer school website:
<https://bioinfo2025.splet.arnes.si/things-to-do-before-summer-school/>
 - *Vina.exe*
 - *Vina_license.rtf*
 - *Vina_split.exe*
 - *Vina_windows.pl*

ChimeraX for visualisation of results

ChimeraX, download from:

<https://www.cgl.ucsf.edu/chimerax/download.html>

Download UCSF ChimeraX

ChimeraX is the state-of-the-art visualization program from the [Resource for Biocomputing, Visualization, and Informatics](#) at UC San Francisco. It is free for academic, government, nonprofit, and personal use; commercial users, please see [commercial licensing](#). Please [cite ChimeraX](#) in publications.

See also:

- [ChimeraX Documentation](#)
- [System Requirements](#)
- [Change Log](#)
- [Download & Citation Counts](#)
- [Older Releases](#)
- [Common Problems](#)

Current releases:

- [Production Builds](#)
- [Daily Builds](#)

ChimeraX 1.10

Production releases are stable versions for [ChimeraX Toolshed](#) bundles to work with. You may need to use an [older release](#) if a bundle you wish to use has not been updated yet. Showing releases for Windows 10.

Operating System	Distribution	Date	Notes
Windows	ChimeraX-1.10.exe	26. jun. 2025	Download is a Windows (Inno Setup based) installer. Tested on Windows 10 and Windows 11. ► More Info...

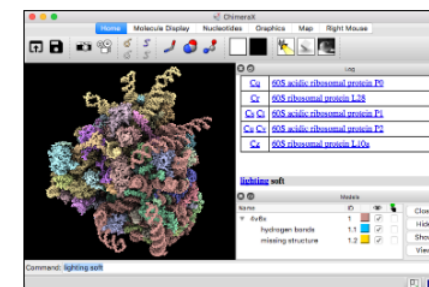
► Other releases

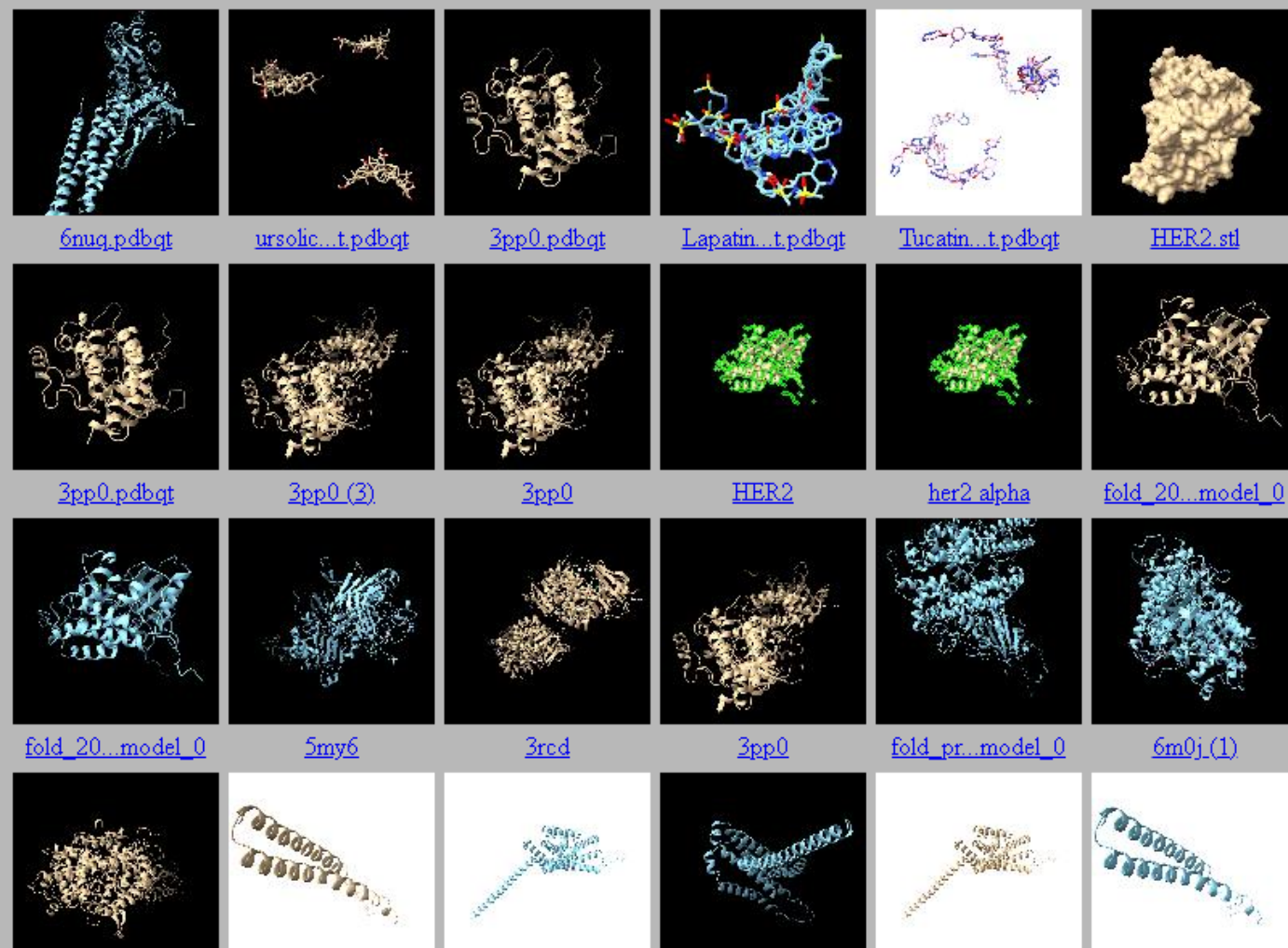
Daily Build

Daily builds are generated automatically each night from the [development source code](#) (see the [change log](#)). While a given build may have unforeseen problems, these are often fixed by the next day. Showing releases for Windows 10.

Operating System	Distribution	Date	Notes
Windows	chimerax-daily.exe	7. jul. 2025	Download is a Windows (Inno Setup based) installer. Tested on Windows 10 and Windows 11. ► More Info...

► Other releases





Comma delete /D

Welcome to ChimeraX

Log

Startup Messages

<i>note</i>	available bundle cache has not been initialized yet
-------------	---

UCSF ChimeraX version: 1.9 (2024-12-11)

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[How to cite UCSF ChimeraX](#)

Models

Name	Age	Gender	Marital Status	Education	Occupation	Income	Health Status	Smoking Status	Alcohol Consumption	Exercise Frequency	Dietary Habits	Stress Level	Sleep Pattern	Mental Health	Family History	Genetic Predisposition	Environmental Factors	Lifestyle Choices	Healthcare Access	Insurance Status	Compliance with Treatment	Quality of Life	Overall Health Score
John Doe	45	Male	Married	High School	Construction Worker	\$35,000	Good	Smoker	Occasional	Weekly	Fast Food	High	Irregular	Anxious	None	None	Urban	Unhealthy	Public	Medicare	Low	65	
Jane Smith	32	Female	Single	Bachelor's	Software Engineer	\$75,000	Excellent	Non-Smoker	None	Daily	Vegetarian	Low	Regular	Stable	None	None	Suburban	Healthy	Private	Medicaid	High	85	
Michael Johnson	58	Male	Divorced	College	Teacher	\$45,000	Fair	Former Smoker	Occasional	Monthly	Mixed	Medium	Semi-Regular	Mild Depression	None	None	Urban	Unhealthy	Public	Medicare	Medium	70	
Emily Davis	28	Female	Single	Master's	Research Scientist	\$90,000	Excellent	Non-Smoker	None	Daily	Organic	Low	Regular	Stable	None	None	Suburban	Healthy	Private	Medicaid	High	90	
Robert Brown	62	Male	Married	High School	Retired	\$25,000	Fair	Smoker	Occasional	Weekly	Fast Food	High	Irregular	Anxious	None	None	Urban	Unhealthy	Public	Medicare	Low	60	
Sarah Wilson	41	Female	Married	Bachelor's	Nurse	\$55,000	Good	Non-Smoker	Occasional	Daily	Mixed	Medium	Regular	Stable	None	None	Suburban	Healthy	Private	Medicaid	High	80	
David Miller	37	Male	Single	College	Marketing Executive	\$65,000	Good	Former Smoker	Occasional	Weekly	Mixed	Medium	Semi-Regular	Mild Depression	None	None	Urban	Unhealthy	Public	Medicare	Medium	75	
Lisa Anderson	52	Female	Divorced	Master's	Professor	\$85,000	Excellent	Non-Smoker	None	Daily	Organic	Low	Regular	Stable	None	None	Suburban	Healthy	Private	Medicaid	High	95	
Christopher Lee	68	Male	Married	High School	Retired	\$20,000	Fair	Smoker	Occasional	Weekly	Fast Food	High	Irregular	Anxious	None	None	Urban	Unhealthy	Public	Medicare	Low	55	
Amanda Taylor	35	Female	Single	Bachelor's	Graphic Designer	\$50,000	Good	Non-Smoker	Occasional	Daily	Mixed	Medium	Regular	Stable	None	None	Suburban	Healthy	Private	Medicaid	High	82	
Kevin White	55	Male	Married	College	Engineer	\$60,000	Good	Former Smoker	Occasional	Weekly	Mixed	Medium	Semi-Regular	Mild Depression	None	None	Urban	Unhealthy	Public	Medicare	Medium	78	
Nicole Green	48	Female	Single	Master's	Business Analyst	\$70,000	Good	Non-Smoker	Occasional	Daily	Organic	Low	Regular	Stable	None	None	Suburban	Healthy	Private	Medicaid	High	88	
Brandon Hall	30	Male	Single	High School	Warehouse Worker	\$30,000	Fair	Smoker	Occasional	Weekly	Fast Food	High	Irregular	Anxious	None	None	Urban	Unhealthy	Public	Medicare	Low	62	
Stephanie King	50	Female	Married	Bachelor's	Accountant	\$58,000	Good	Non-Smoker	Occasional	Daily	Mixed	Medium	Regular	Stable	None	None	Suburban	Healthy	Private	Medicaid	High	84	
Gregory Scott	60	Male	Divorced	College	Teacher	\$42,000	Fair	Former Smoker	Occasional	Weekly	Mixed	Medium	Semi-Regular	Mild Depression	None	None	Urban	Unhealthy	Public	Medicare	Medium	72	
Michelle Adams	33	Female	Single	Master's	Software Engineer	\$78,000	Excellent	Non-Smoker	None	Daily	Organic	Low	Regular	Stable	None	None	Suburban	Healthy	Private	Medicaid	High	92	
Timothy Baker	57	Male	Married	High School	Construction Worker	\$38,000	Fair	Smoker	Occasional	Weekly	Fast Food	High	Irregular	Anxious	None	None	Urban	Unhealthy	Public	Medicare	Low	68	
Christina Clark	43	Female	Single	Bachelor's	Marketing Executive	\$62,000	Good	Non-Smoker	Occasional	Daily	Mixed	Medium	Regular	Stable	None	None	Suburban	Healthy	Private	Medicaid	High	86	
Jonathan Evans	65	Male	Married	College	Retired	\$28,000	Fair	Former Smoker	Occasional	Weekly	Mixed	Medium	Semi-Regular	Mild Depression	None	None	Urban	Unhealthy	Public	Medicare	Medium	74	
Victoria Harris	38	Female	Single	Master's	Research Scientist	\$82,000	Excellent	Non-Smoker	None	Daily	Organic	Low	Regular	Stable	None	None	Suburban	Healthy	Private	Medicaid	High	94	
Benjamin Ives	53	Male	Divorced	High School	Warehouse Worker	\$32,000	Fair	Smoker	Occasional	Weekly	Fast Food	High	Irregular	Anxious	None	None	Urban	Unhealthy	Public	Medicare</			

ID



Close

Hide

Show

