

# Molecular Docking Tutorial

Tutorial to prepare PDBQT files for docking by  
Vina and Autodock



SAPIENZA  
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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.

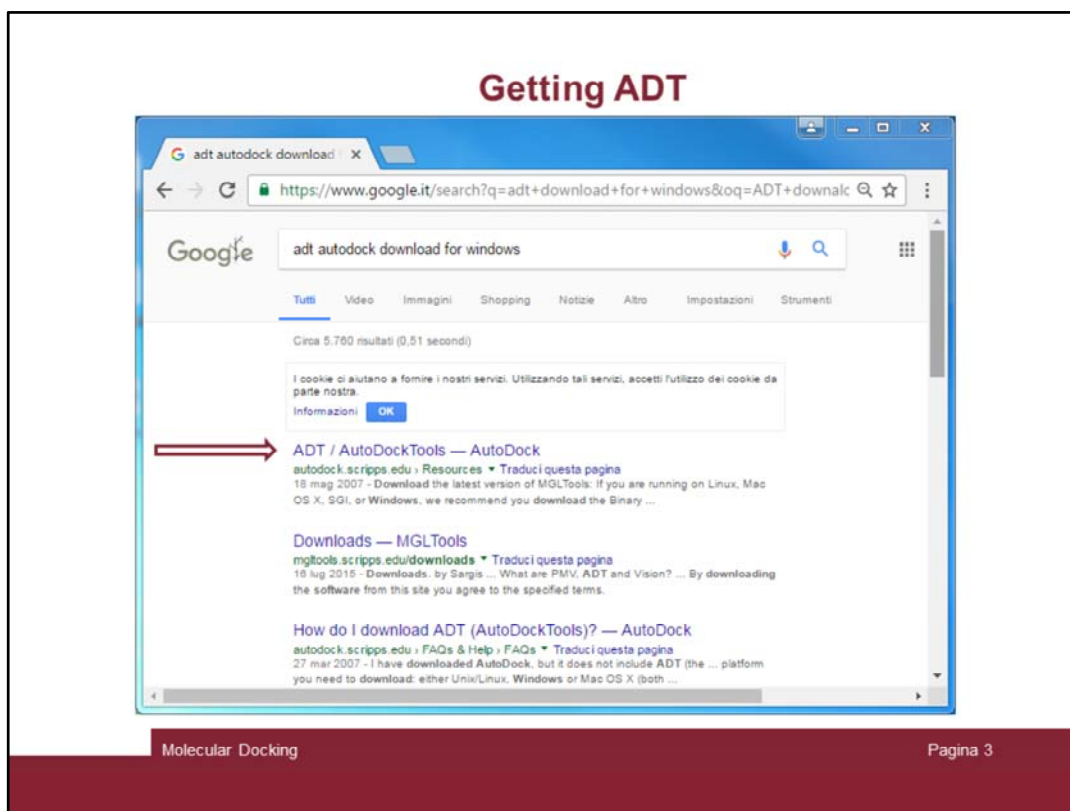
## Overview

- Download of ADT (AutoDock Tools)
- Installation of ADT
- Key preparation (ligand)
- Lock preparation (protein or macromolecule)

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 ...

## Getting ADT

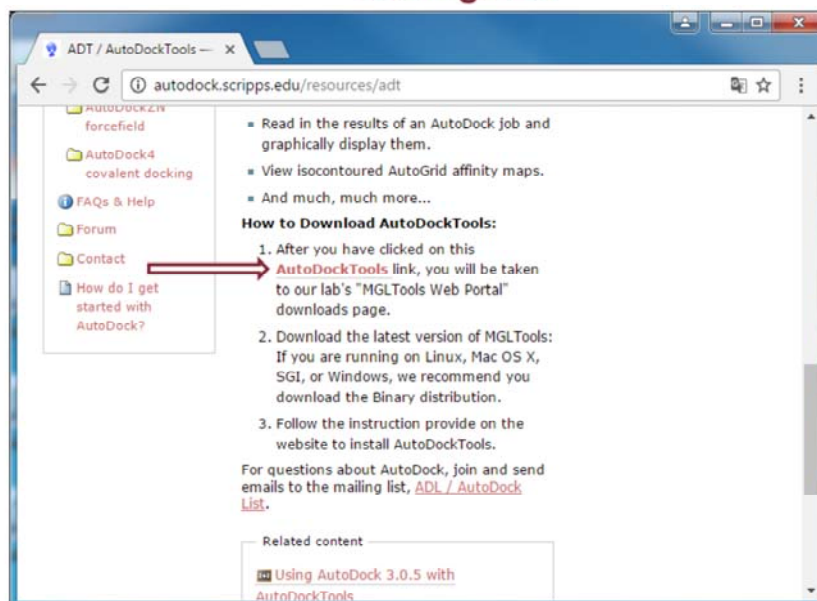
The screenshot shows a web browser window displaying the AutoDock website. The browser's address bar shows the URL `autodock.scripps.edu/resources/adt`. The page features the AutoDock logo and a navigation menu with links for `home`, `downloads`, `resources`, `faq's & help`, `forum`, and `contact`. A search bar is located in the top right corner. The main content area is titled "ADT / AutoDockTools" and includes a sub-header "by [morris](#) — last modified 2007-05-18 07:39". The text describes ADT as a free GUI for AutoDock, developed by the same laboratory. It lists various capabilities: "You can use it to set up, run and analyze AutoDock dockings and isocontour AutoGrid affinity maps, as well as compute molecular surfaces, display secondary structure ribbons, compute hydrogen-bonds, and do many more useful things." Below this, it states: "AutoDockTools, or ADT, is the ultimate GUI to set up, launch and analyze AutoDockruns. With ADT you can...". To the right of the main text is a "news" section with several entries. A red arrow points to the entry: "AutoDock Vina now has an Open Source version" dated 2010-04-20.

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... the AutoDock home page will be reached.  
Scroll down the page ...

## Getting ADT



... and look for the AutodockTools link as indicated by the arrow.  
Click on the link and ...

## Getting ADT



... the MGL Tools web page will open.

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

In the example the windows version will be clicked ...

## Getting ADT



The screenshot shows a web browser window displaying the MGLTools website. The browser's address bar shows the URL `mglttools.scripps.edu/downloads`. The website header includes the MGLTools logo and navigation links: Home, Downloads, Screenshots, Documentation, Packages, eBMV, Support, Forum, and Log in. The main content area is titled "Downloads" and lists various installation packages. A red arrow points to the download link for `mglttools_win32_1.5.6_Setup.exe` in the browser's download bar at the bottom of the window.

Operating System	Package Name
Windows	<code>mglttools_win32_1.5.6_Setup.exe</code>
Windows	<code>mglttools_win32_1.5.6.zip</code>
Linux (x86)	<code>mglttools_Linux-x86_1.5.6_Install</code>
Linux (x86)	<code>mglttools_Linux-x86_1.5.6.tar.gz</code>
Linux (i86)	<code>mglttools_i86Linux2_1.5.6.tar.gz</code>
Linux (x86_64)	<code>mglttools_x86_64Linux2_1.5.6.tar.gz</code>

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And the browser will start downloading it.

## Getting ADT



The screenshot shows the MGLTools website's Downloads page. The page title is "Downloads" and it lists various installation packages for Windows and Linux. A red arrow points to the download link for "mglttools\_win32\_1.5.6\_Setup.exe" in the Windows section.

Operating System	Package Name	Description
Windows	mglttools_win32_1.5.6_Setup.exe	Windows installer
Windows	mglttools_win32_1.5.6.zip	Windows zip file
Linux (x86)	mglttools_Linux-x86_1.5.6_Install	GUI installer (GLIBC_2.3, libstdc++5.X)
Linux (x86)	mglttools_Linux-x86_64Linux2_1.5.6.tar.gz	Tarball installer (GLIBC_2.3, libstdc++5.X)

Navigation: Home, Downloads, Updates, Latest Builds, Screenshots

Footer: Molecular Docking, Pagina 8

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



## Getting ADT



The screenshot shows the MGLTools website's Downloads page. The page title is "Downloads" and it lists various installation packages for different operating systems. A red arrow points to the download link for "mglttools\_win32\_1.5.6\_Setup.exe".

Operating System	Package Name	Description
Windows	mglttools_win32_1.5.6_Setup.exe	Windows Setup
Windows	mglttools_win32_1.5.6.zip	Windows Zip
Linux (x86)	mglttools_Linux-x86_1.5.6_Install	GUI installer (GLIBC_2.3, libstdc++5.X)
Linux (x86)	mglttools_Linux-x86_64Linux2_1.5.6.tar.gz	Tarball installer (GLIBC_2.3, libstdc++5.X)

Navigation: Home, Downloads, Updates, Latest Builds, Screenshots


Footer: Molecular Docking, Pagina 9

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

## Getting ADT



The screenshot shows the MGLTools website's Downloads page. The browser's address bar is at `mglttools.scripps.edu/downloads`. The page header includes navigation links: Home, Downloads, Screenshots, Documentation, Packages, eBMV, Support, Forum, and Log in. The main content area is titled "Downloads" and lists various installation packages. A table of download links is shown below:

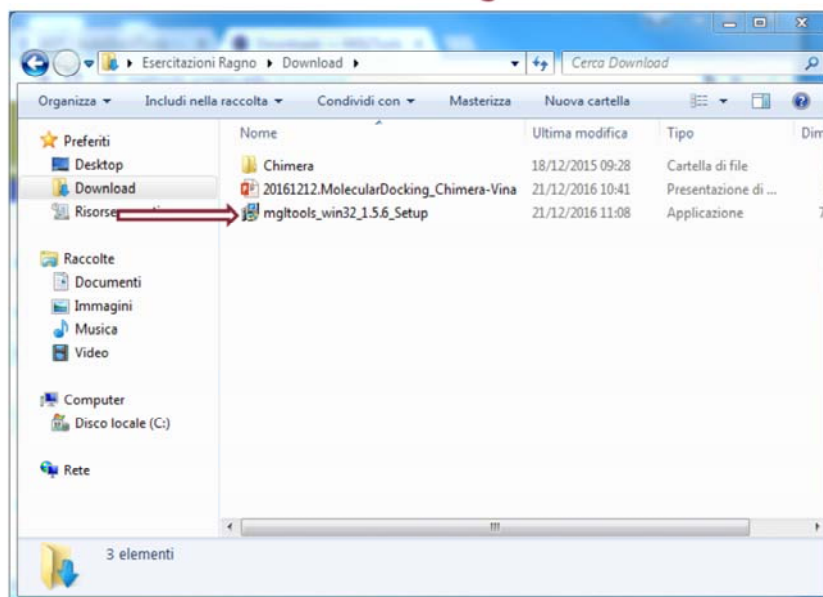
	<a href="#">mgltools_win32_1.5.6_Setup.exe</a>	<a href="#">mgltools_win32_1.5.6.zip</a>
	<a href="#">mgltools_Linux-x86_1.5.6_Install</a> GUI installer (GLIBC_2.3, libstdc++5.X)	<a href="#">mgltools_i86Linux2_1.5.6.tar.gz</a> Tarball installer (GLIBC_2.3, libstdc++5.X)
	<a href="#">mgltools_Linux-x86_64Linux2_1.5.6.tar.gz</a>	

A red arrow points to the download bar at the bottom of the browser window, which shows the file `mgltools_win32_1.5.6_Setup.exe` has been downloaded.

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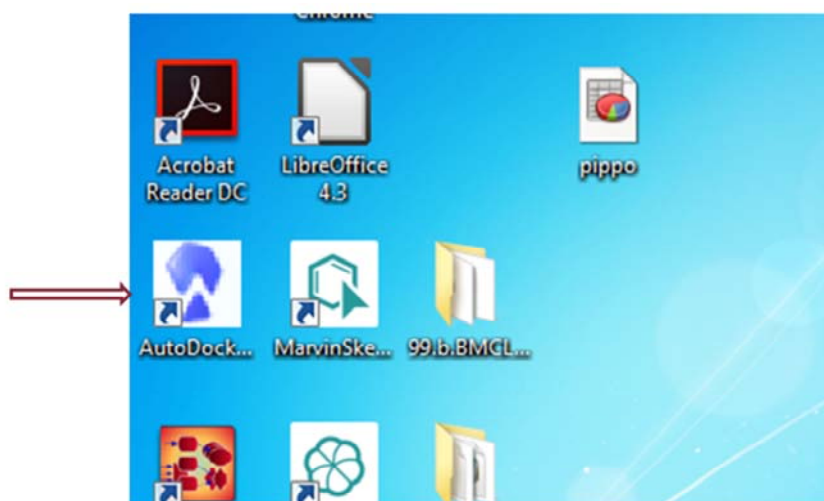
It will take some time (if you have a slow computer or net)

## Installing ADT

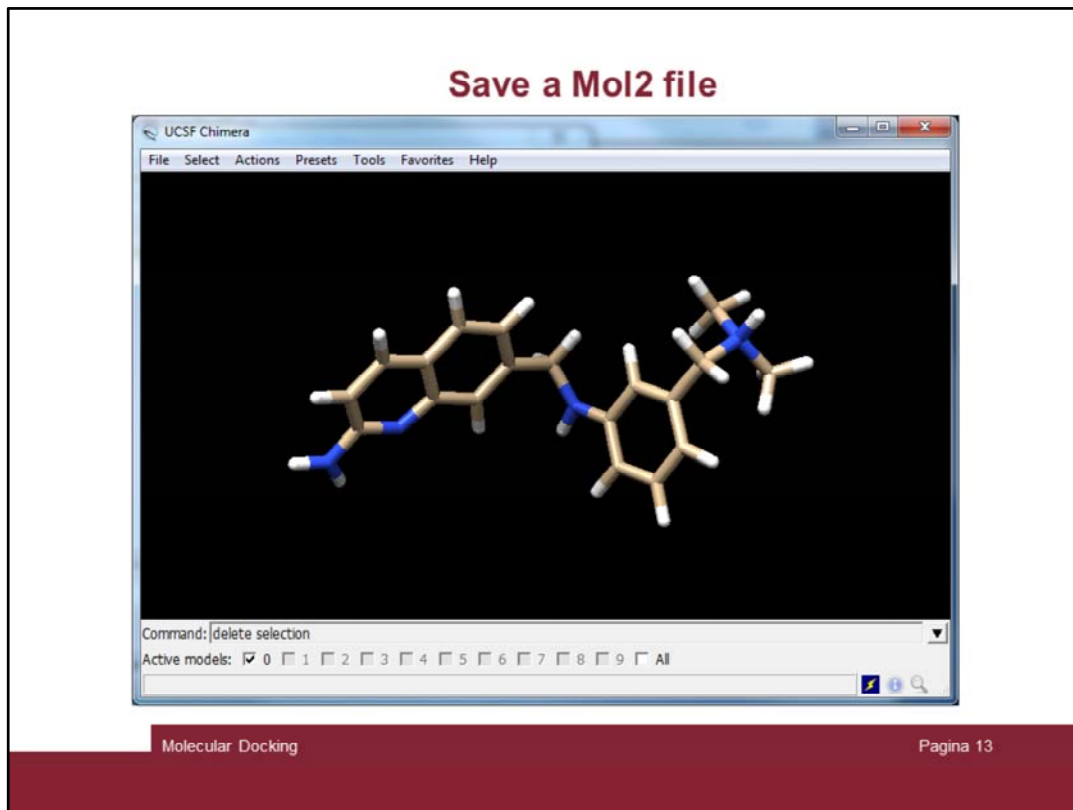


Go to the folder containing the downloaded file and click twice on it and install the program and answer «yes» all the questions the installation program asks

## Installing ADT



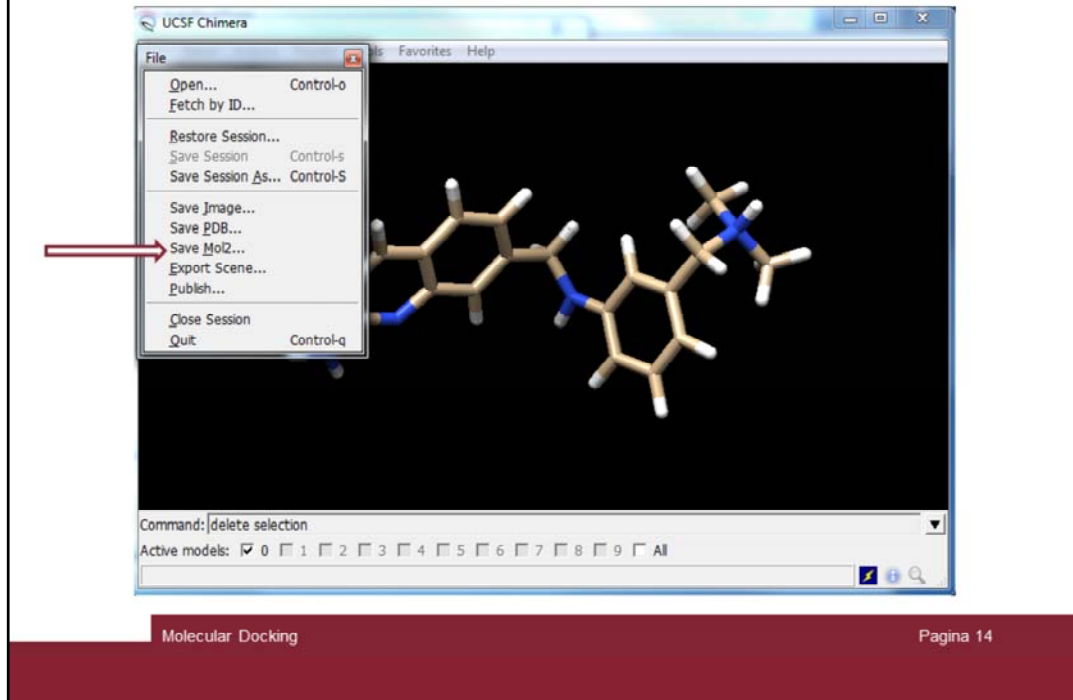
After the installation is finished a some new icons will appear on your desktop. That indicated by the arrow it is the one you need.



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

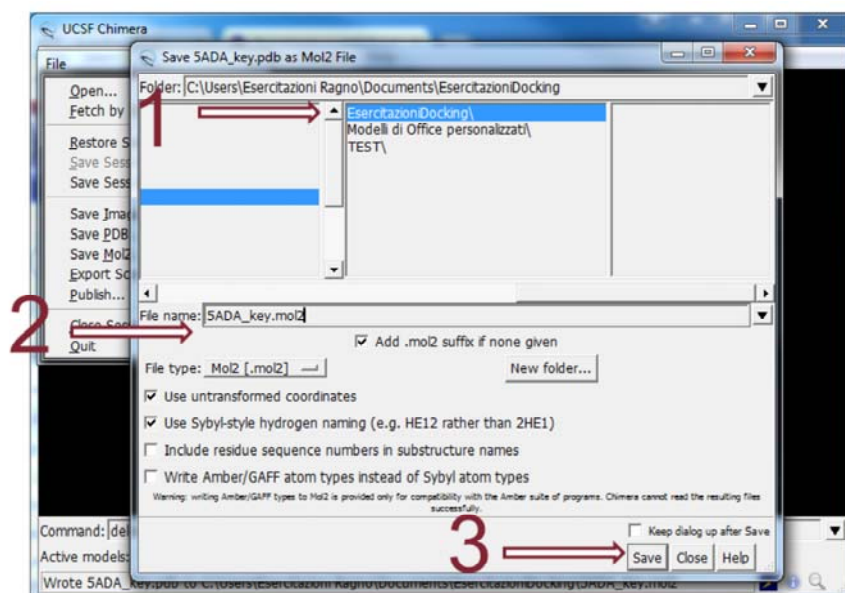
With chimera add all the hydrogens to it and ...

## Save a Mol2 file



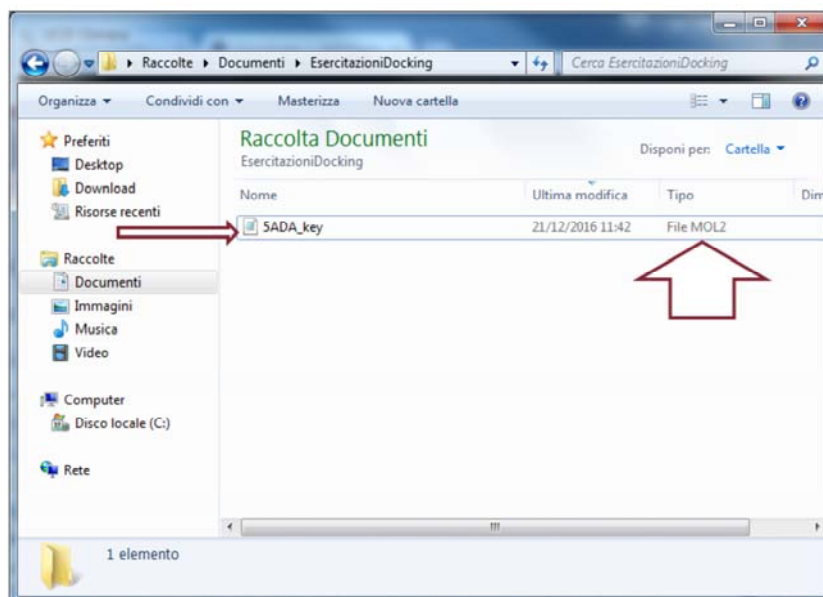
... save the mol in Mol2 (File → Save Mol2 ...)

## Save a Mol2 file



Select the folder, give a name and save it.

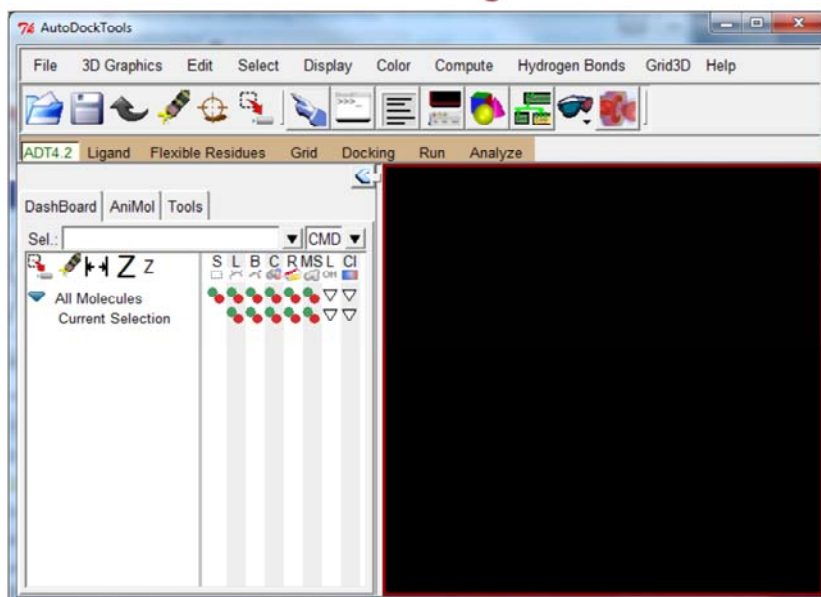
## Save a Mol2 file



Check the mol2 file was created



## Executing ADT

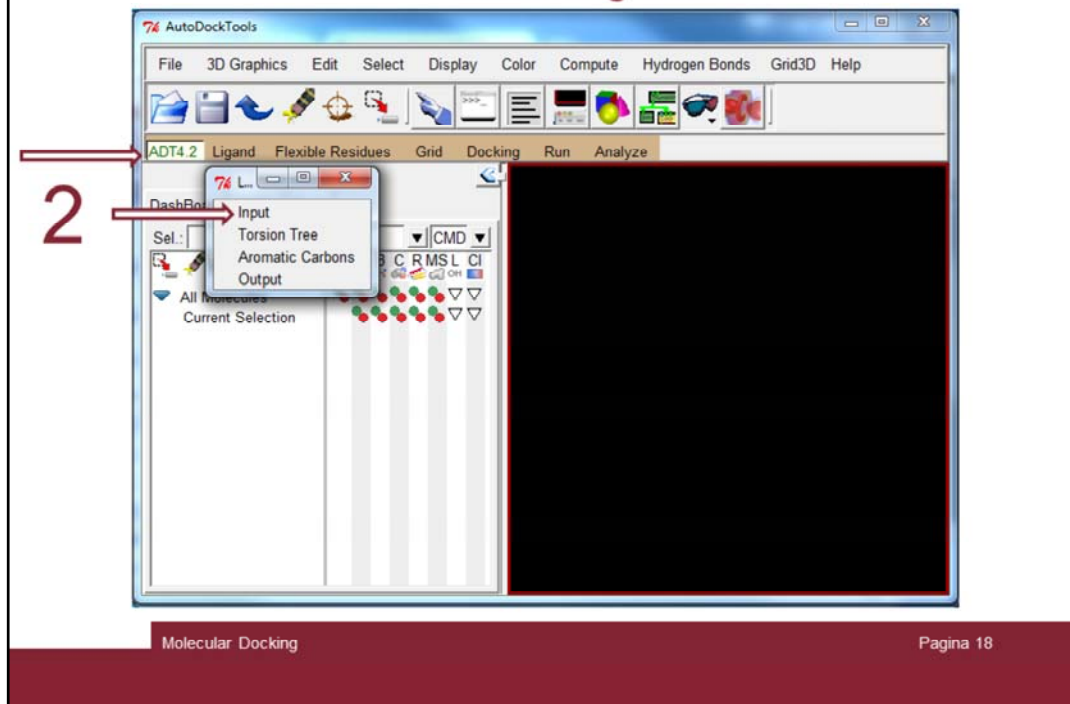


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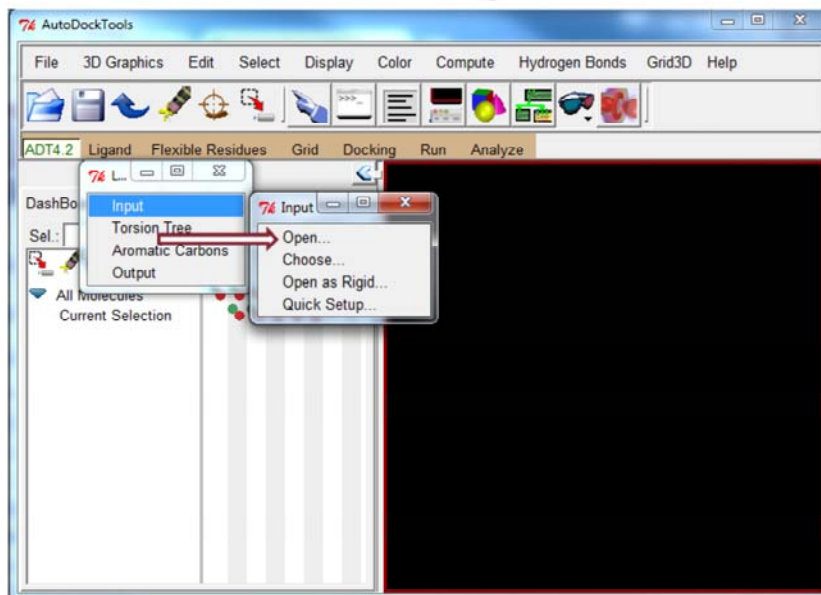
Now click twice on the ADT icon and start the program.

## Executing ADT



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

## Executing ADT

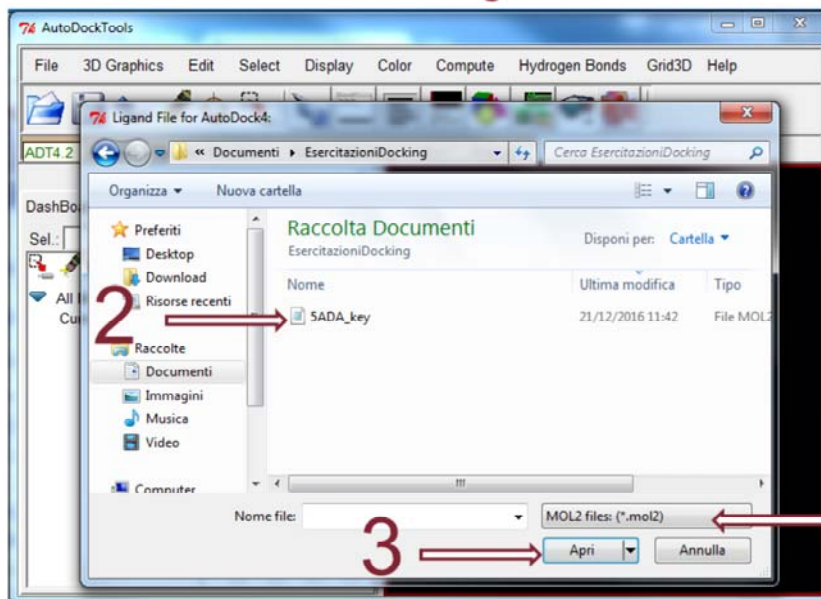


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Then open

## Executing ADT

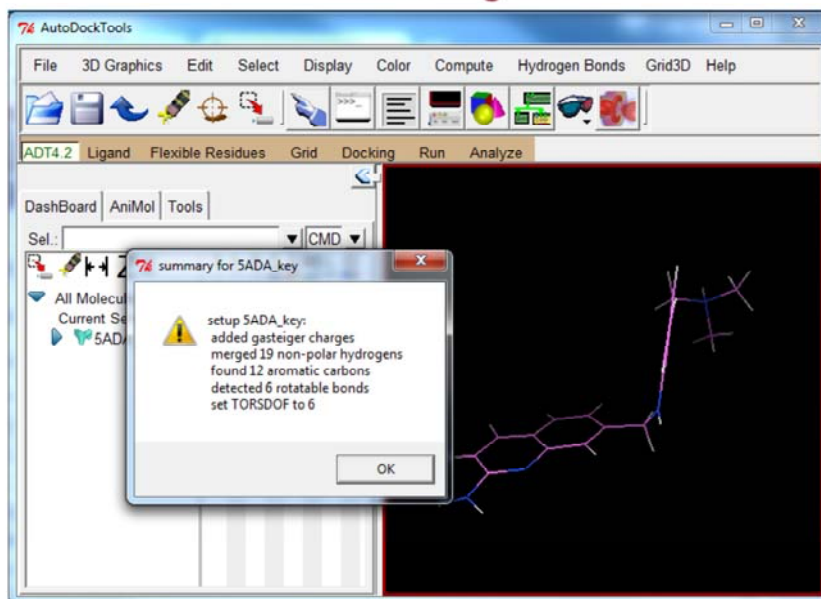


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A windows will pop up. Set the file format to «Mol2 files», Select the file you've created by means of Chimera and open it

## Executing ADT

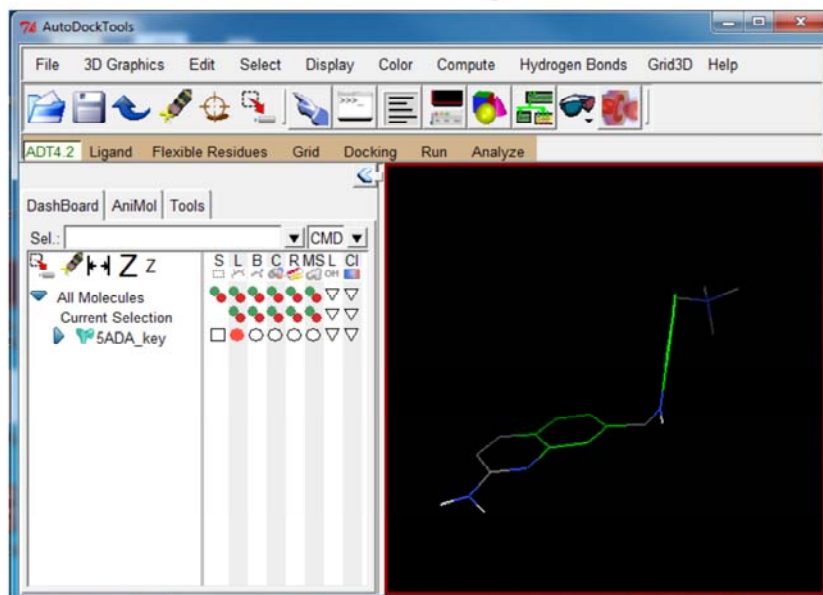


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The program will inform you about some action it applied to the loaded molecule

## Executing ADT

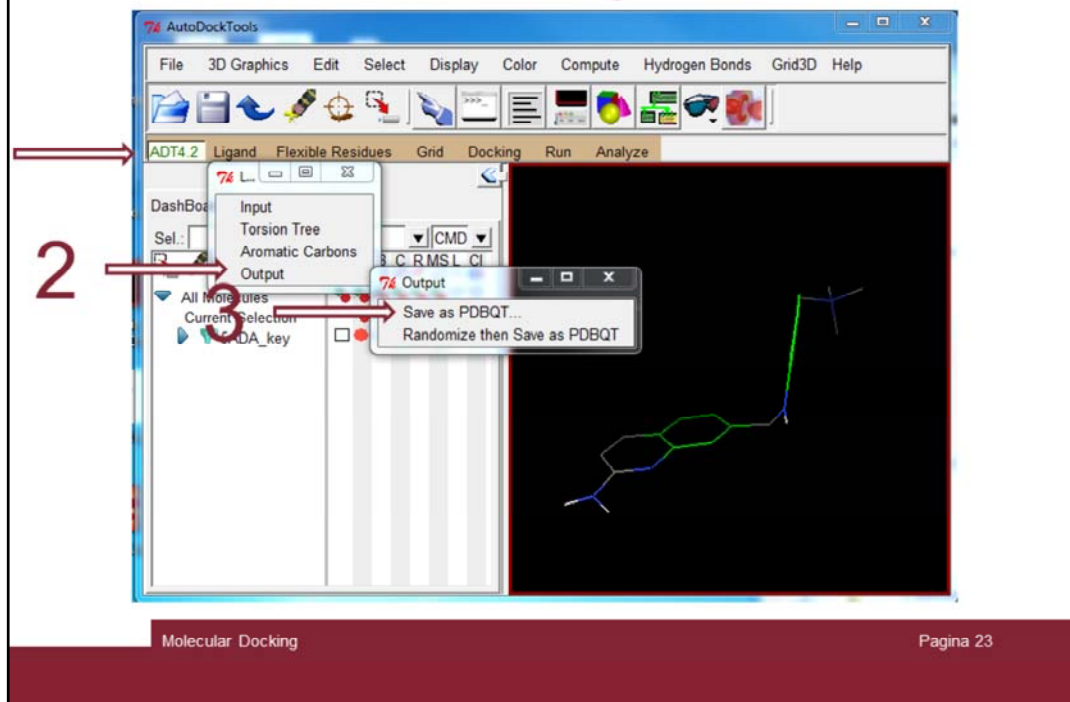


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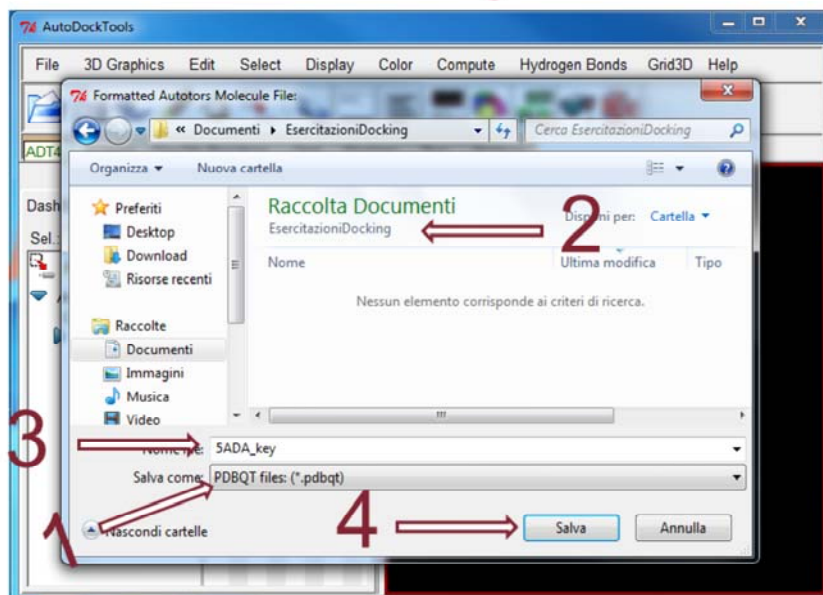
And will show the molecule in the right window (aromatic carbon atoms are colored in green)

## Executing ADT



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

## Executing ADT



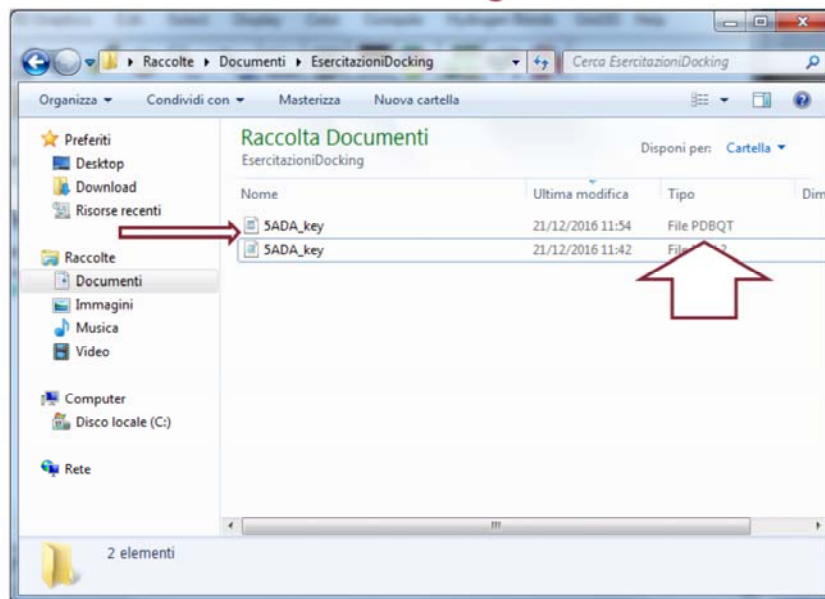
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A windows will pop up. Set the file format to «PDBQT files».  
Set the folder, the name of the file and save it.



## Executing ADT



Check the PDBQT file was created

## The Mol2 file

```
SADA_key - Blocco note
File Modifica Formato Visualizza ?
@<TRIPOS>MOLECULE
SADA_key.pdb
46 48 1 0 0
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C26 47.9130 -1.8860 6.2000 C.3 1 25N 0.0000
2 N24 46.8660 -2.2360 5.1690 N.4 1 25N 0.0000
3 C25 47.2170 -3.5730 4.5890 C.3 1 25N 0.0000
4 C23 45.4750 -2.1880 5.7570 C.3 1 25N 0.0000
5 C16 45.0940 -4.4710 6.8120 C.ar 1 25N 0.0000
6 C15 45.2440 -3.0780 6.9410 C.ar 1 25N 0.0000
7 C14 45.1810 -2.4360 8.1970 C.ar 1 25N 0.0000
8 C13 44.9880 -3.2340 9.3460 C.ar 1 25N 0.0000
9 C12 44.7790 -4.6280 9.1830 C.ar 1 25N 0.0000
10 C11 44.8460 -5.2360 7.9310 C.ar 1 25N 0.0000
11 N22 44.6830 -6.5520 7.7710 N.p13 1 25N 0.0000
12 C21 44.2410 -7.2300 6.5820 C.3 1 25N 0.0000
13 C10 40.5870 -8.0350 7.4350 C.ar 1 25N 0.0000
14 C09 41.9820 -7.8370 7.5710 C.ar 1 25N 0.0000
15 C08 42.7300 -7.3230 6.5110 C.ar 1 25N 0.0000
16 C07 42.0380 -6.9320 5.3830 C.ar 1 25N 0.0000
17 C06 40.6610 -7.1080 5.2320 C.ar 1 25N 0.0000
18 C05 39.9040 -7.6360 6.2720 C.ar 1 25N 0.0000
19 C04 38.5070 -7.7280 6.1800 C.ar 1 25N 0.0000
20 C03 37.8140 -8.3250 7.2320 C.ar 1 25N 0.0000
21 C02 38.5400 -8.8180 8.3100 C.ar 1 25N 0.0000
22 N02 38.0140 -9.4660 9.3670 N.p13 1 25N 0.0000
23 N01 39.8710 -8.6660 8.3910 N.ar 1 25N 0.0000
24 H24 46.8860 -1.5400 4.3960 H 1 25N 0.0000
25 H232 45.2230 -1.1130 5.9610 H 1 25N 0.0000
26 H233 44.8110 -2.5390 4.9770 H 1 25N 0.0000
```

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

## The PDBQT file

```
SADA_key - Blocco note
File Modifica Formato Visualizza ?
REMARK 6 active torsions:
REMARK status: ('A' for Active; 'I' for Inactive)
REMARK 1 A between atoms: C23_4 and N24_2
REMARK 2 A between atoms: C15_6 and C23_4
REMARK 3 A between atoms: C11_10 and N22_11
REMARK 4 A between atoms: C21_12 and N22_11
REMARK 5 A between atoms: C08_15 and C21_12
REMARK 6 A between atoms: C02_21 and N02_22
ROOT
ATOM 1 C26 25N A 47.913 -1.886 6.200 0.00 0.00 0.269 C
ATOM 2 N24 25N A 46.866 -2.236 5.169 0.00 0.00 -0.075 N
ATOM 3 C25 25N A 47.217 -3.573 4.589 0.00 0.00 0.269 C
ATOM 4 H24 25N A 46.886 -1.540 4.396 0.00 0.00 0.279 HD
ENDROOT
BRANCH 2 5
ATOM 5 C23 25N A 45.475 -2.188 5.757 0.00 0.00 0.272 C
BRANCH 5 6
ATOM 6 C15 25N A 45.244 -3.078 6.941 0.00 0.00 -0.030 A
ATOM 7 C14 25N A 45.181 -2.436 8.197 0.00 0.00 0.009 A
ATOM 8 C13 25N A 44.988 -3.234 9.346 0.00 0.00 0.003 A
ATOM 9 C12 25N A 44.779 -4.628 9.183 0.00 0.00 0.029 A
ATOM 10 C11 25N A 44.846 -5.236 7.931 0.00 0.00 0.028 A
ATOM 11 C16 25N A 45.094 -4.471 6.812 0.00 0.00 0.038 A
BRANCH 10 12
ATOM 12 N22 25N A 44.683 -6.552 7.771 0.00 0.00 -0.386 N
ATOM 13 H22 25N A 44.682 -7.051 8.588 0.00 0.00 0.160 HD
BRANCH 12 14
ATOM 14 C21 25N A 44.241 -7.230 6.582 0.00 0.00 0.158 C
BRANCH 14 15
ATOM 15 C08 25N A 42.730 -7.323 6.511 0.00 0.00 -0.038 A
ATOM 16 C07 25N A 42.038 -6.932 5.383 0.00 0.00 0.010 A
ATOM 17 C06 25N A 40.661 -7.108 5.232 0.00 0.00 0.014 A
ATOM 18 C05 25N A 39.904 -7.636 6.272 0.00 0.00 -0.007 A
ATOM 19 C04 25N A 38.507 -7.728 6.180 0.00 0.00 0.017 C
```

ADT stands for AutoDock Tools.

## Executing ADT

- The molecule has been converted into pdbqt format
- Apply the procedure to all small molecules that have to be docked by means of Autodock Vina

ADT stands for AutoDock Tools.