MoPro.11   Tutorial

** 1 **   Fill in the registration form on the website:

http://www.crystallography.fr/crm2/fr/labo/equipes/emqc/mopro-download.html

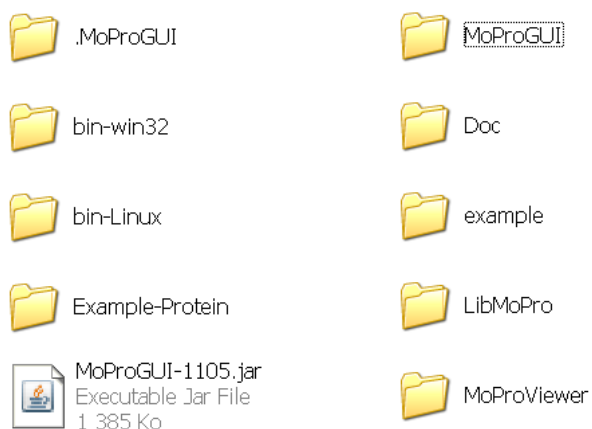**After obtaining the password, download the MoProSuite package on the website**

and unzip the file MoProSuite.zip

A "MoProSuite" directory containing the package will be extracted.

** 2 ** Execute the MoProGUI.jar   Graphical User Interface

MoProGUI.jar requires JAVA version 5 to be installed on your computer.
It is downloadable at http://java.sun.com/javase/downloads/index.jsp

On windows double click on MoProGUI.jar

|	
.MoProGUI	MoProGUI
bin-win32	Doc
bin-Linux	example
Example-Protein	LibMoPro
MoProGUI-1105.jar Executable Jar File 1 385 Ko	MoProViewer

Under DOS or linux/unix, go to the directory MoProSuite containing the java executable

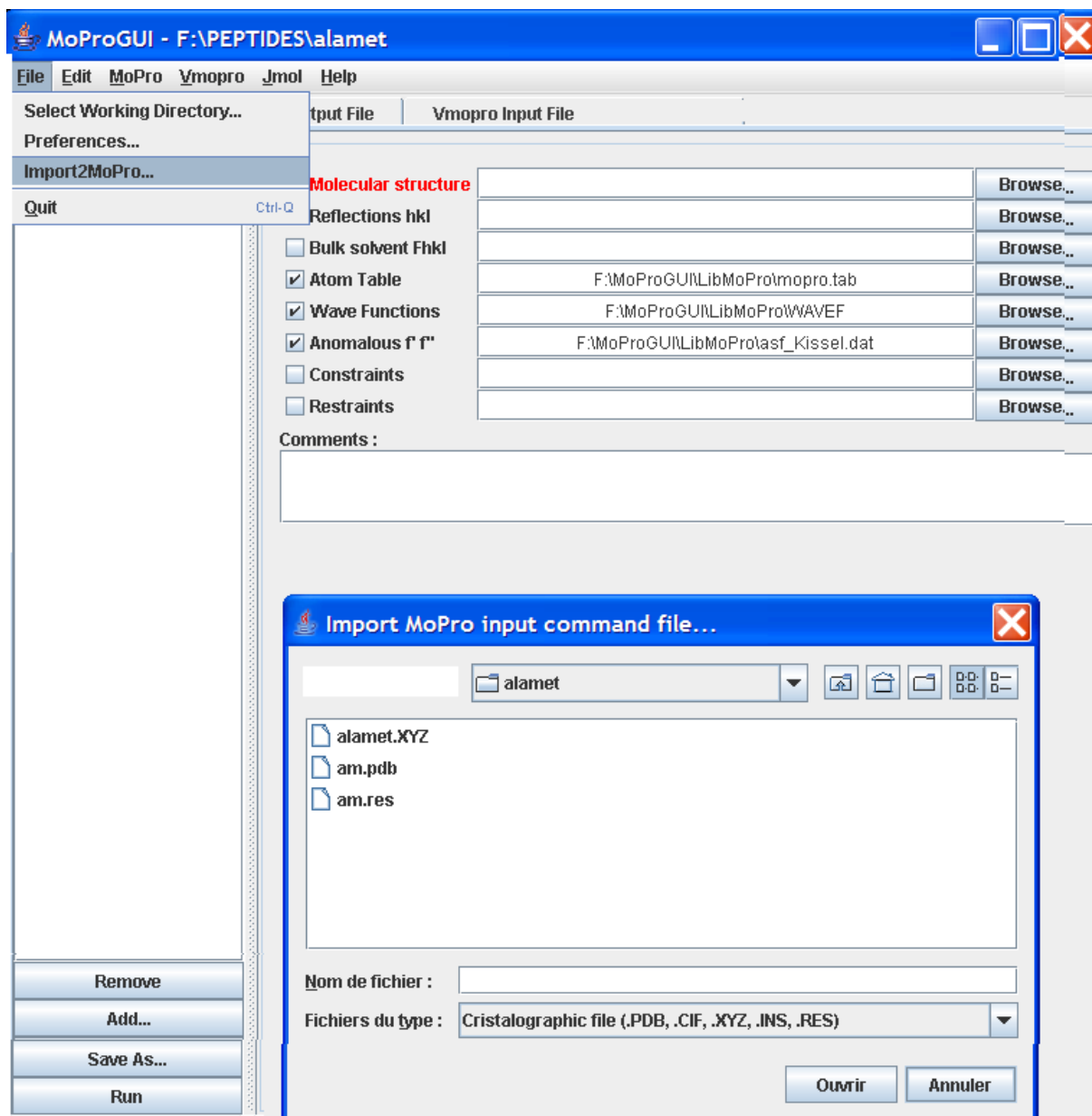file MoProGUI.jar and type :

 java –jar MoProGUI.jar

** 3 ** Select the Working Directory
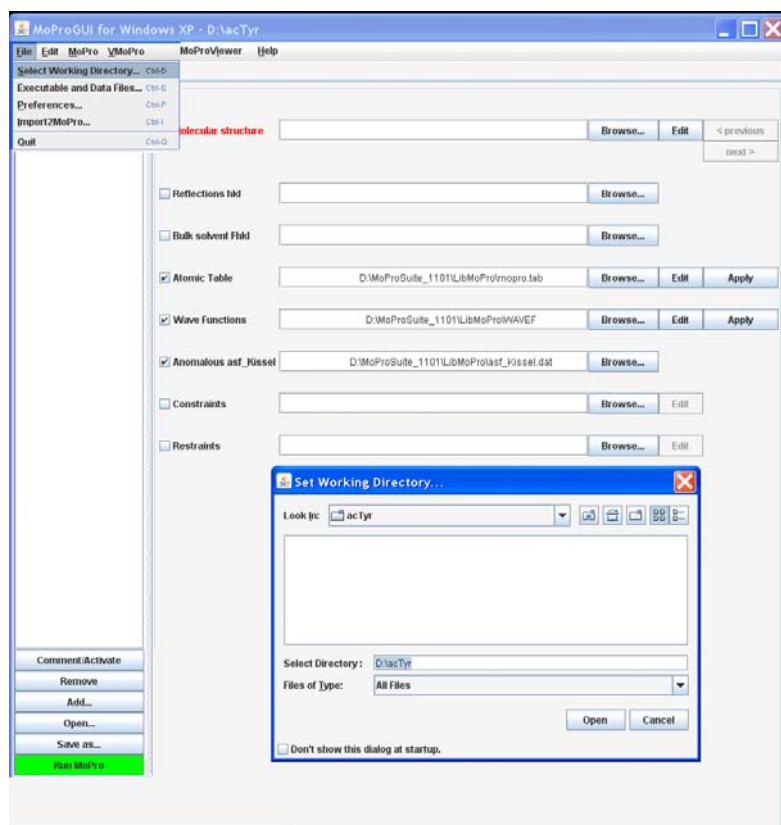
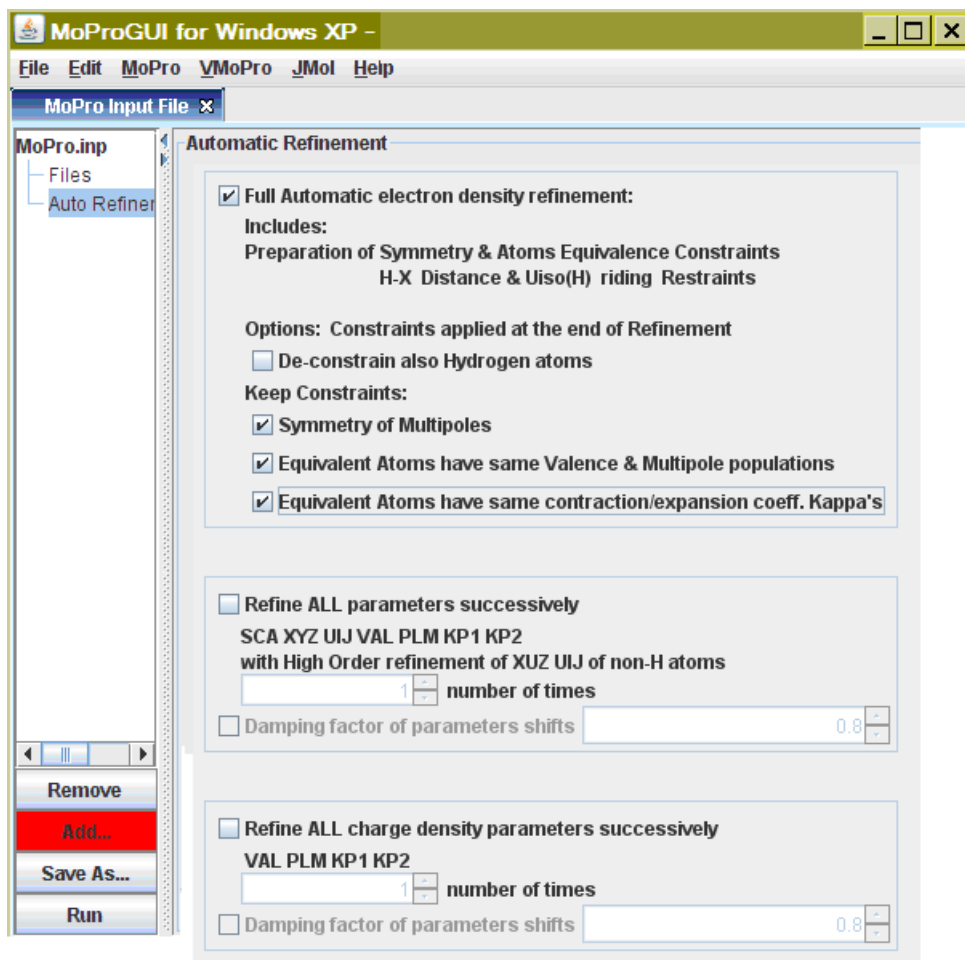**** 4 **** Check if the executable files in the "FILE" menu are correctly assigned.
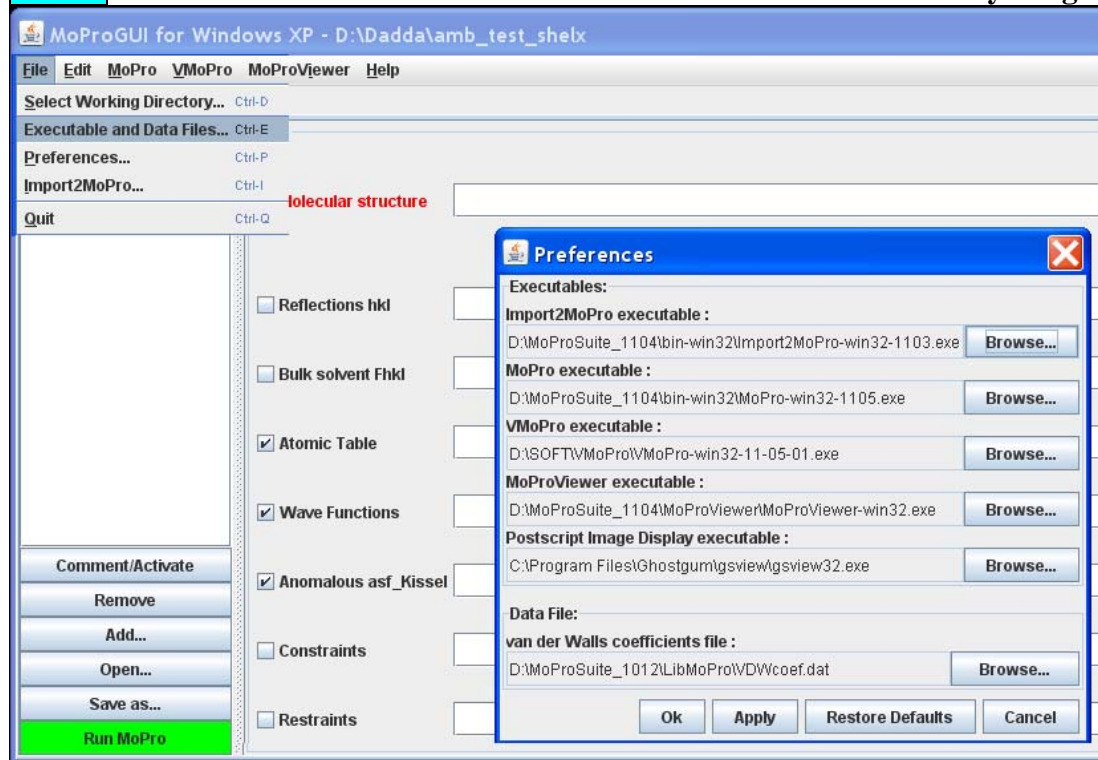
** 5 ** **Import a molecular structure file to MoPro format.**
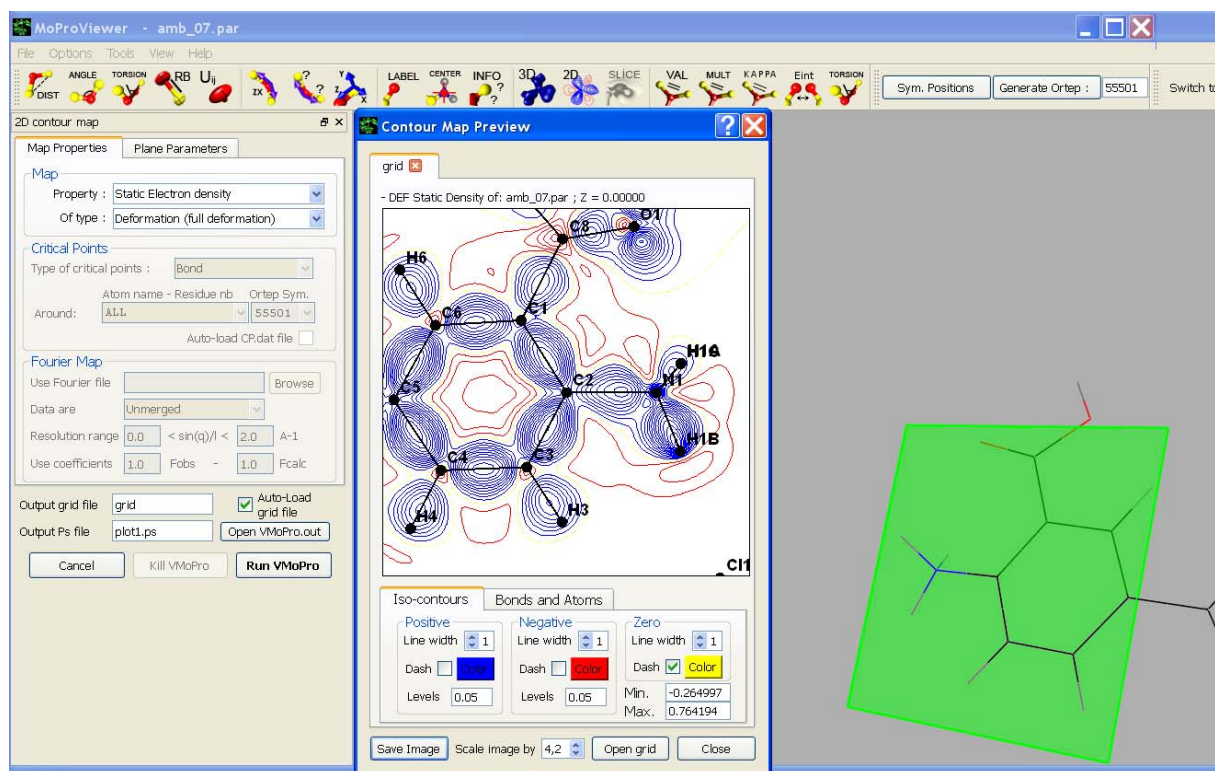
6 **Run MoPro for an automatic electron density refinement**

** 7 ** **Molecule can be displayed with MoProViewer.**

Menus for computation of 2D or 3D molecular properties maps
are available in MoProViewer.

** 8 ** **Run VMoPro to compute molecular properties**

DOS window appears :

When running directly VMoPro, all its functionalities appear.

Enter the selected command and reply to interactive questions.

When VMoPro is finished, a "vmopro.inp" file is created, which contains all the answers entered.

For a Fourier map calculation, a .FOUR file is necessary,
It is generated by MoPro command "WRIT FOUR", in Output Files Menu.

VMoPro can also be run in batch using an input commands file (vmopro.inp).

Postscript files may be displayed notably
with GSview 4.8.
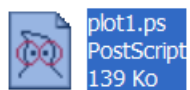
.cube maps can be displayed
with MoProViewer or Molekel

Xplor-CNS 3D maps can be displayed
with MoproViewer or Pymol.