MOLECULAR DOCKING

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

Molecular Docking with AutoDock Vina

Download softwares:

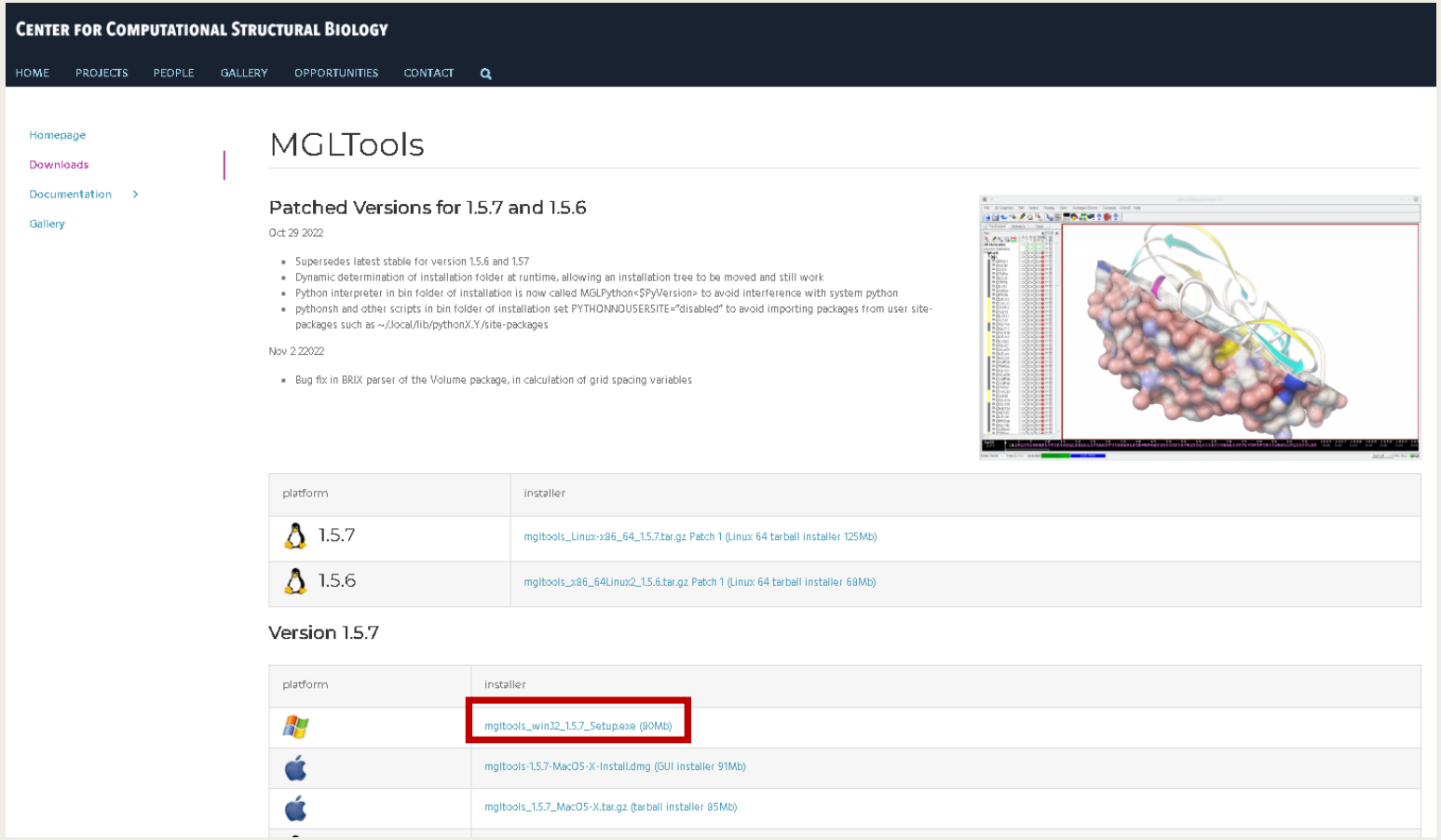
- Pearl: https://padre.perlide.org/download.html
- MGL Tools: https://ccsb.scripps.edu/mgltools/downloads/
- OpenBabel GUI: https://github.com/openbabel/openbabel/releases
- AutoDock Vina: https://bioinfo2025.splet.arnes.si/things-to-do-before-summer-school/
  - *.zip file on the official website of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

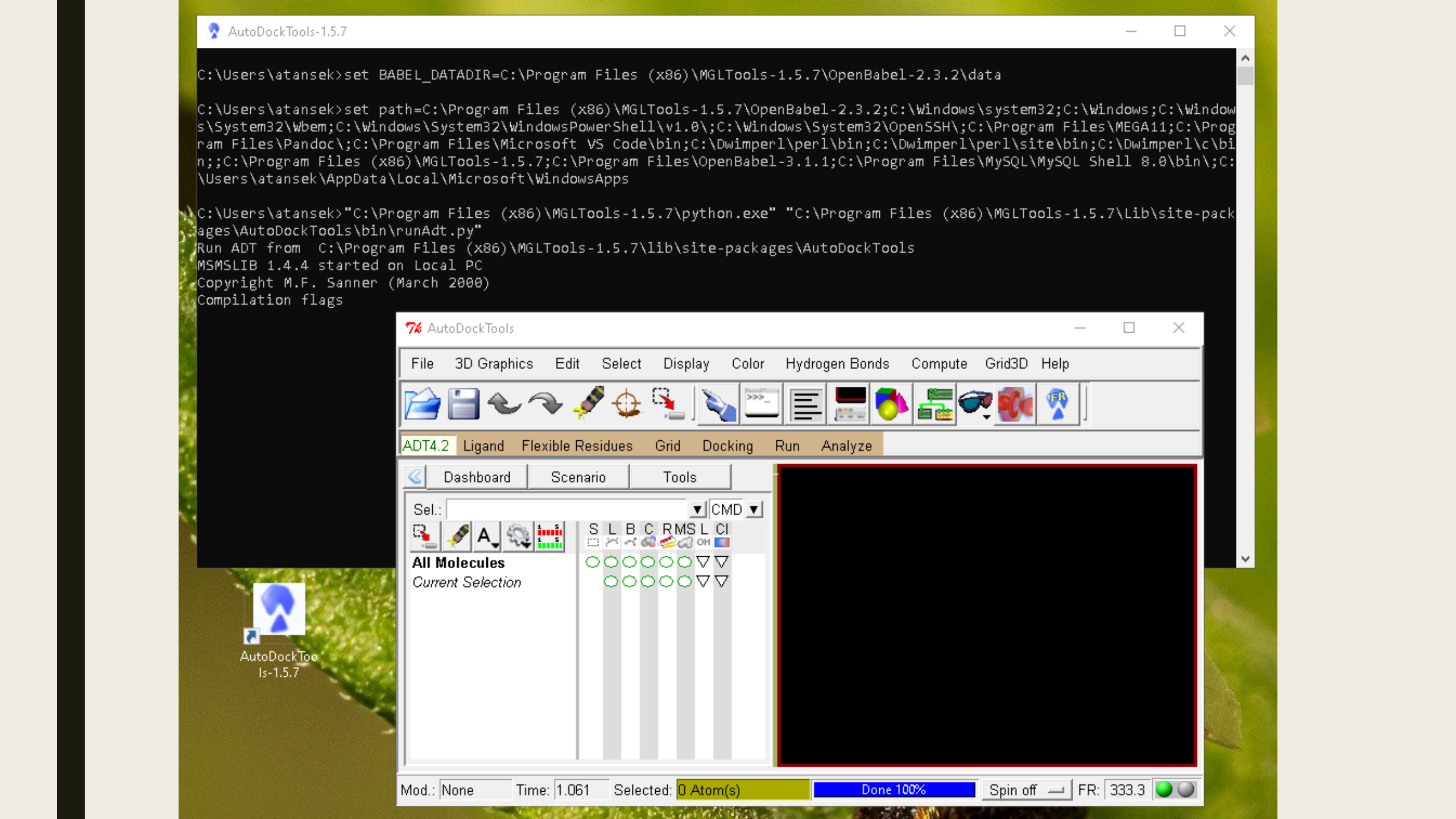
Pearl

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

MGL Tools

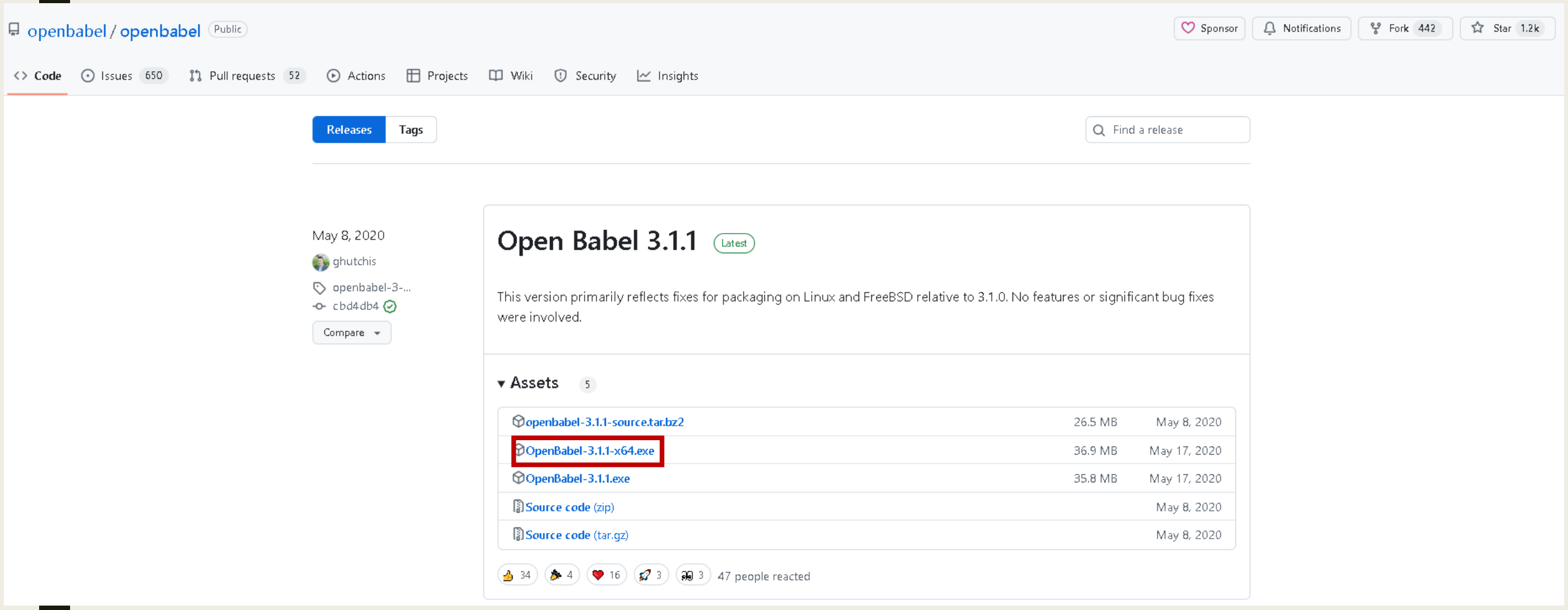
https://ccsb.scripps.edu/mgltools/downloads/

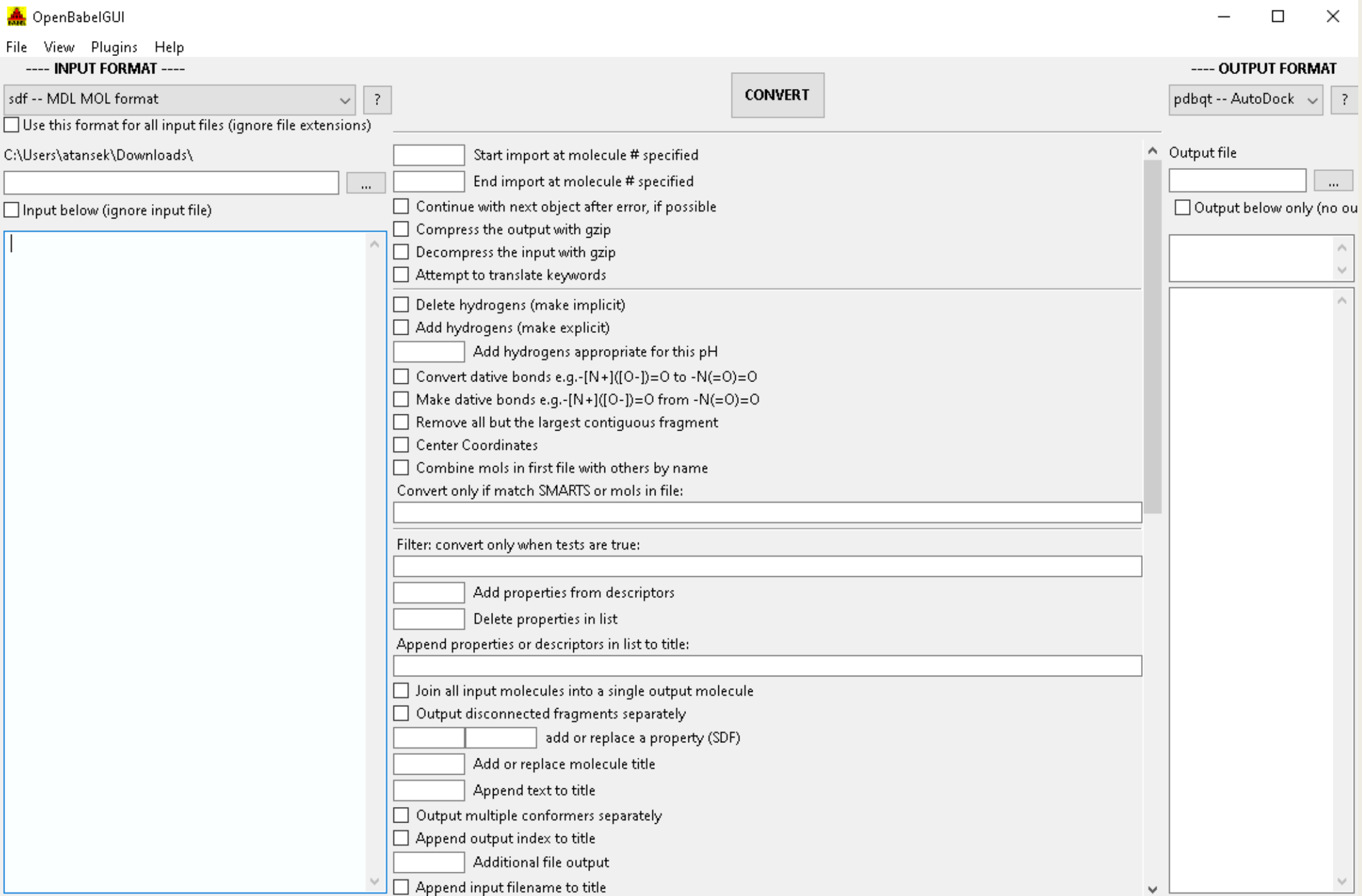



AutoDockTools-1.5.7
C:\Users\atansek>set BABEL_DATADIR=C:\Program Files (x86)\MGLTools-1.5.7\OpenBabel-2.3.2\data
C:\Users\atansek>set path=C:\Program Files (x86)\MGLTools-1.5.7\OpenBabel-2.3.2;C:\Windows\system32;C:\Windows;C:\Windows\System32\Wbem;C:\Windows\System32\WindowsPowerShell\v1.0\;C:\Windows\System32\OpenSSH\;C:\Program Files\MEGA11;C:\Program Files\Pandoc\;C:\Program Files\Microsoft VS Code\bin;C:\Dwimperl\perl\bin;C:\Dwimperl\perl\site\bin;C:\Dwimperl\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
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 R MS L Cl
All Molecules
Current Selection
Mod.:
None
Time:
1.061
Selected:
0 Atom(s)
Done 100%
Spin off
FR:
333.3
AutoDockTools-1.5.7

OpenBabel GUI

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




OpenBabelGUI
File View Plugins Help
---- 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
?
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
Output file
...
Output below only (no ou

AutoDock Vina

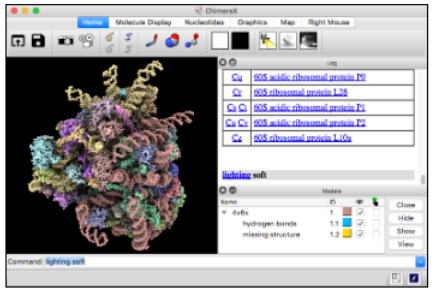
- Download from official summer school website: https://bioinfo2025.splet.arnes.si/things-to-do-before-summer-school/
  - *Vina.exe*
  - *Vina_license.rtf*
  - *Vina_split.exe*
  - *Vina_windows.pl*

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...

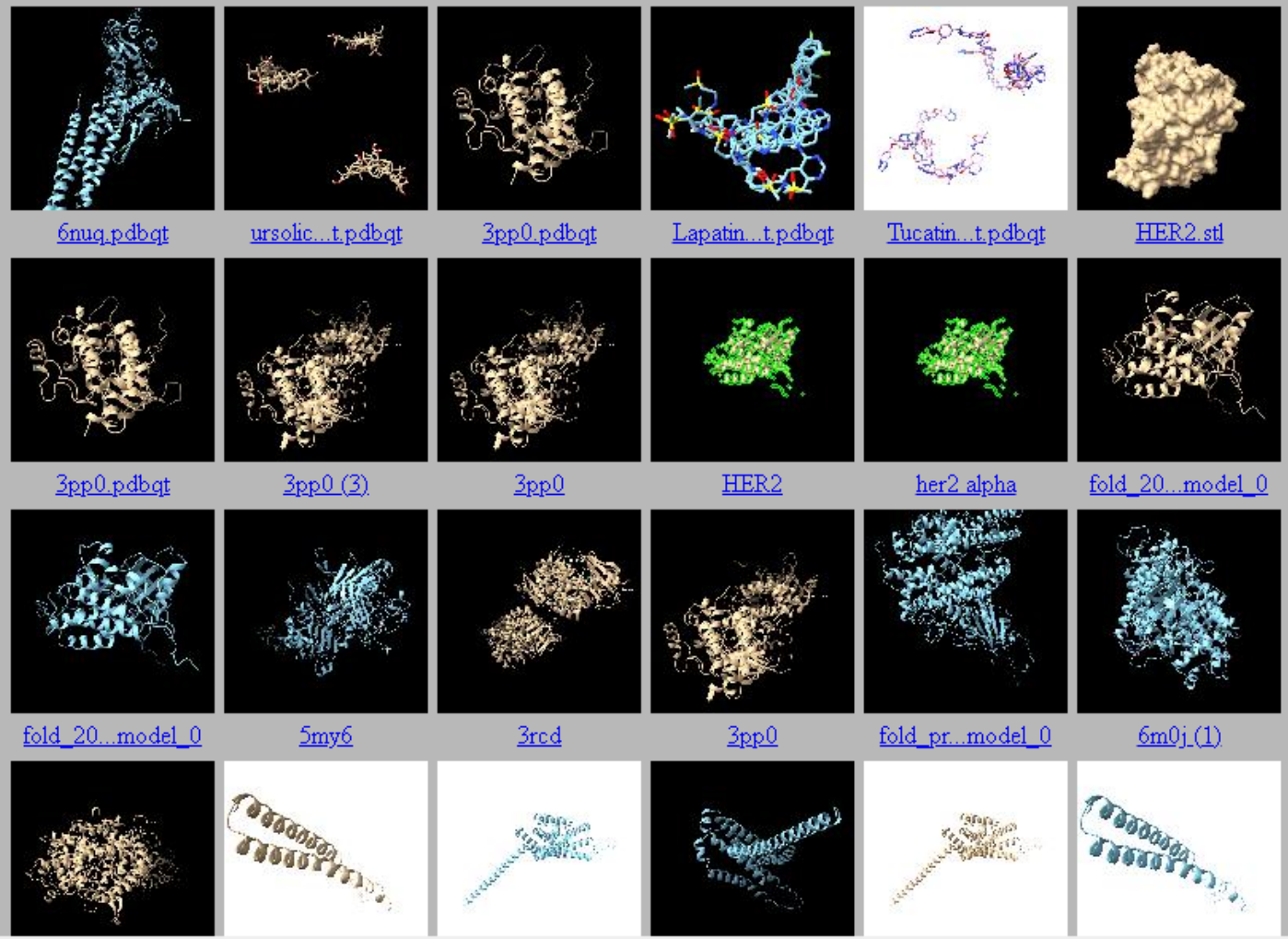
▶ Other releases

ChimeraX

File Edit Select Actions Tools Favorites Presets Help

Home | Molecule Display | Nucleotides | Graphics | Map | Medical Image | Markers | Right Mouse

Open Recent Save — File
Snapshot Spin movie — Images
Show Hide — Atoms
Show Hide — Cartoons
Stick Sphere Ball stick — Styles
White Black — Background
Simple Soft Full — Lighting
Inspect — Selection



Log

Startup Messages

note	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	ID			

Close Hide Show

Comma delete /D

Welcome to ChimeraX