

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

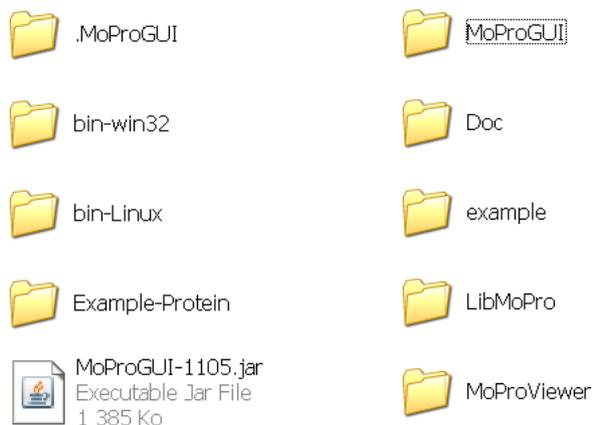
and unzip the file **MoProSuite.zip**

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>

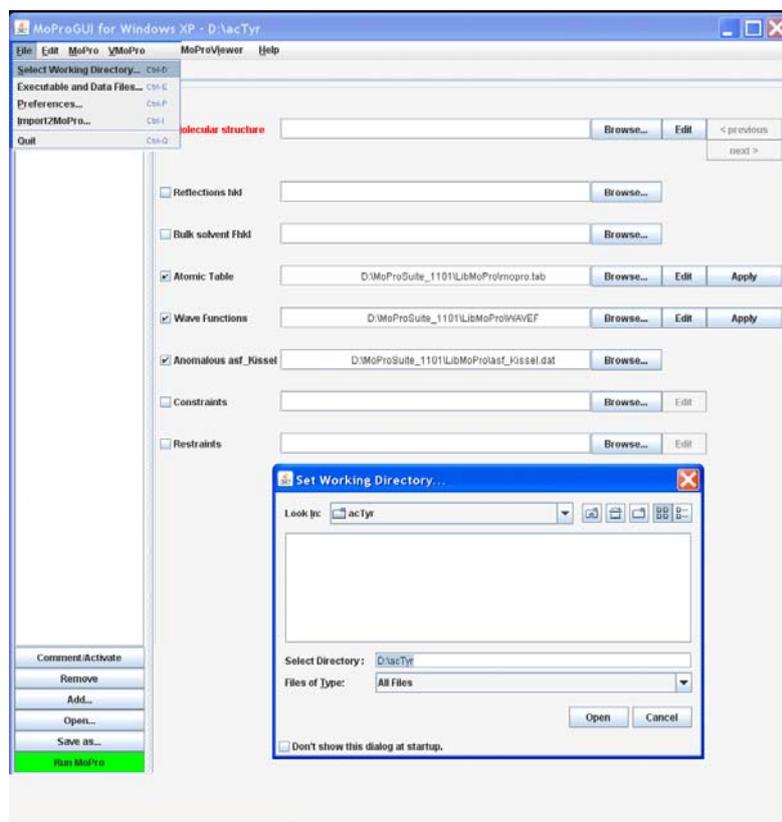
On windows double click on **MoProGUI.jar**



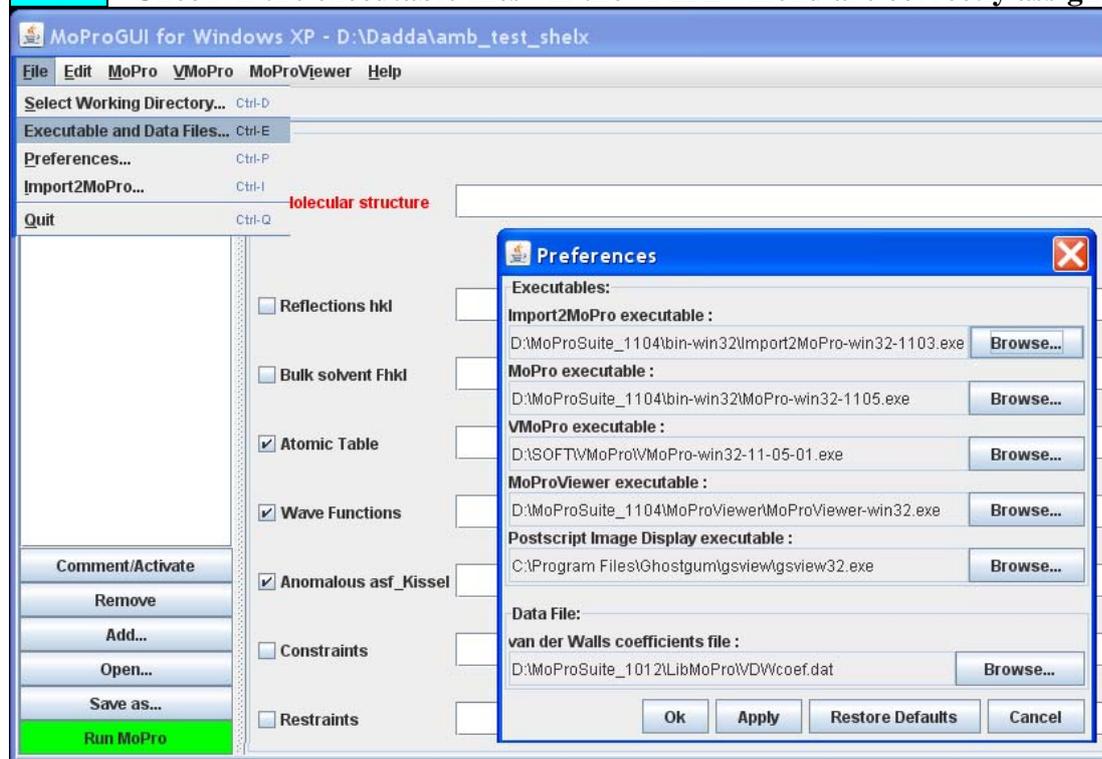
Under DOS or linux/unix, go to the directory **MoProSuite** containing the java executable file **MoProGUI.jar** and type :

java -jar MoProGUI.jar

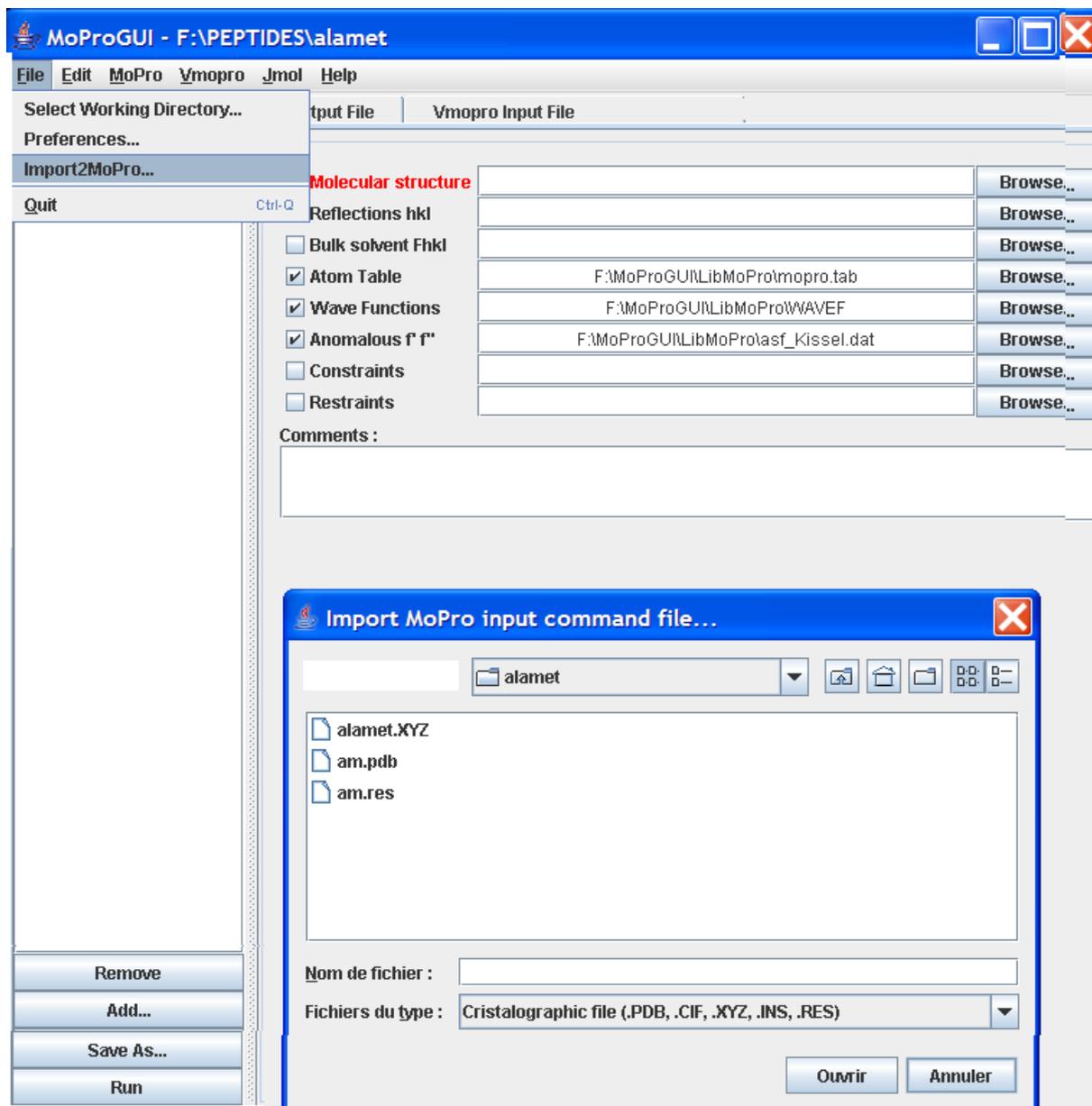
**** 3 **** Select the Working Directory



**** 4 **** Check if the executable files in the "FILE" menu are correctly assigned.

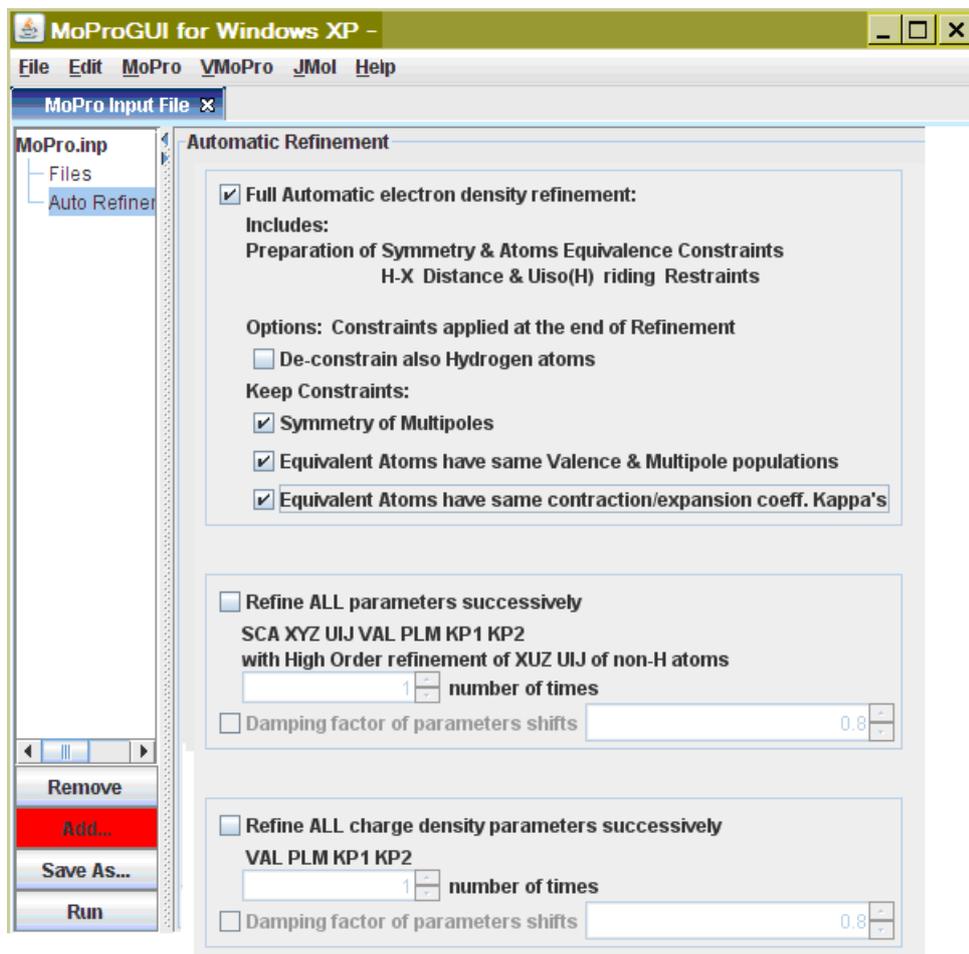


**** 5 **** Import a molecular structure file to MoPro format.

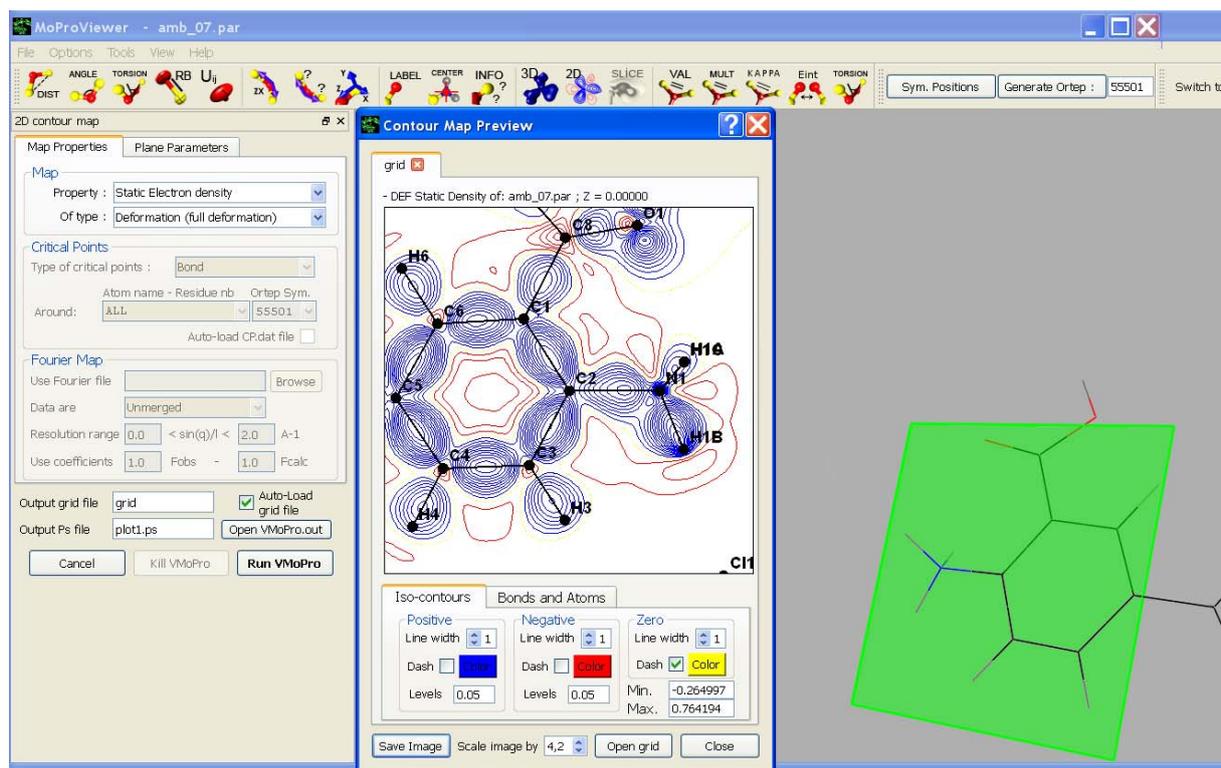


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Run MoPro for an automatic electron density refinement

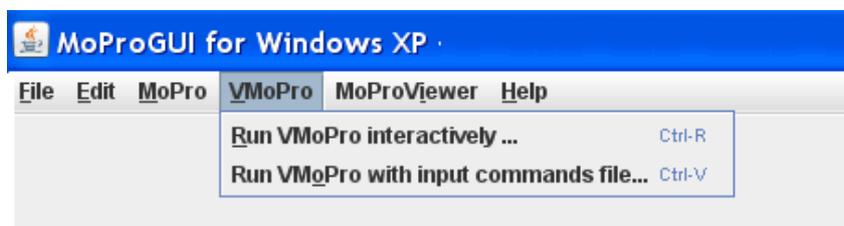


**** 7 **** Molecule can be displayed with MoProViewer.



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

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



DOS window appears :

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vmopro > Possible commands:
INIT : initialize VMoPro Library & Graphics Display

STAT : STATic (deformation) electron density
ELEC : ELECTrostatic potential map
FOUR : FOURier m*Fo-n*Fc electron density
LAPL : LAPLacian of total electron density
GRAN : GRADient Norm of electron density or electrostatic potential
CRIT : find CRITical points
ENER : ENERgy computations
INTE : INTEgrations of density or potential

SELE : define atoms SELECTION for property calculation
PARA : read new MoPro molecular parameters file
PLOT : create & PLOT postscript image from 2D grid
GRID : GRIDs handling
CONT : set Gradient / Basin / IsoCONTOur lines options

SYST command : call system to apply a command e.g.: SYST ls SYST dir
HELP ? : help, list of commands
QUIT EXIT STOP END
vmopro > _
```

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.

