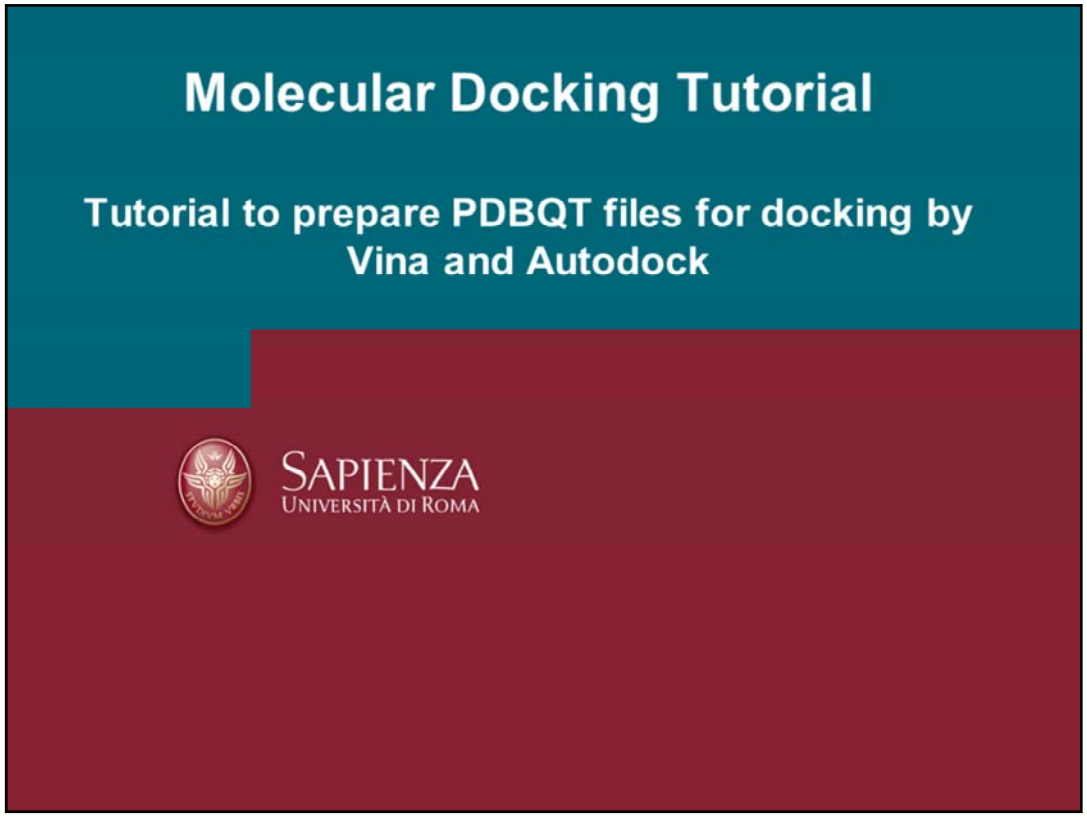
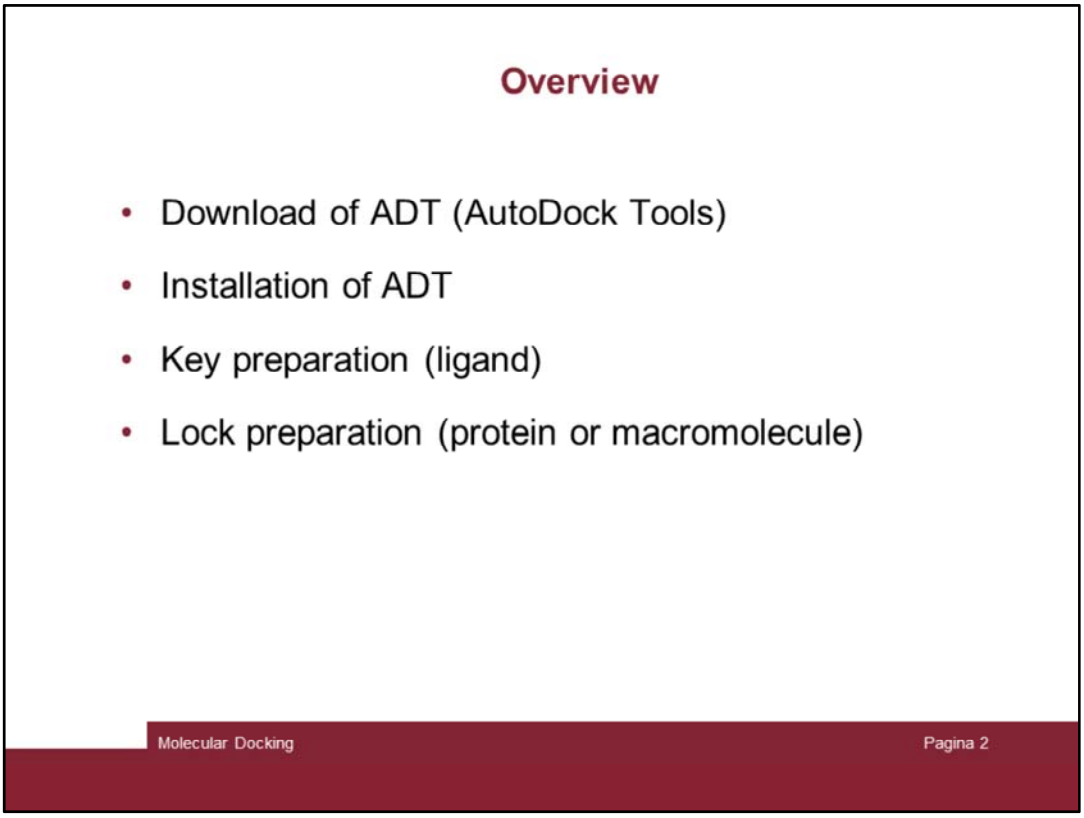


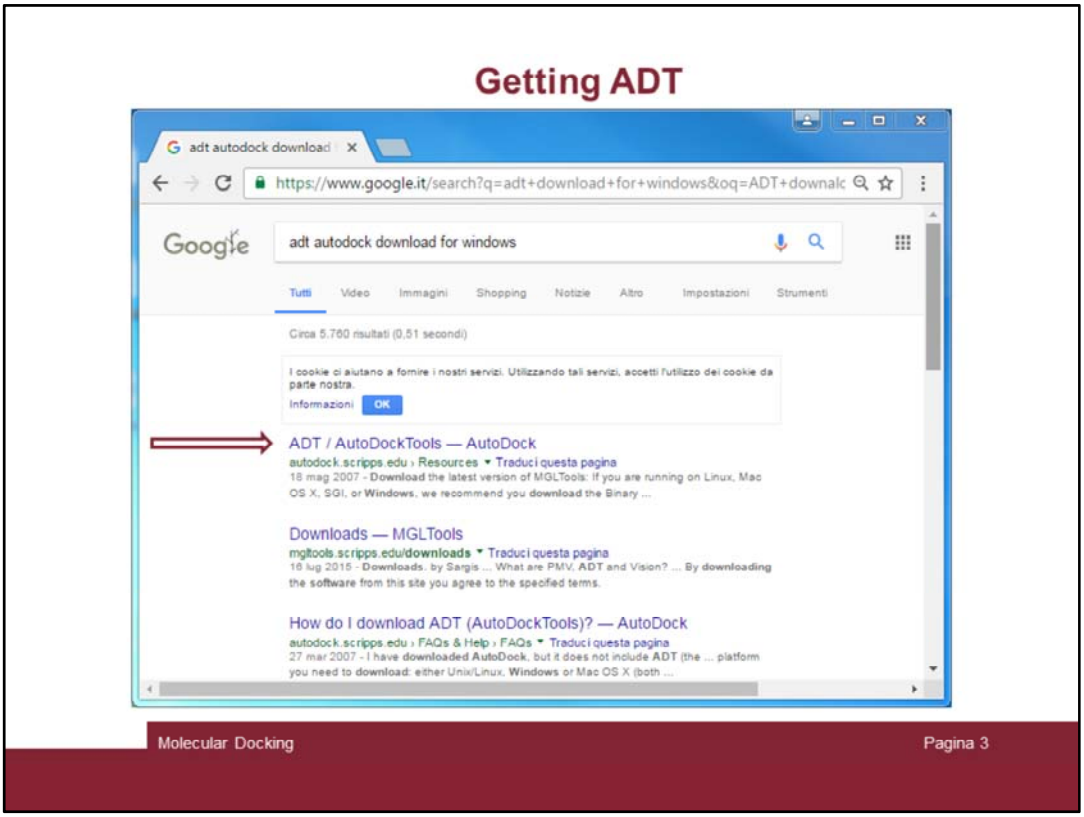
By following this tutorial the user will learn how to prepare the needed files for molecular docking by means of Autodock Vina and Autodock programs.



Here is the sequence of minimal operation to set up a docking study.

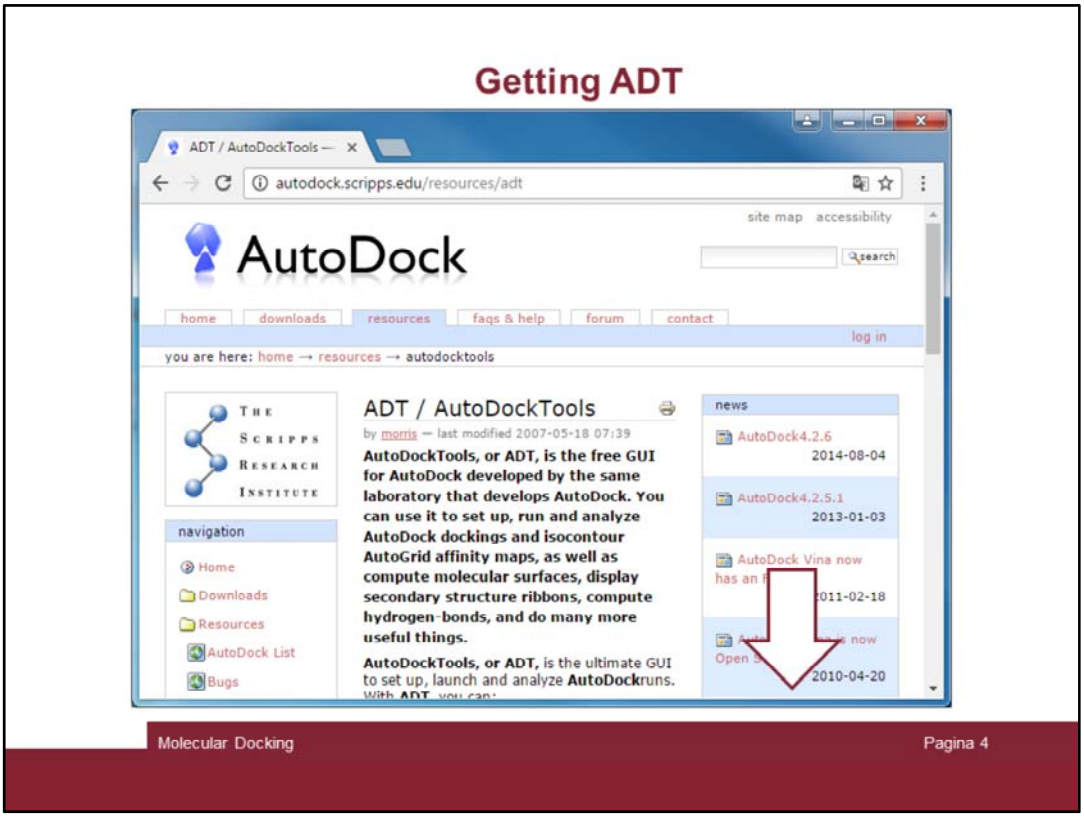
First the target and its role has to be inspected.

Then a series of actions are to first validate the docking program and apply it



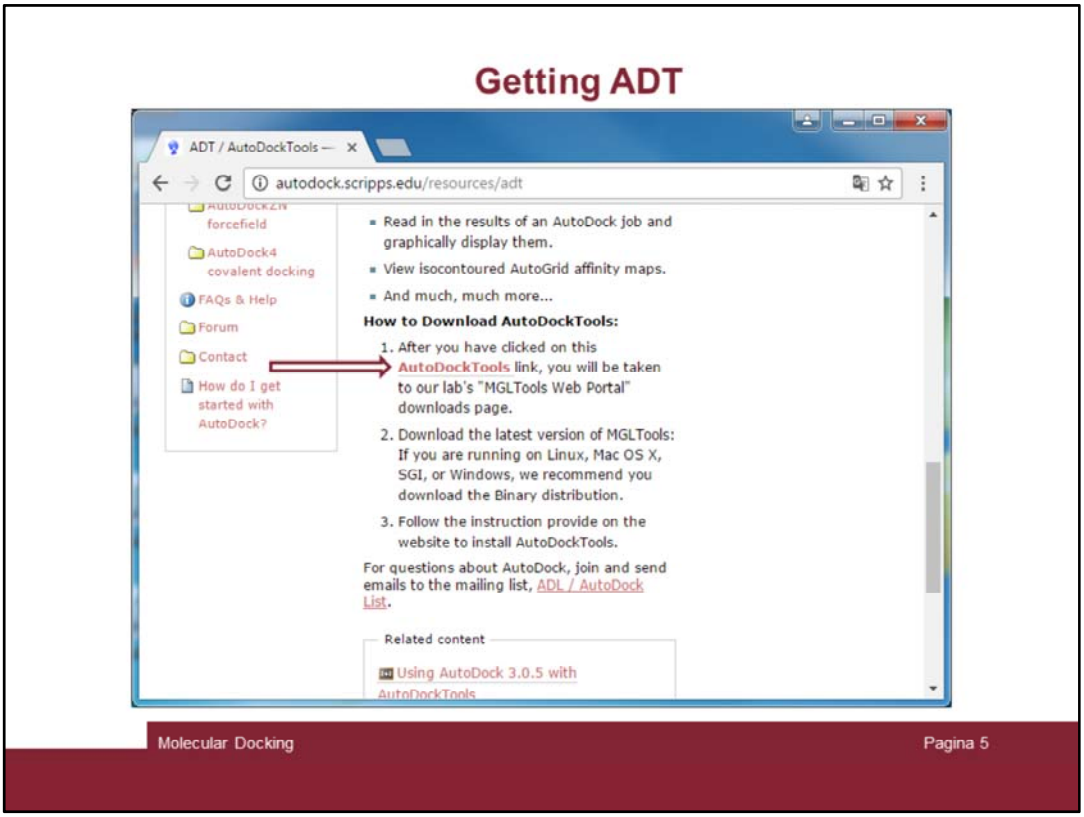
ADT stands for AutoDock Tools.

Google with the «adt autodock download for windows» keys and the first link should be the one you are looking for. Click on that and …



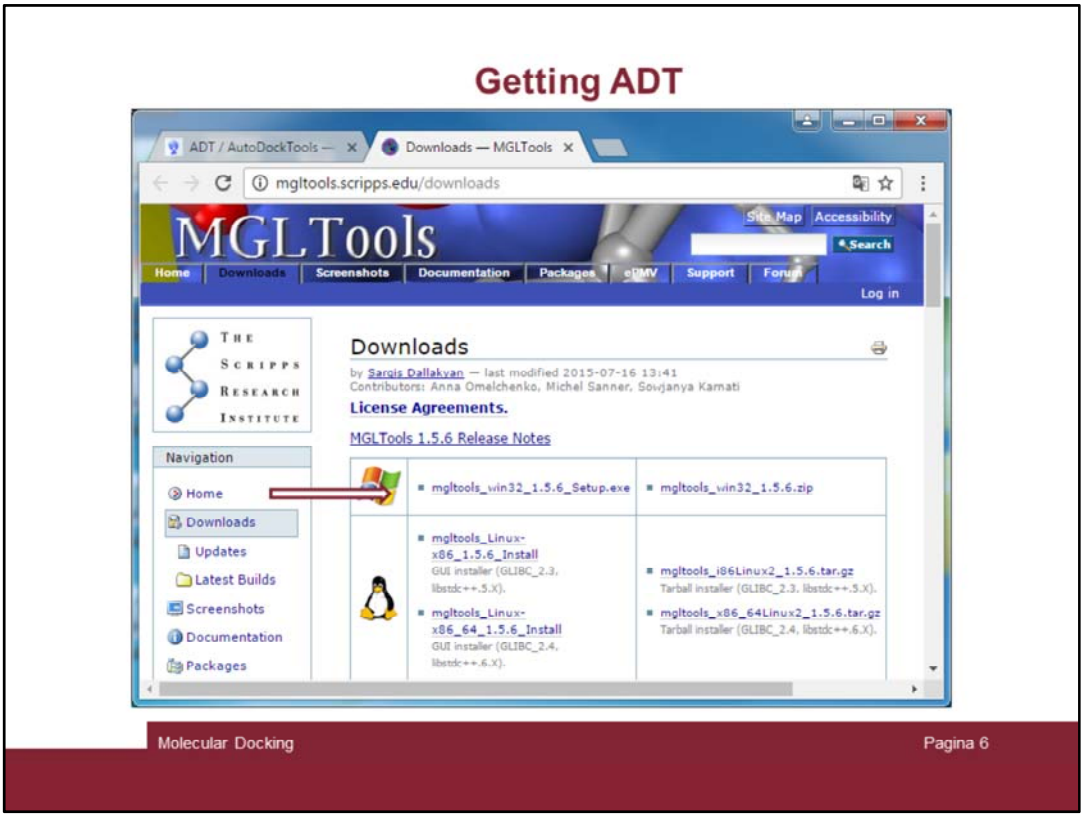
… the AutoDock home page will be reached.

Scroll down the page …



… and look for the AutodockTools link as indicated by the arrow.

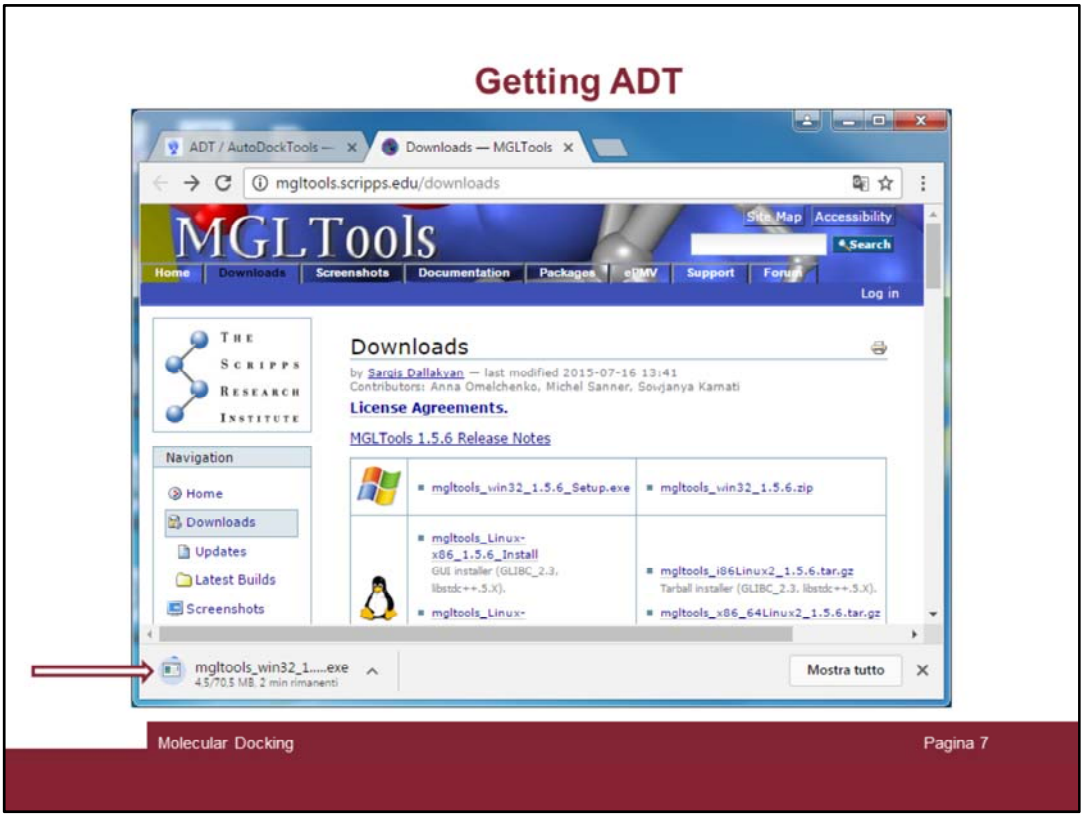
Click on the link and …



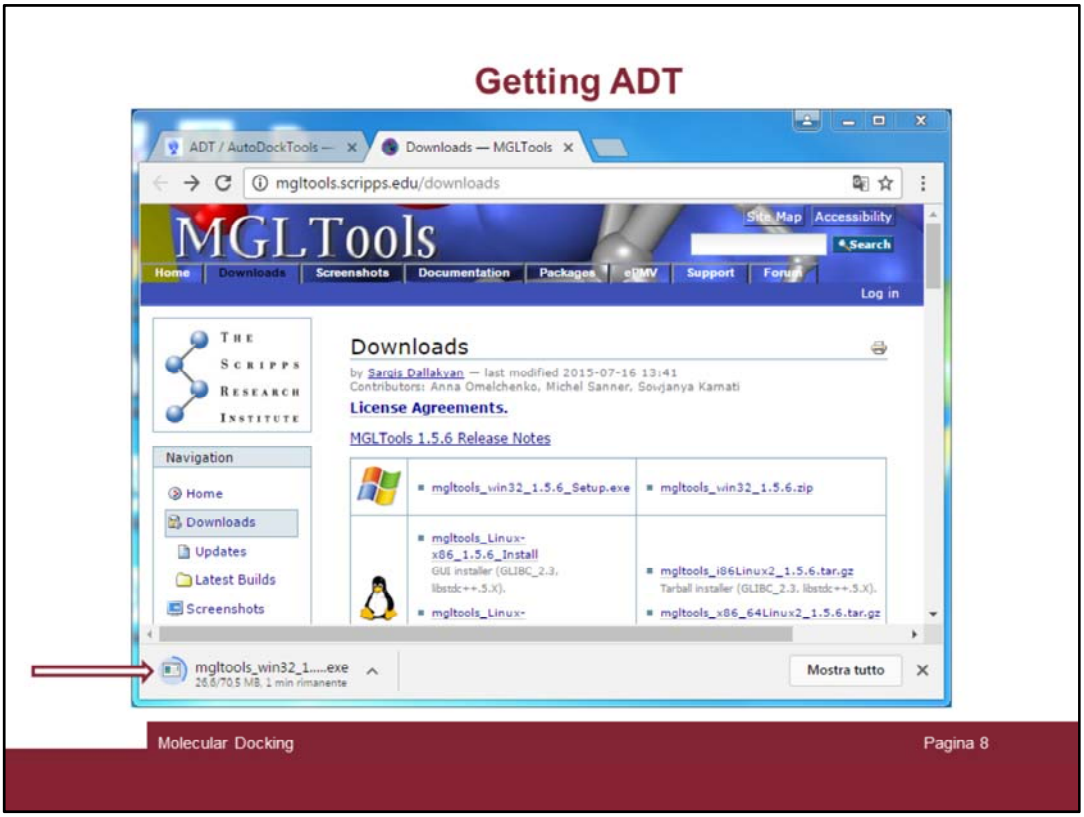
… the MGL Tools web page will open.

Download the program (pay attention if you need 32 or 64 bit version for you r operating system [Windows, Linux or MacOS])

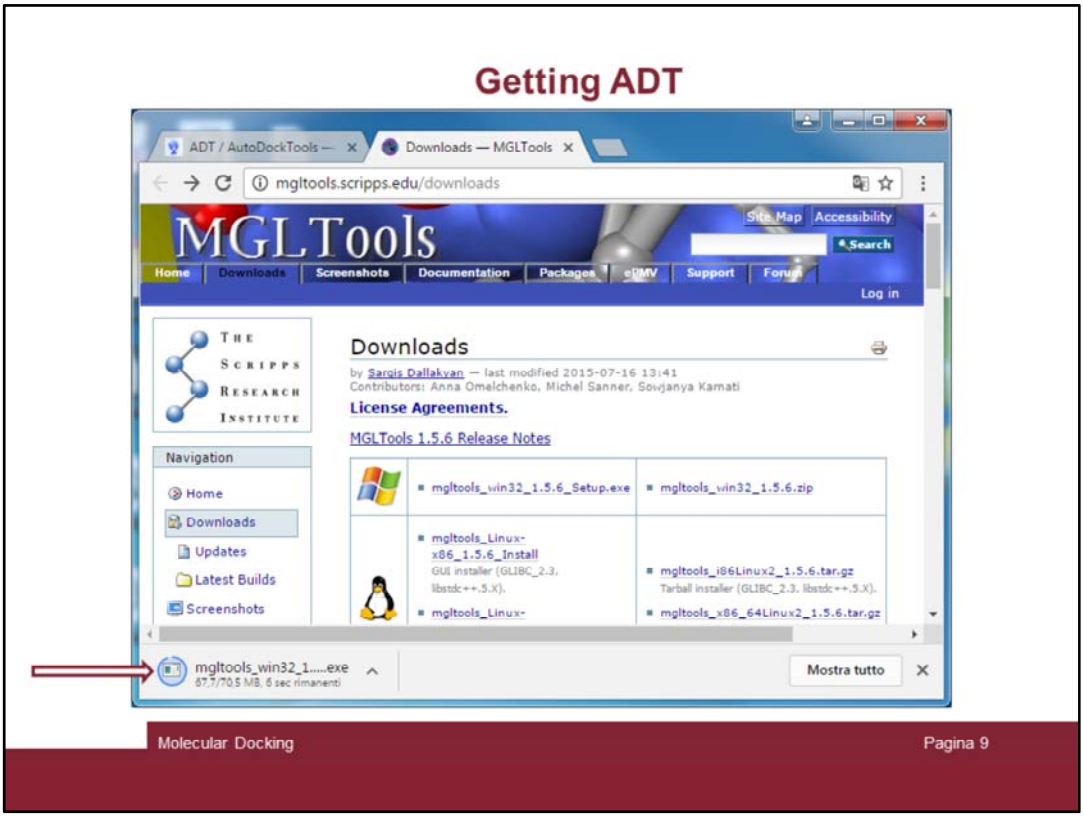
In the example the windows version will be clicked …



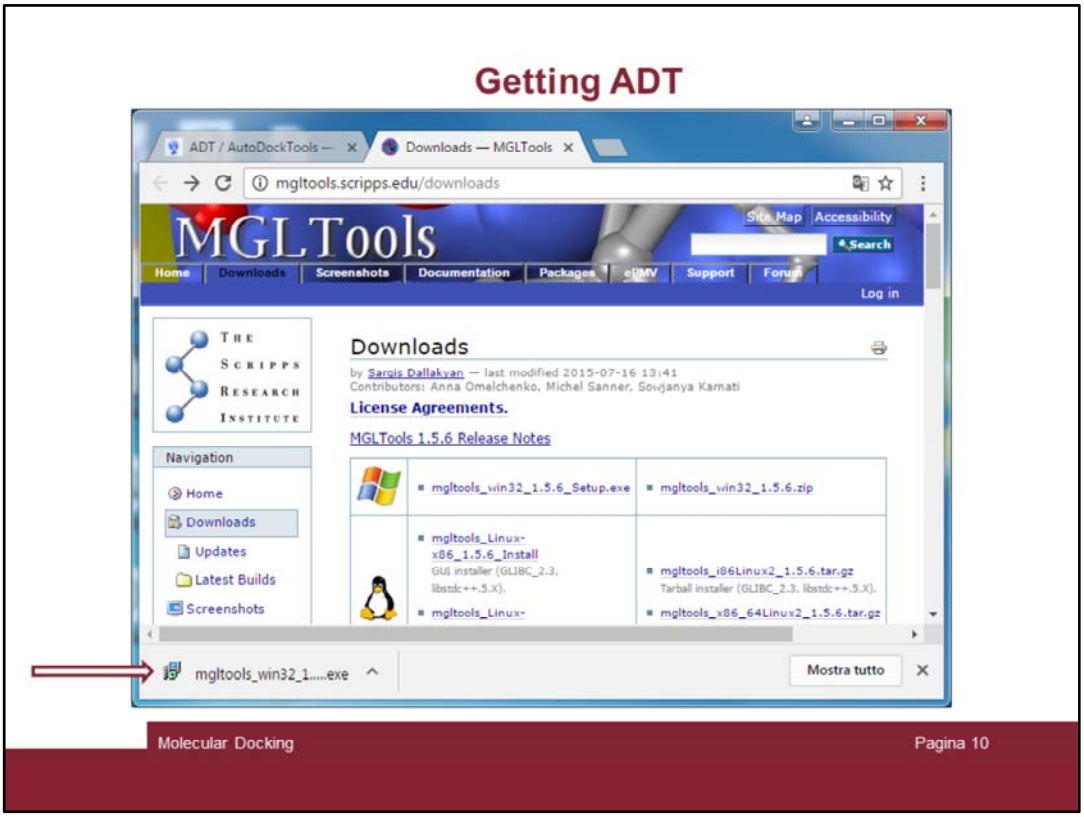
And the browser will start downloading it.



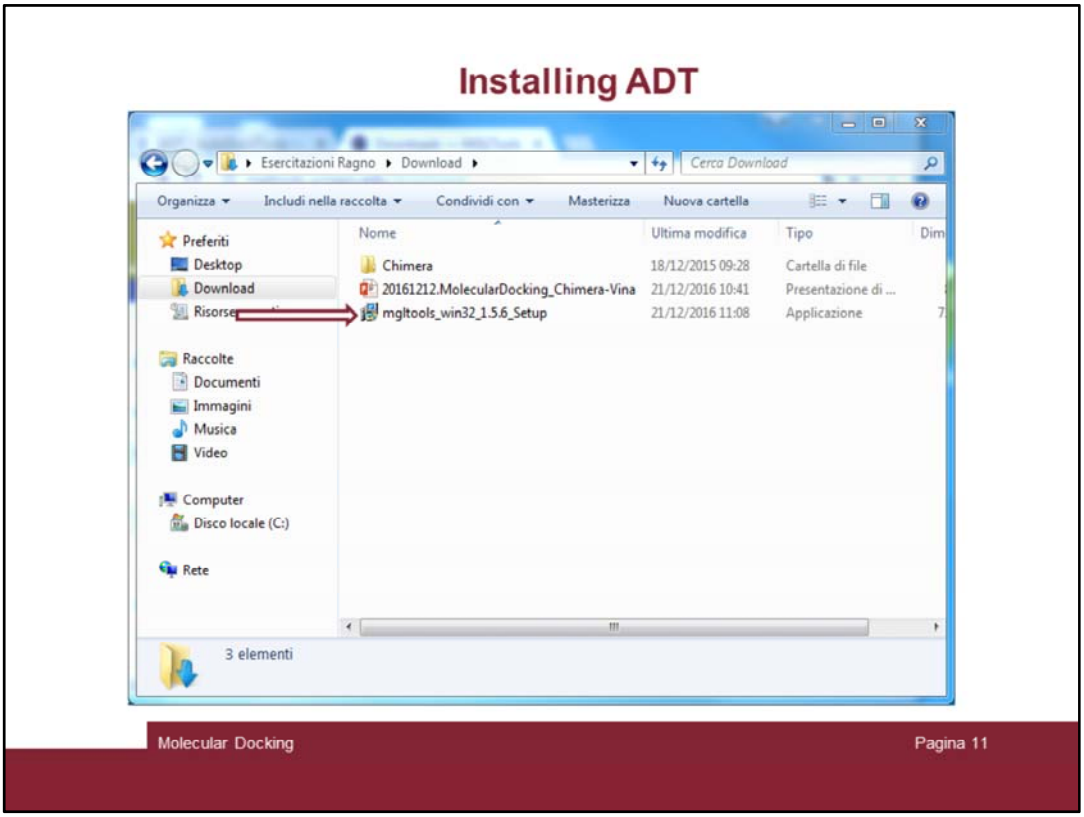
It will take some time (if you have a slow computer or net)



It will take some time (if you have a slow computer or net)



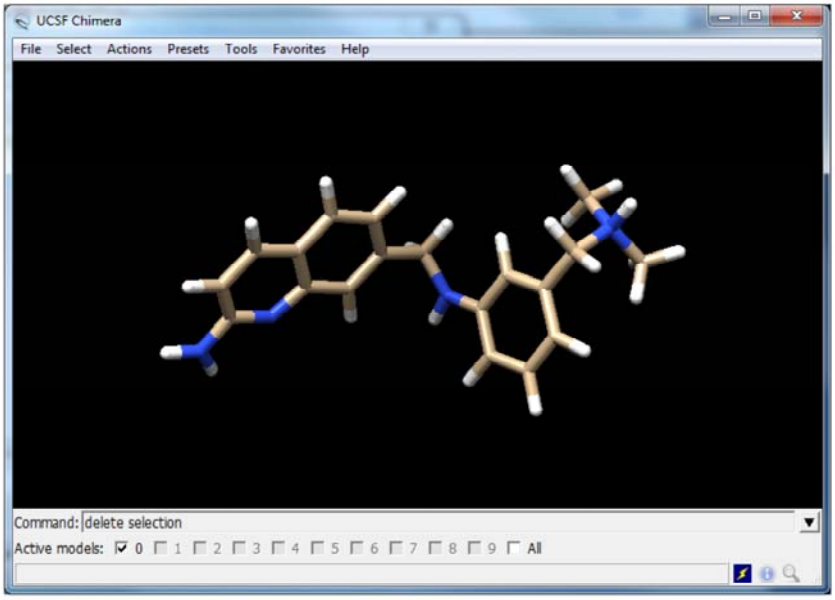
It will take some time (if you have a slow computer or net)



Go to the folder containing the downloaded file and click twice on it and install the program and answer «yes» all the questions the installation program asks

After the installation is finished a some new icons will appear on your desktop. That indicated by the arrow it is the one you need.

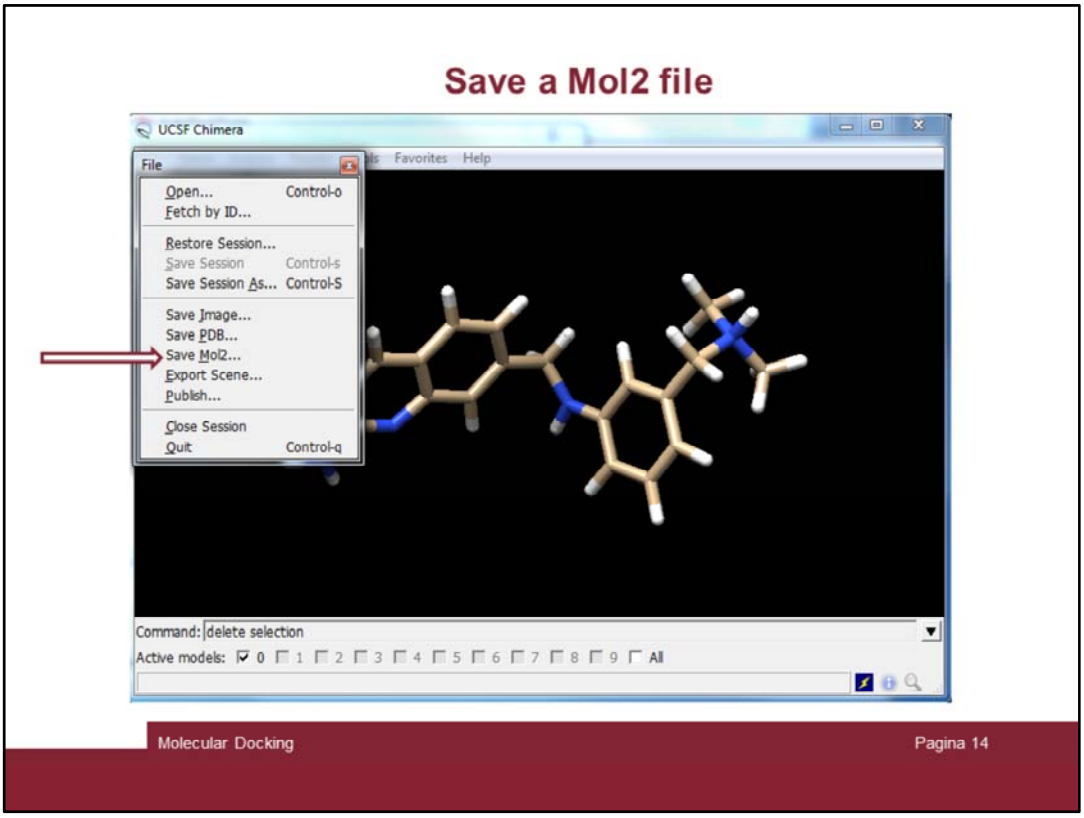
Save a Mol2 file



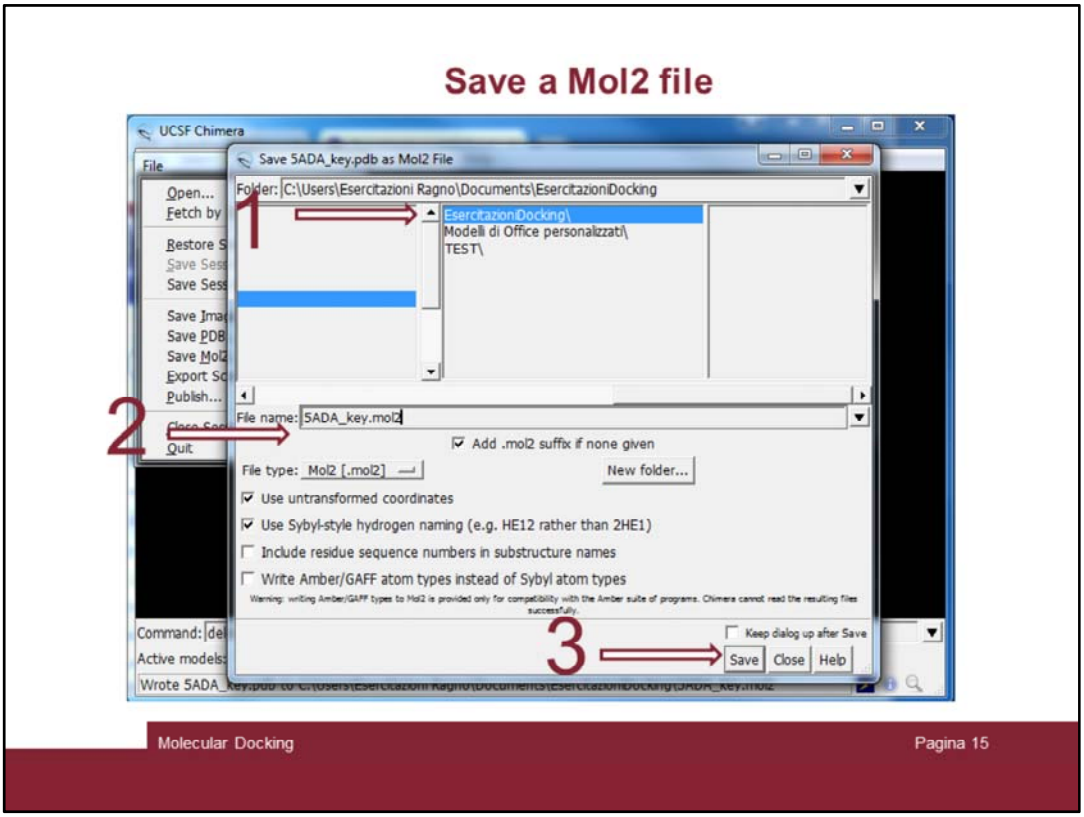
Molecular Docking Pagina 13

Before you start using the ADT program, you need to save a mol2 file format of the ligand.

With chimera add all the hydrogens to it and …

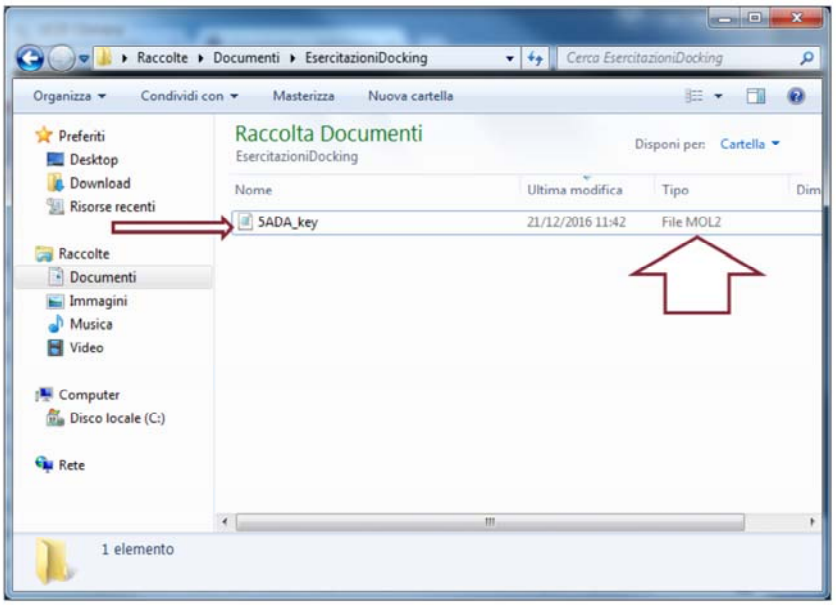


… save the mol in Mol2 (File → Save Mol2 ...)

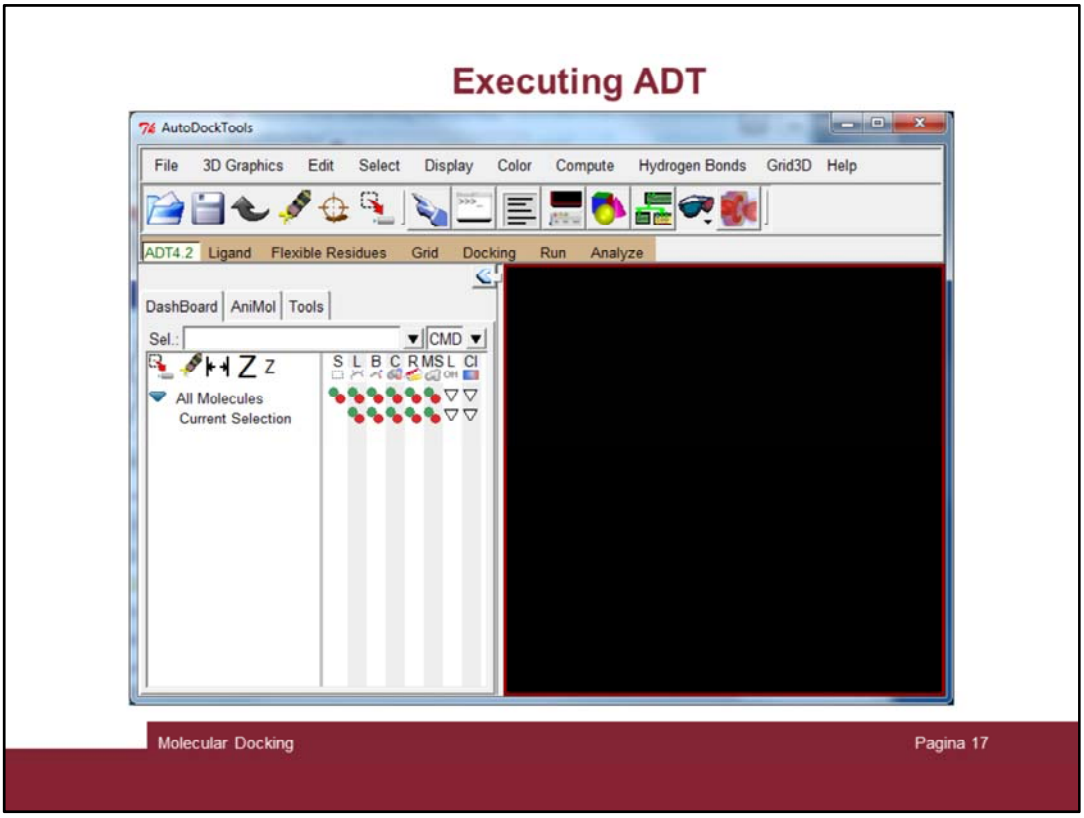


Select the folder, give a name and save it.

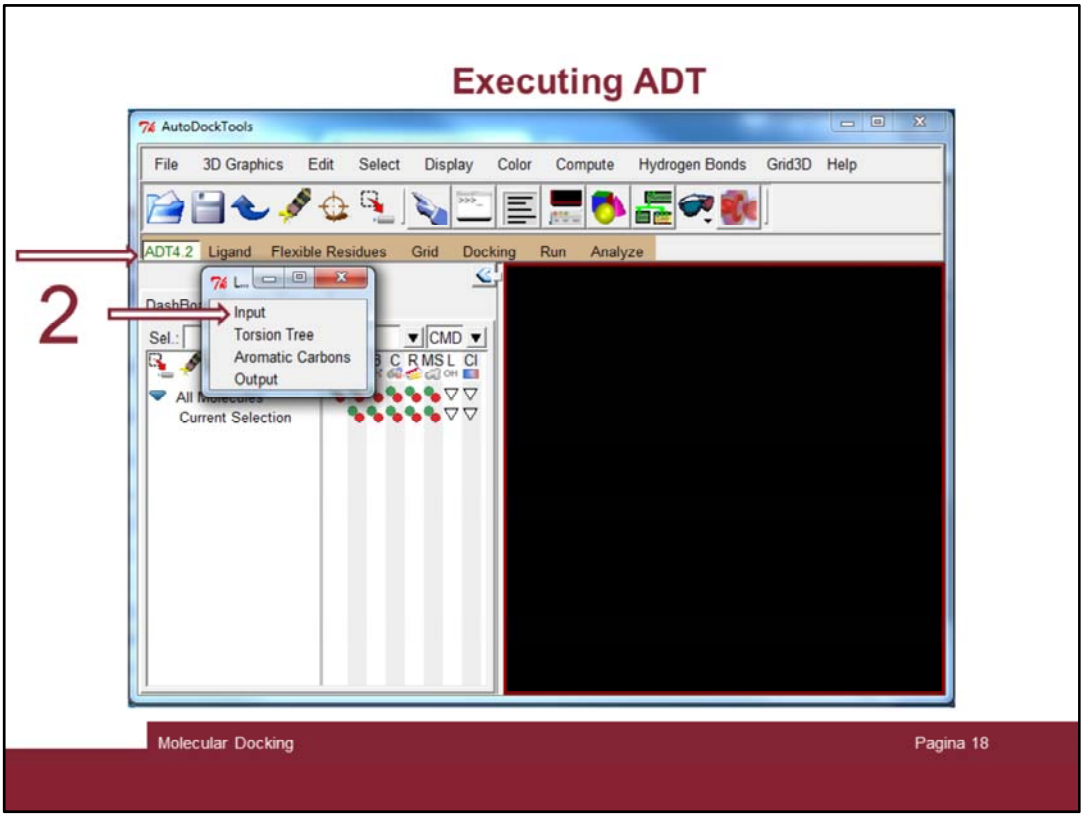
Save a Mol2 file



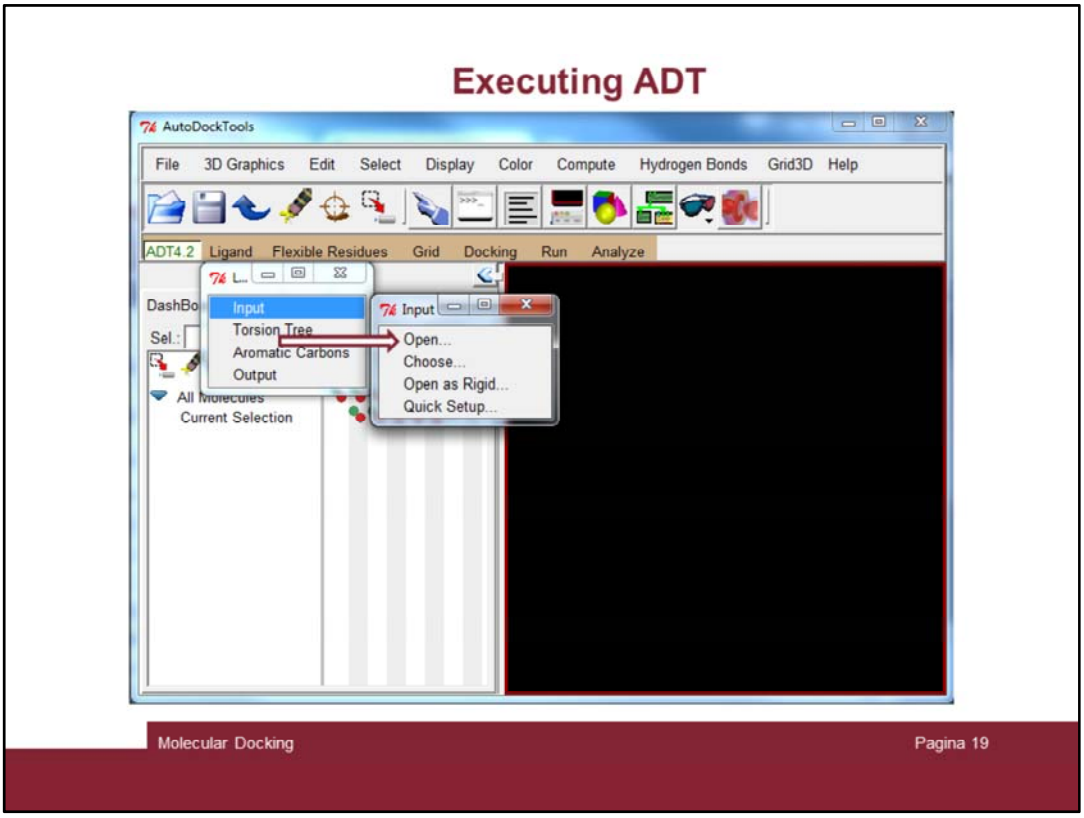
Check the mol2 file was created



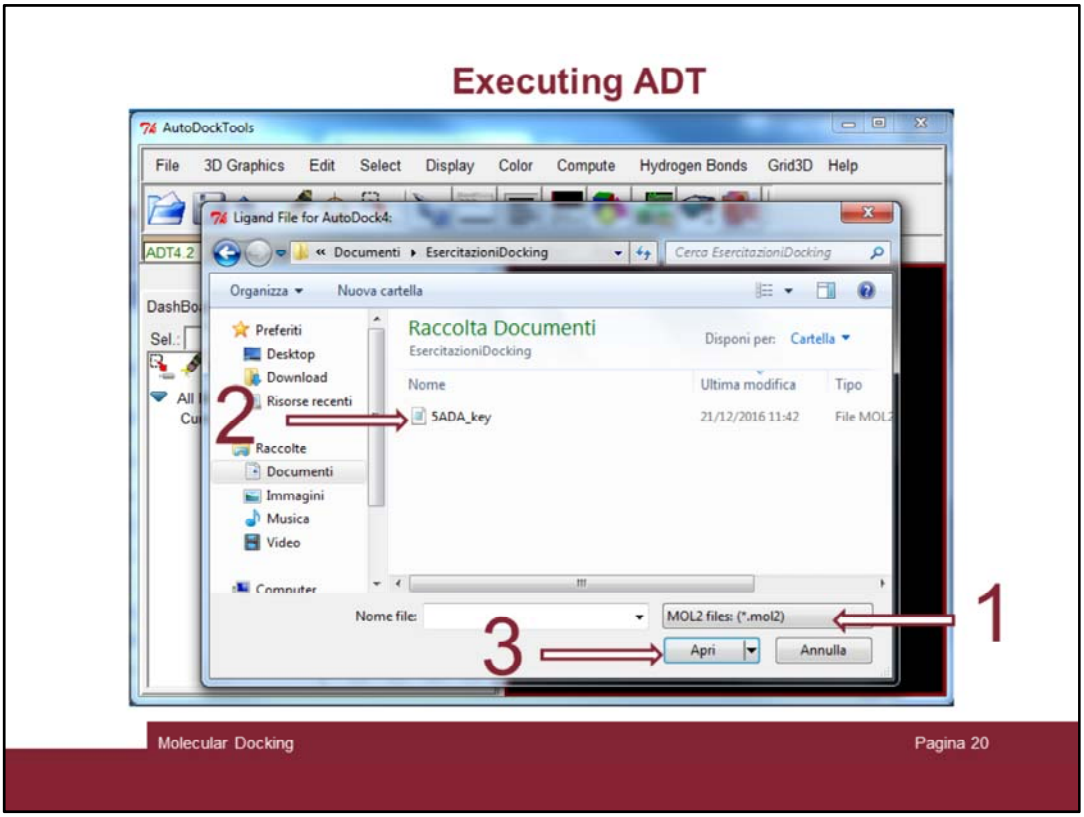
Now click twice on the ADT icon and start the program.



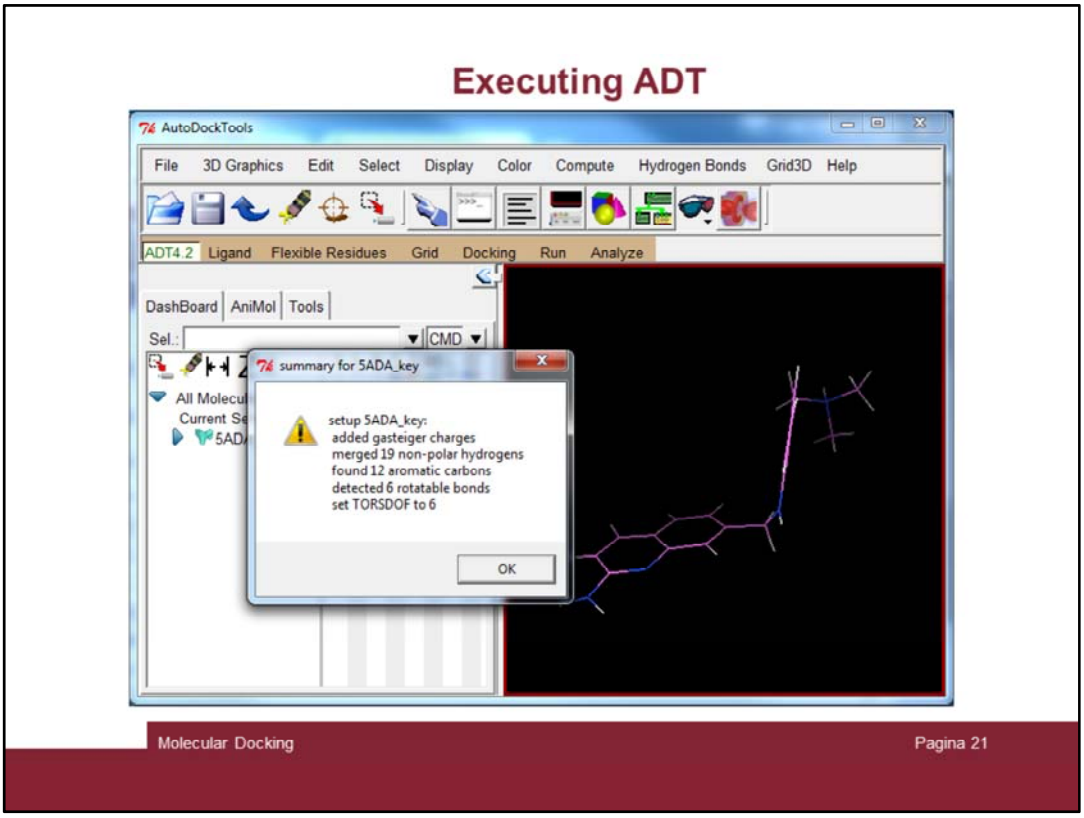
Using the ADT4.2 menu (see the arrow), click on Ligand and select Input.


Executing ADT
AutoDockTools
File
3D Graphics
Edit
Select
Display
Color
Compute
Hydrogen Bonds
Grid3D
Help
ADT4.2
Ligand
Flexible Residues
Grid
Docking
Run
Analyze
Input
Torsion Tree
Aromatic Carbons
Output
Open...
Choose...
Open as Rigid...
Quick Setup...
Current Selection
Molecular Docking
Pagina 19

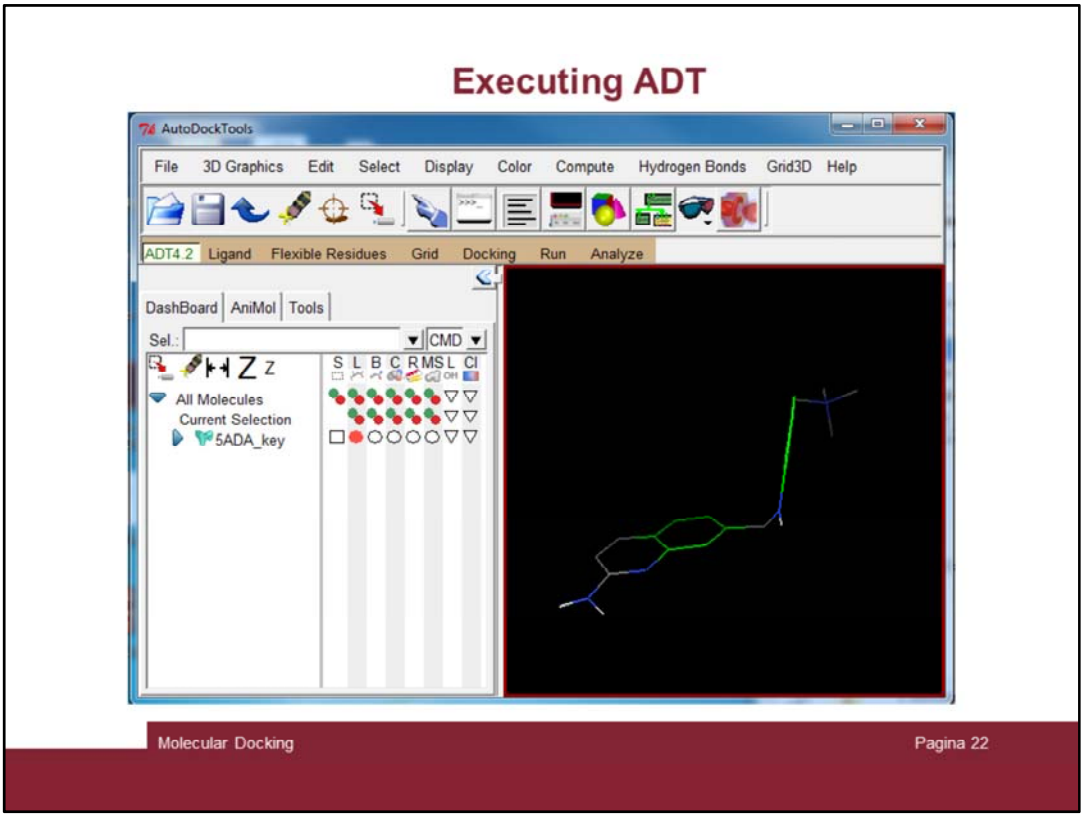
Then open



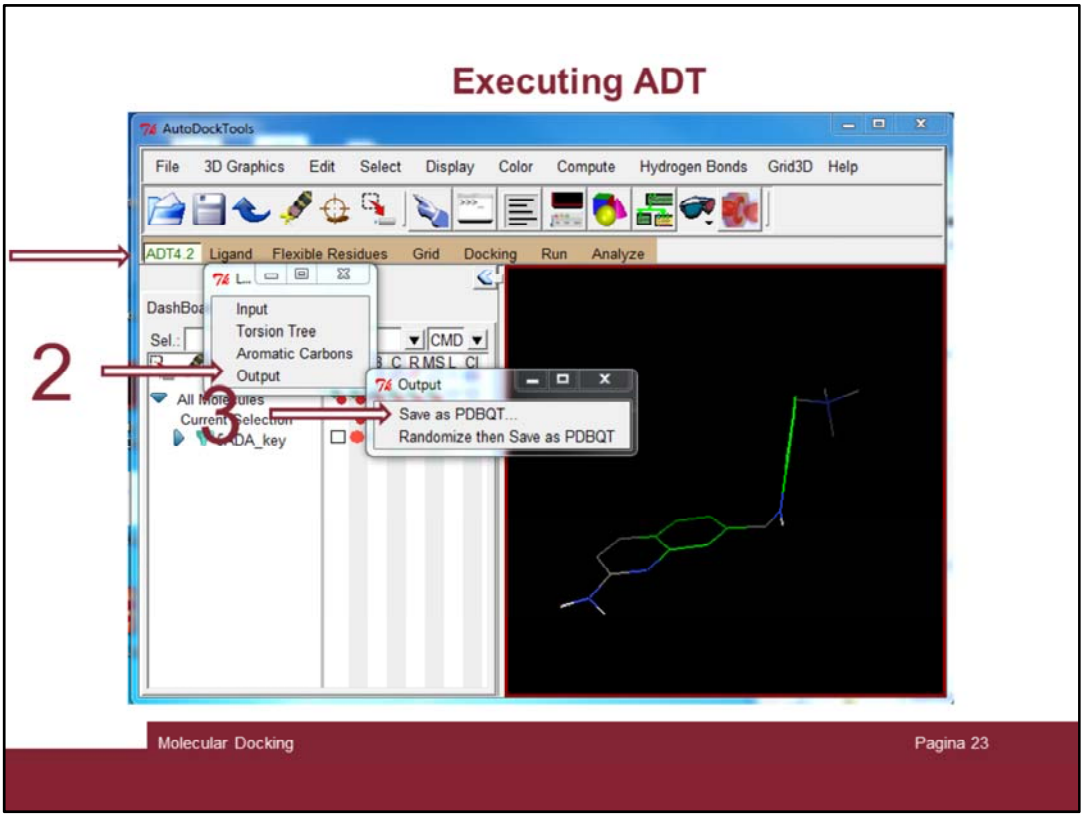
A windows will pop up. Set the file format to «Mol2 files», Select the file you've created by means of Chimera and open it



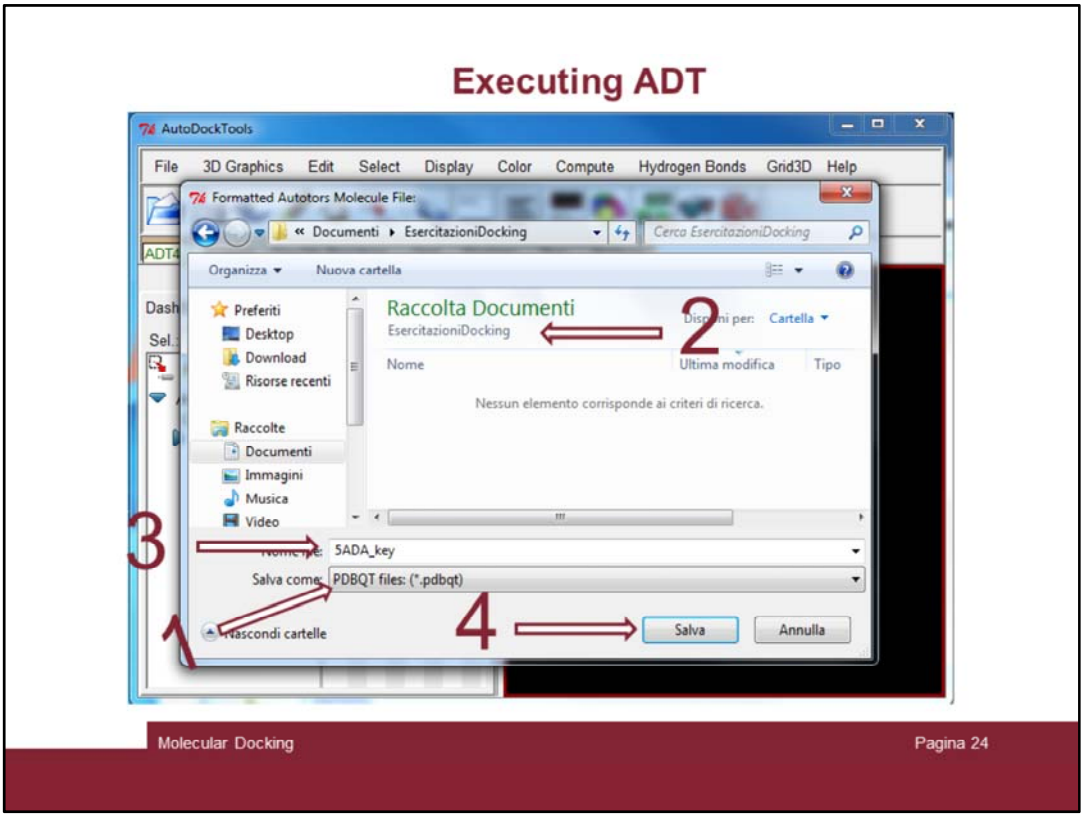
The program will infor you about some action it applied to the loaded molecule



And will show the molecule in the right window (aromatic carbon atoms are colored in green)

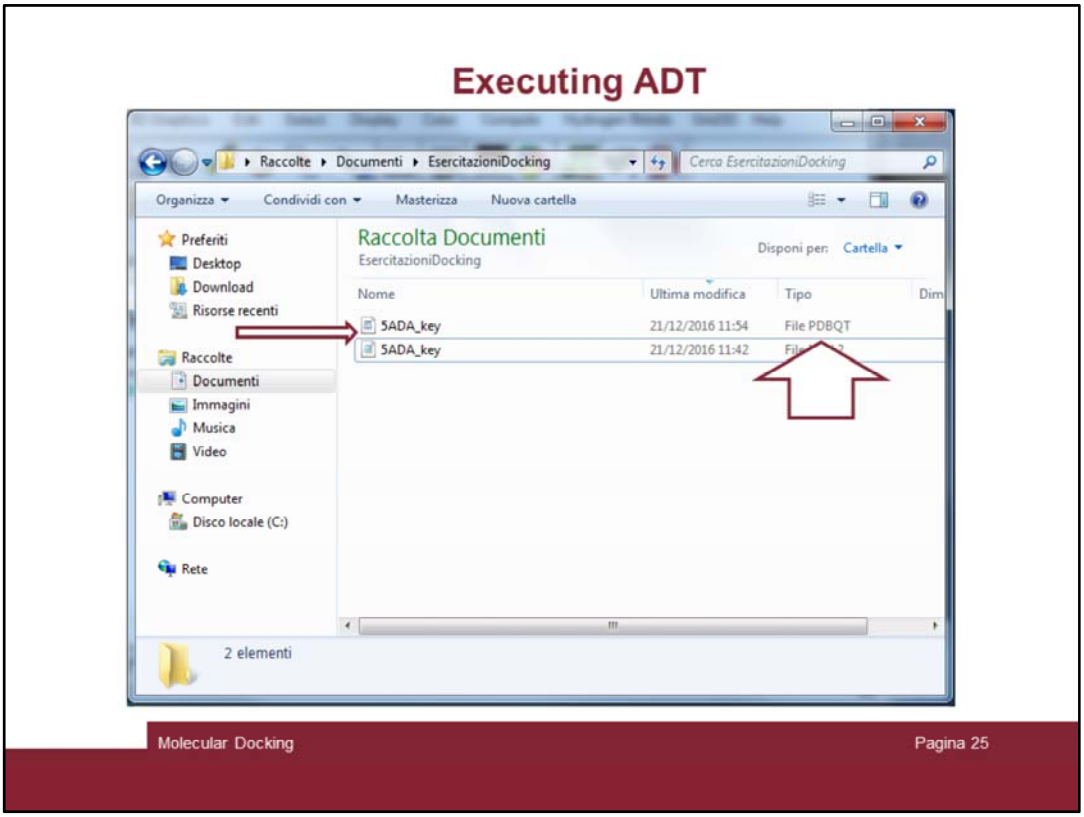


Now let's save the PDBQT file format of the molecule. Click on Ligand → Output → Save as PDBQT …



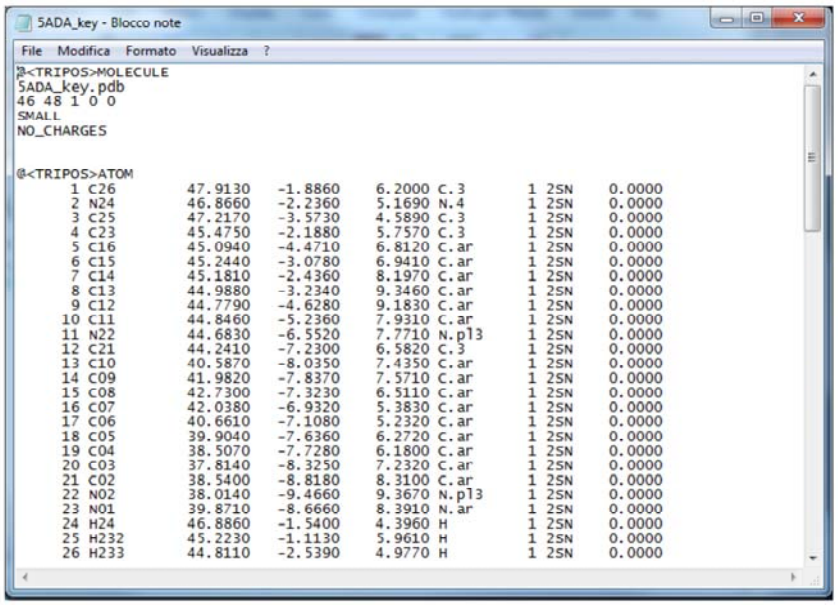
A windows will pop up. Set the file format to «PDBQT files».

Set the folder, the name of the file and save it.



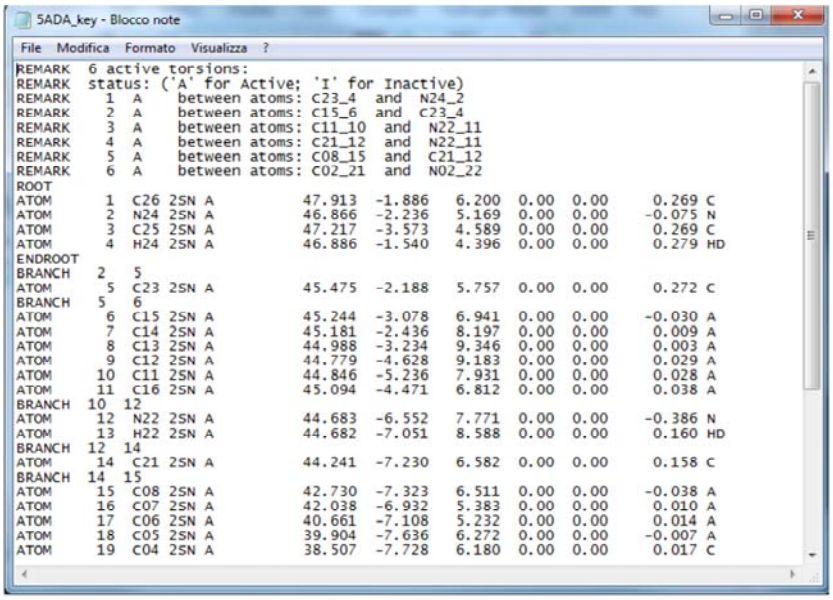
Check the PDBQT file was created

The Mol2 file

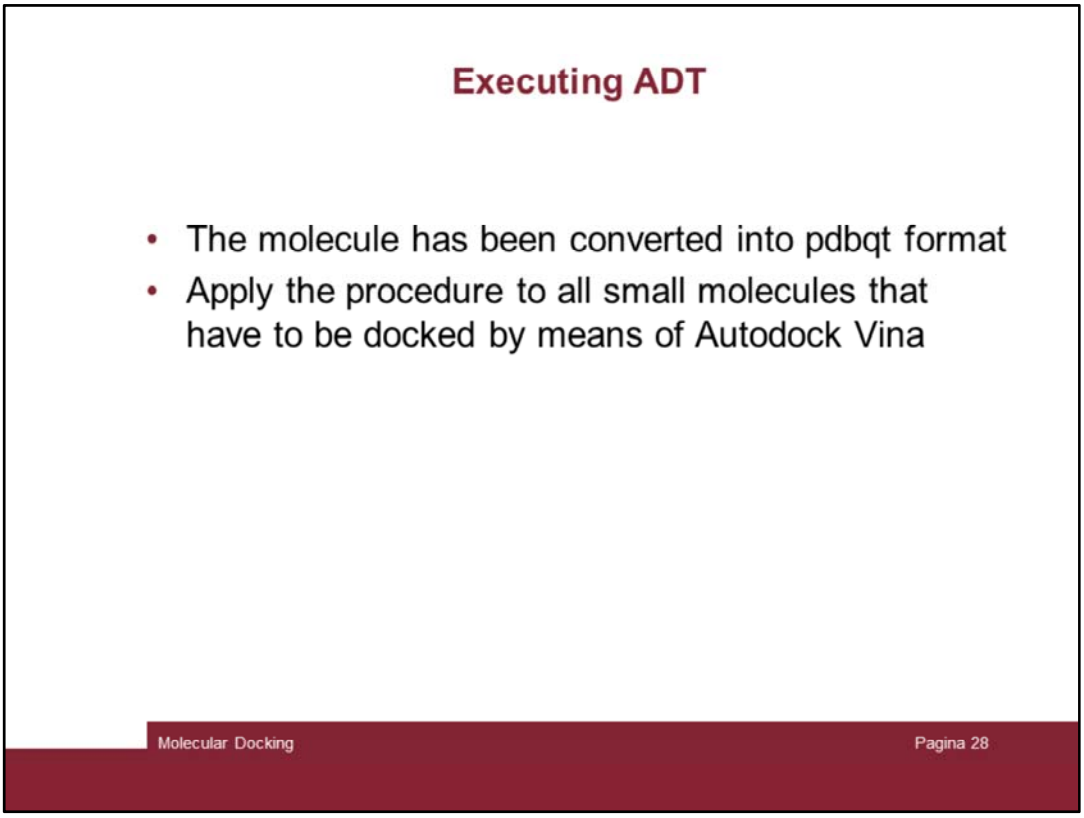


Check the two files by reading them with the Notes Windows program.

The PDBQT file



ADT stands for AutoDock Tools.



ADT stands for AutoDock Tools.