

# Tutorial

## **MoProSuite : Crystallographic software for charge density refinement**

<http://crm2.univ-lorraine.fr/lab/software/mopro/download-mopro/>

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MoProSuite working under Windows, linux & mac.

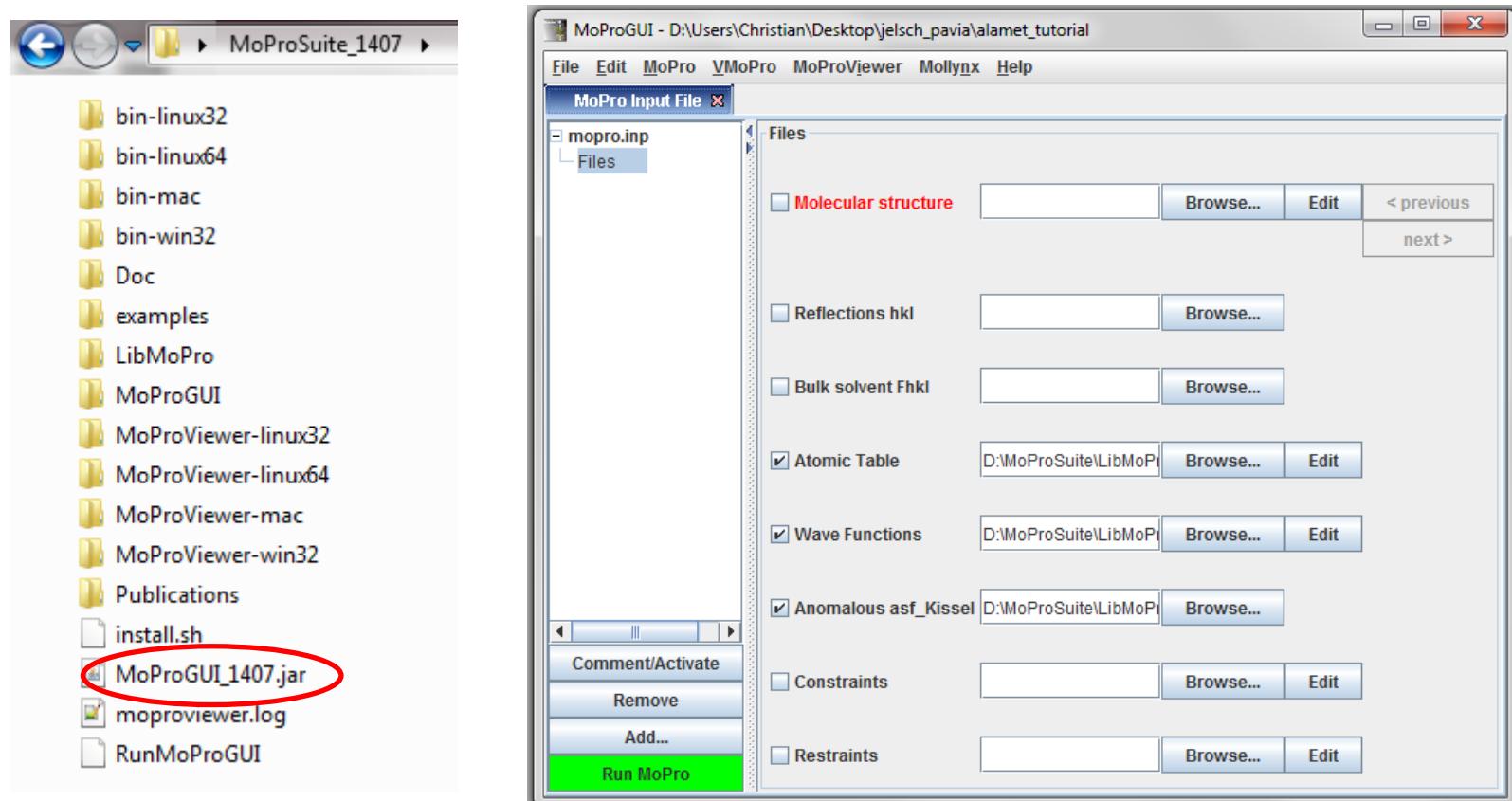
29<sup>th</sup> ECM  
Crystallographic Computing School



Croatia, Rovinj 20th-21st August 2015

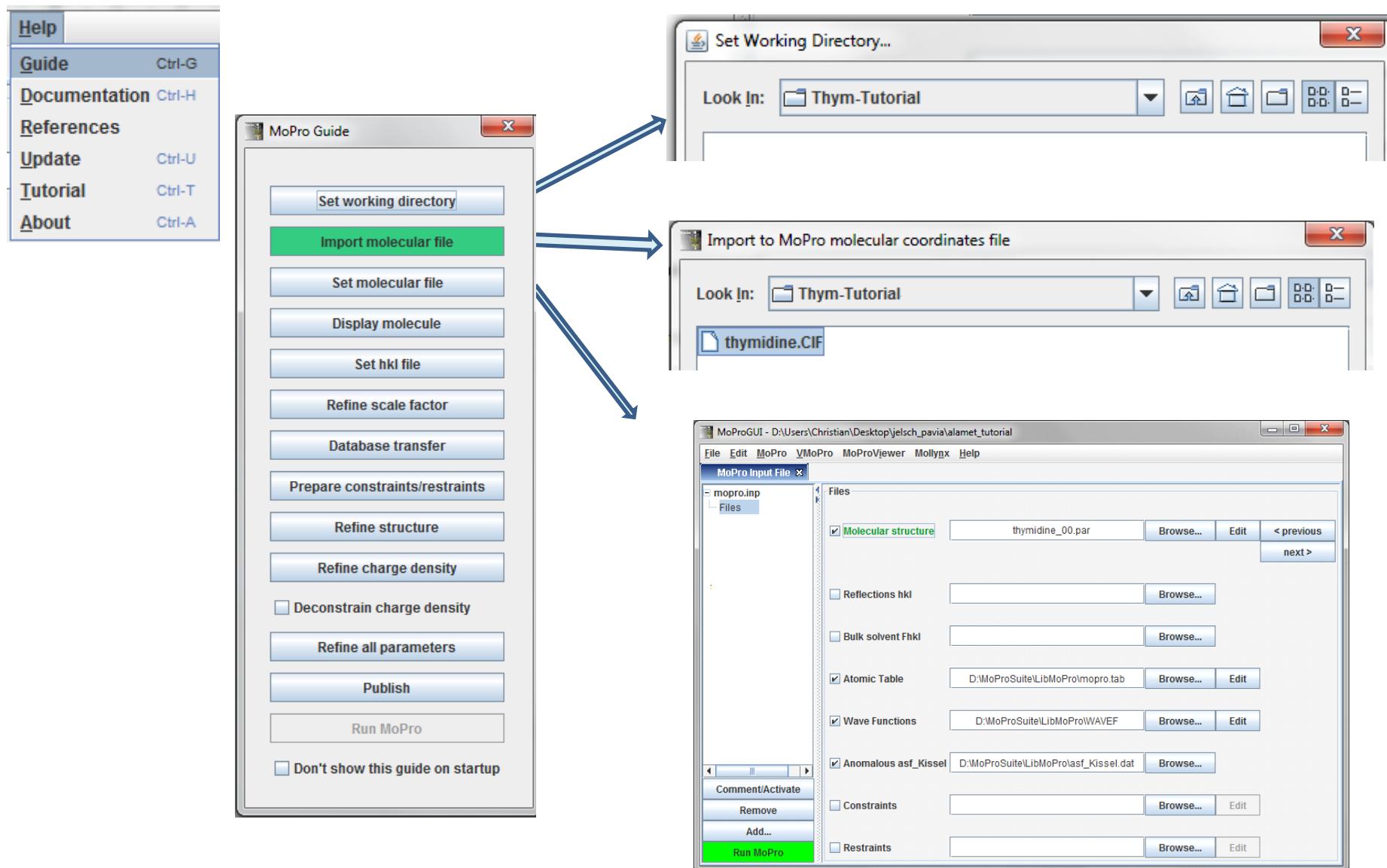
## Step 1 Launch MoProGUI

### MoPro Graphical User Interface



Requires JAVA, which can be downloaded at:  
<https://www.java.com/fr/download/>

## Step 2 initial steps : follow the GUIDE

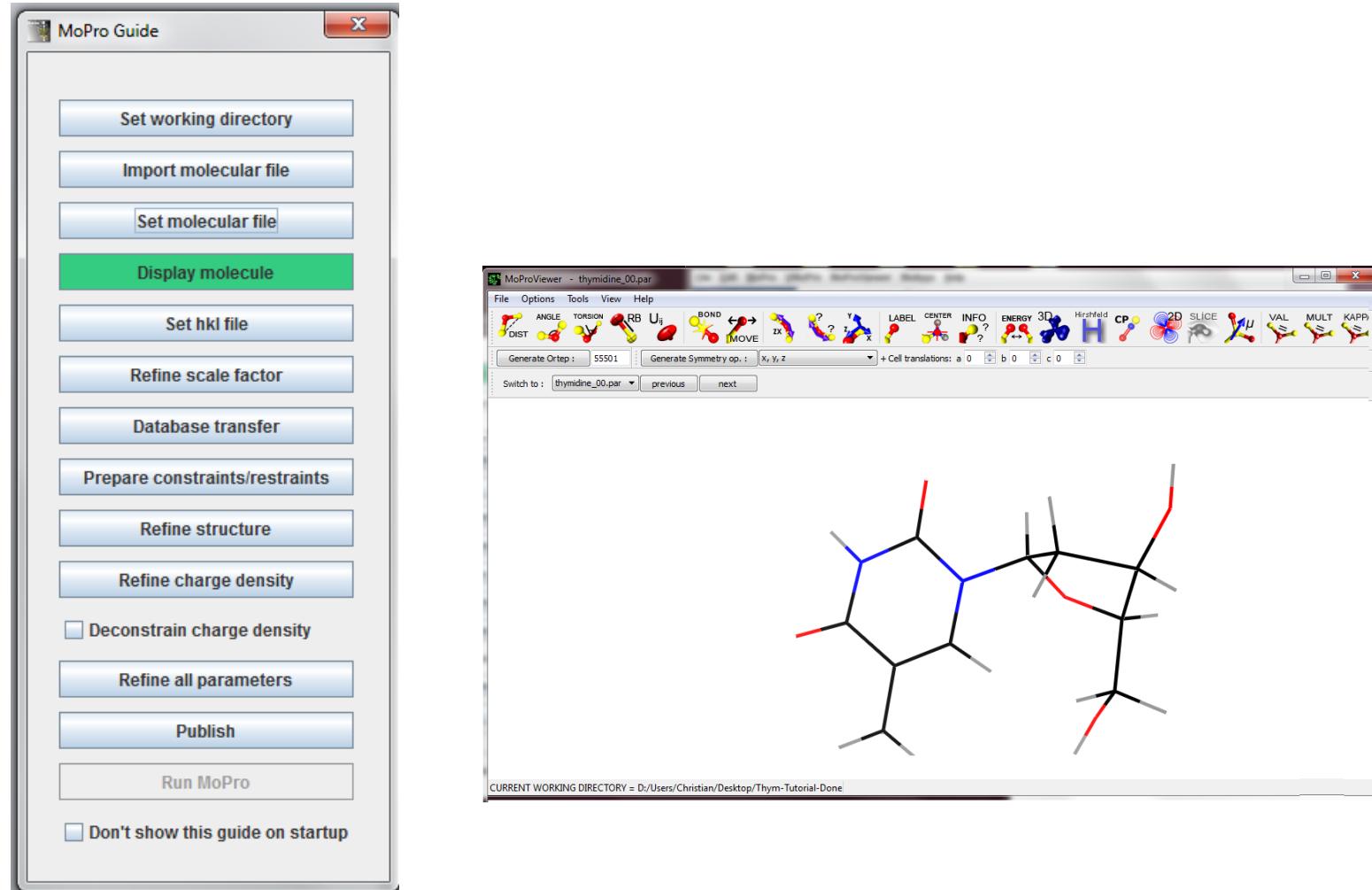


## Step 3 Display molecule with MoProViewer

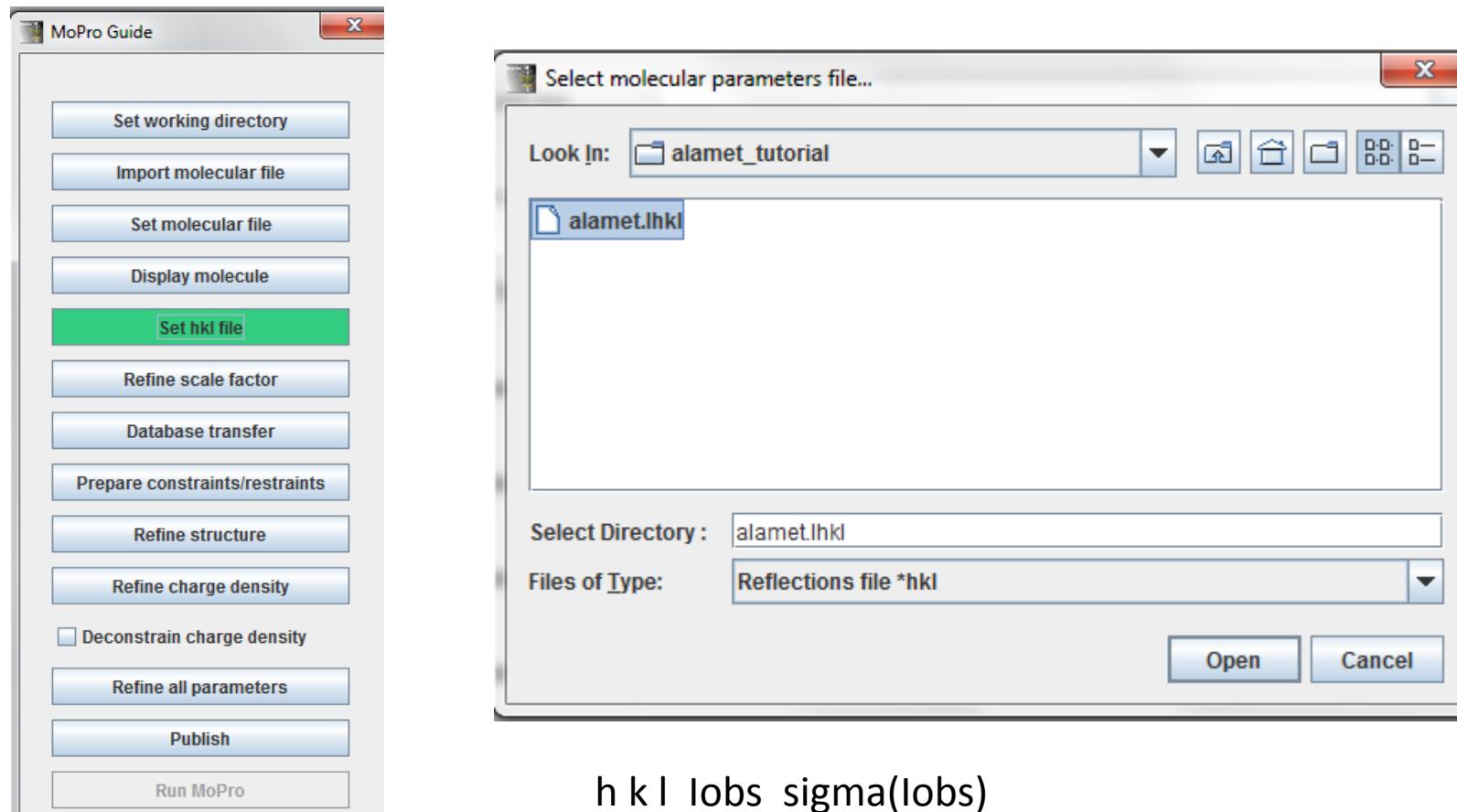
The MoPro Guide window on the left shows the following buttons:

- Set working directory
- Import molecular file
- Set molecular file
- Display molecule** (highlighted in green)
- Set hkl file
- Refine scale factor
- Database transfer
- Prepare constraints/restraints
- Refine structure
- Refine charge density
- Deconstrain charge density
- Refine all parameters
- Publish
- Run MoPro
- Don't show this guide on startup

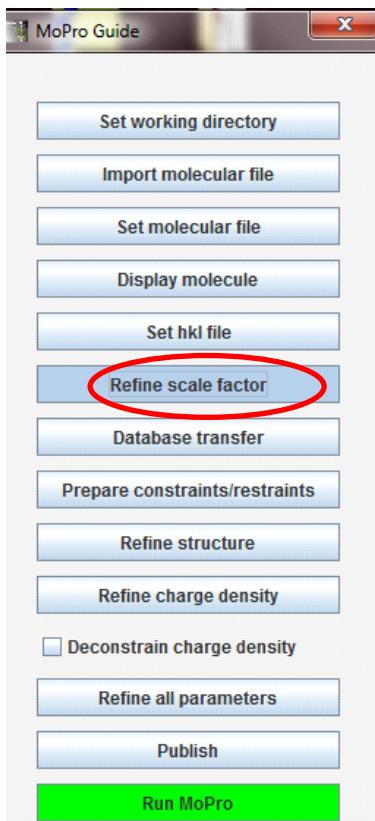
The MoProViewer window on the right displays a 3D molecular model of thymidine. The interface includes a toolbar with various molecular manipulation tools like DIST, ANGLE, TORSION, RB, U<sub>j</sub>, MOVE, and many others. The current working directory is set to D:/Users/Christian/Desktop/Thym-Tutorial-Done.



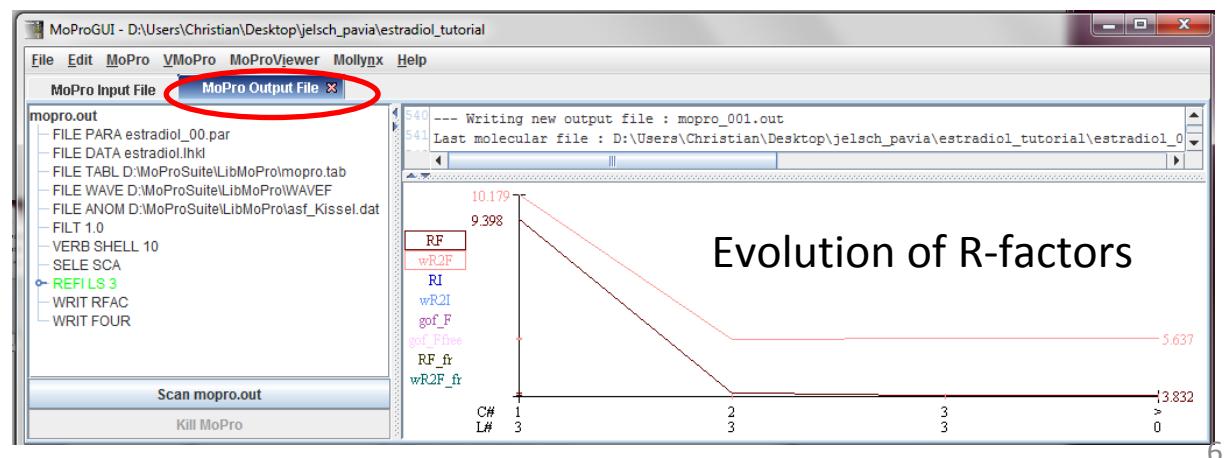
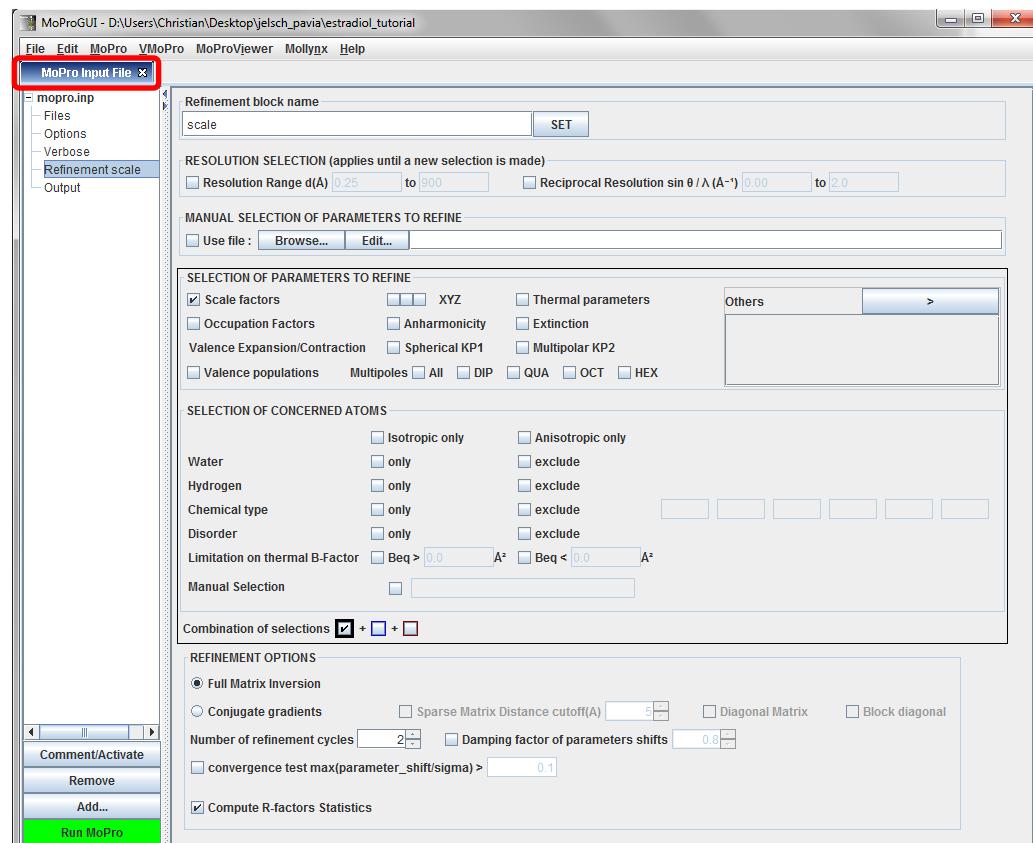
## Step 4 Select reflections file



## Step 5 Refine SCAlE factor

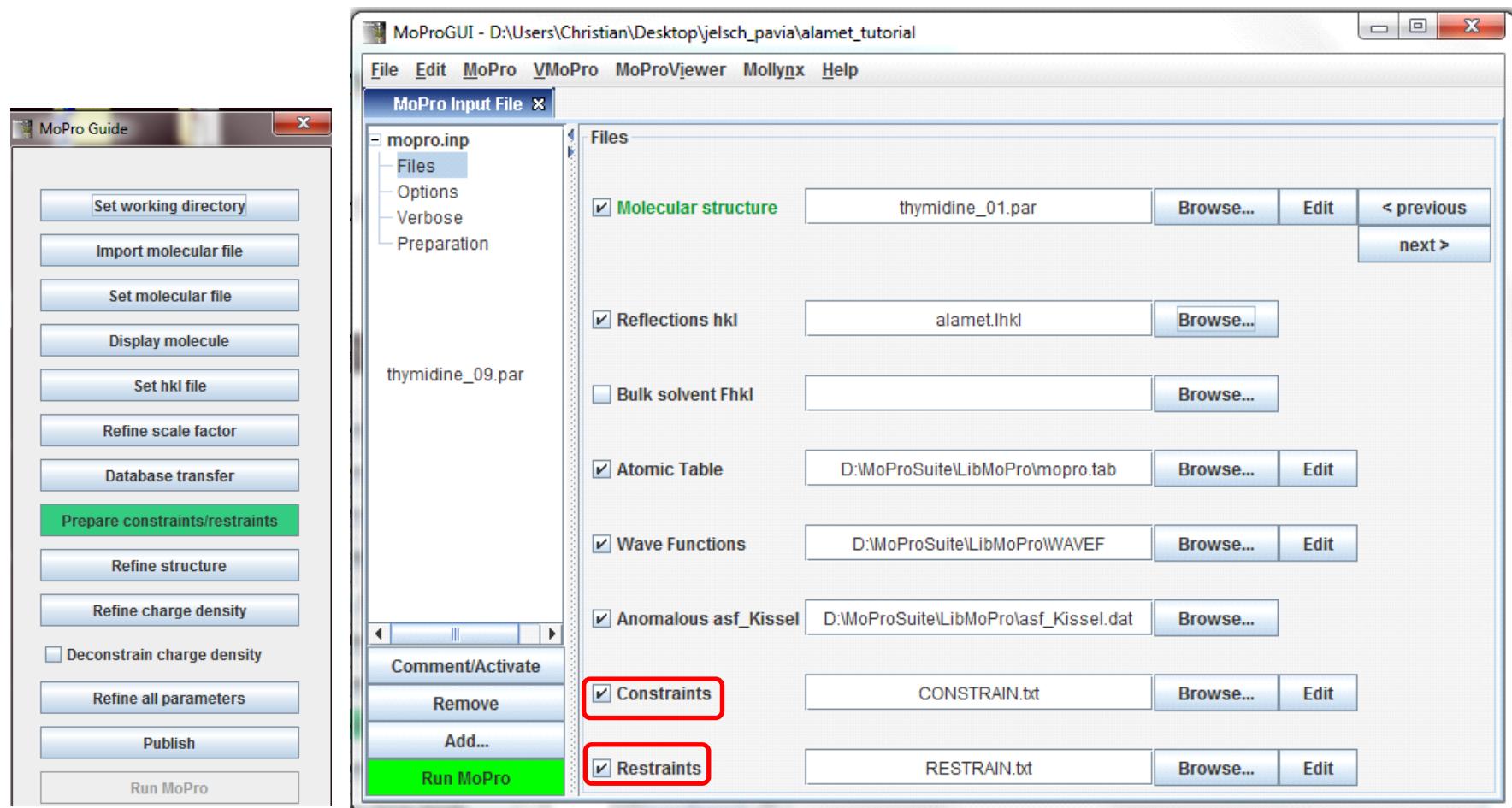


Click on  
"mopro Input file"  
&  
"mopro Output file"



## Step 6 Preparation of constraints & restraints

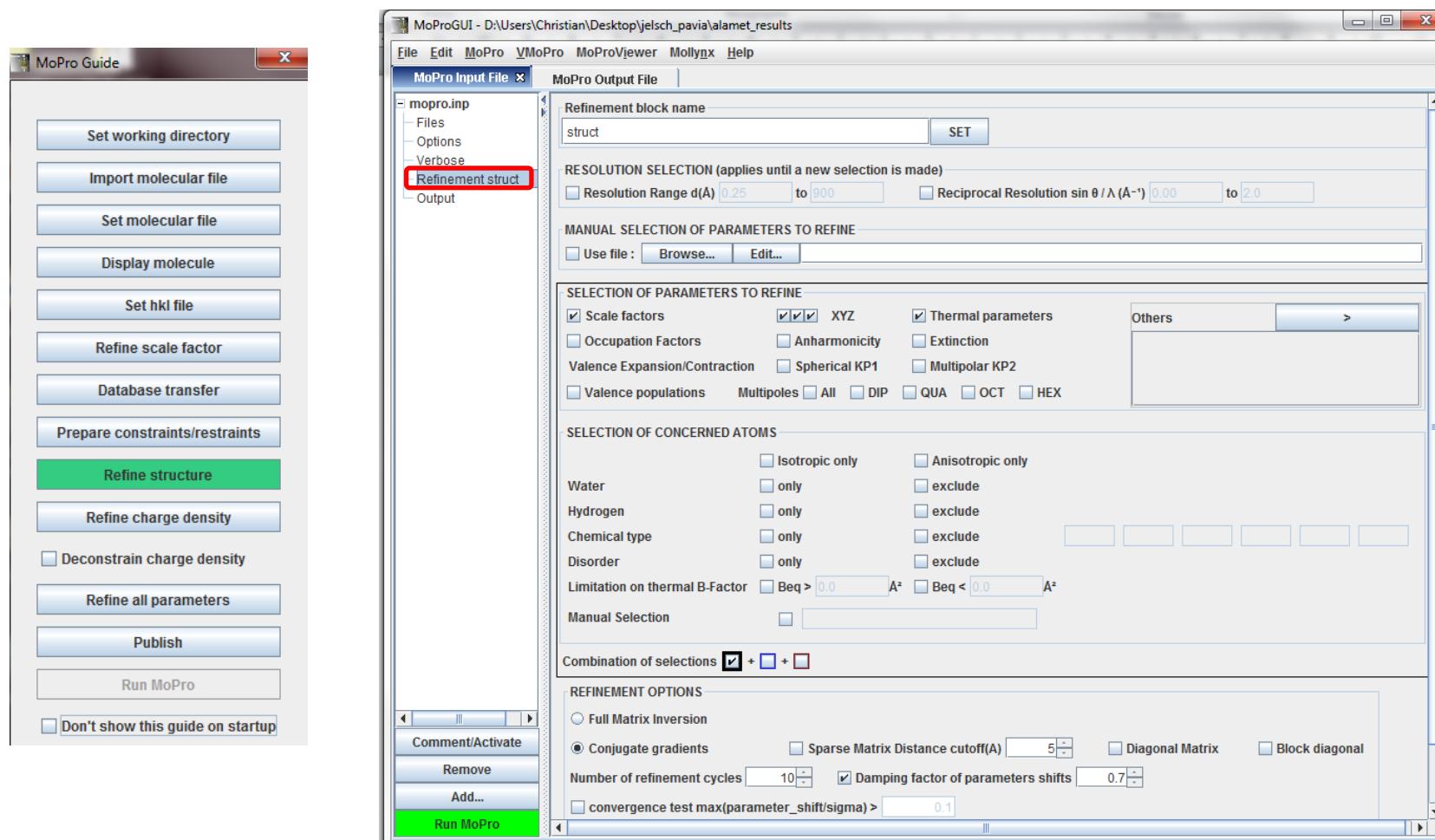
e.g. H-X distances for Hydrogen atoms



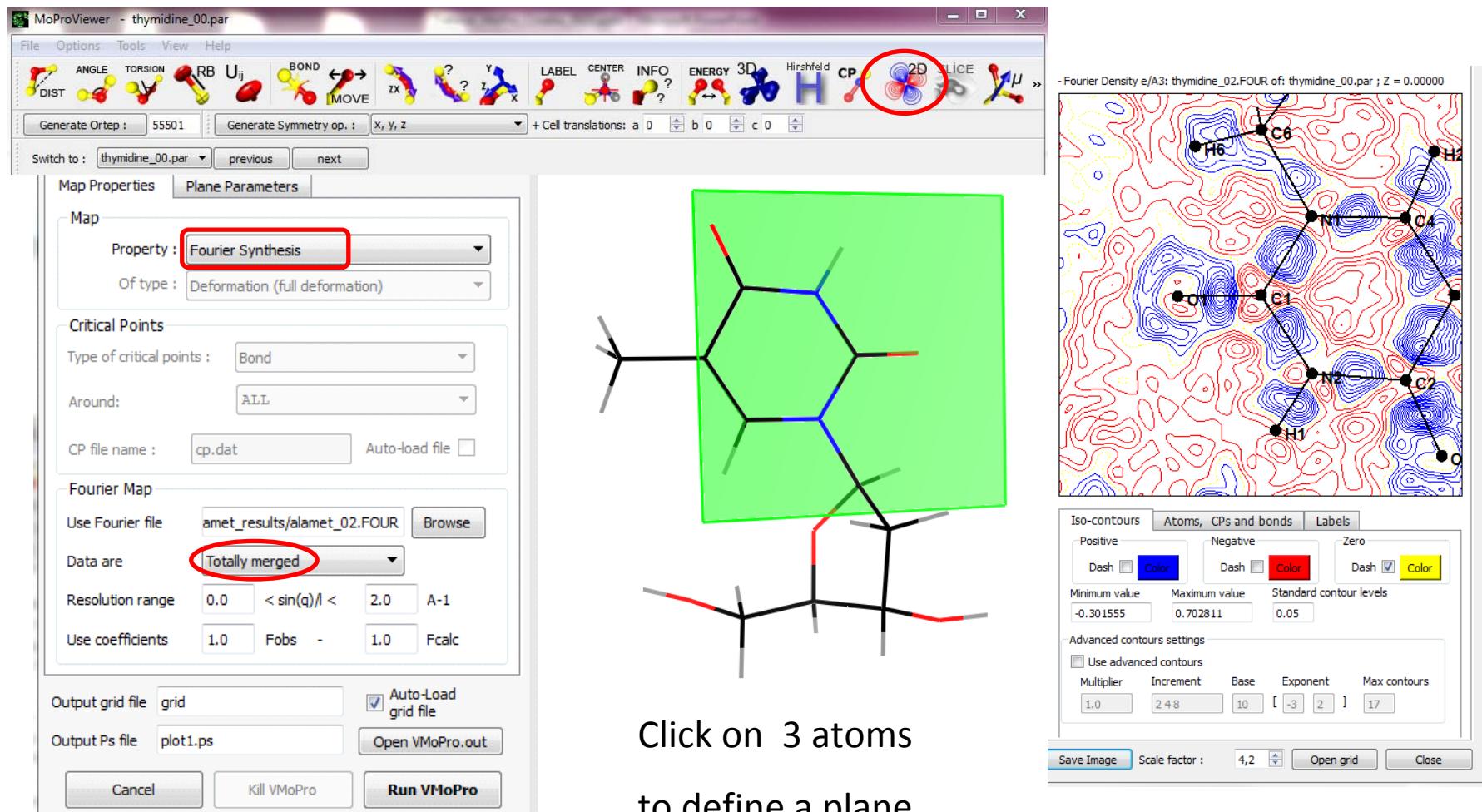
Edit and have a look at the generated  
CONSTRAIN.txt & RESTRAIN.txt files

## Step 7 Refine structure

SCA XYZ UIJ are selected  
SCAle factor, Positions & Thermal motion parameters



## Step 8 Compute a Fourier Residual Electron Density 2D map



Click on 3 atoms  
to define a plane

2D map:

Select Map Property : Fourier Synthesis

Select Fourier file : alamet\_02.FOUR

Data are Merged

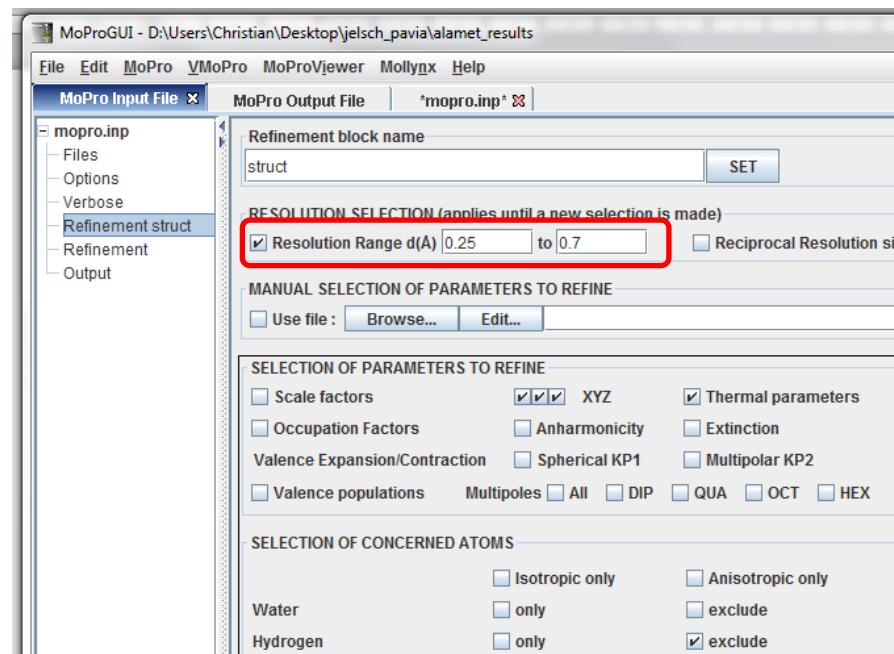
Click on "Run VMoPro" to start calculation

## Step 9 HIGH ORDER refinement of structure

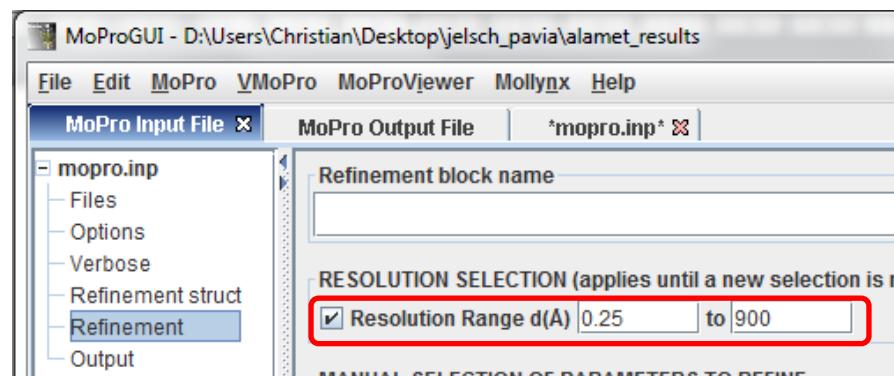
High resolution data  $d < 0.7 \text{ \AA}$ ,  
Hydrogen not refined

*The MoPro commands*

```
!<refinement> structural  
RESO 0.25 0.7  
SELE XYZ UIJ NOH  
REFI CG 10 DAMP 0.7  
WRIT RFAC
```



Write a Fourier reflections file  
for all resolution



## Step 10 Compute a Fourier Residual Electron Density after High-Order refinement

MoProGUI - D:\Users\Christian\Desktop\jelsch\_pavia\alamet\_results

**File Edit MoPro VMoPro MoProViewer Mollynx Help**

**MoPro Input File** x      **MoPro Output File**      \*mopro.inp\* x

**mopro.inp**

- Files
- Options
- Verbose
- Refinement struct
- Refinement**
- Output

**Refinement block name**

**RESOLUTION SELECTION (applies until a new selection is made)**

Resolution Range d(A) **0.25** to **900**

**MANUAL SELECTION OF PARAMETERS TO DEFINE**

**mopro.inp**

- Files
- Options
- Verbose
- Output**

**Write Output Files**

**Reflections**

Type (Format)      Optional filename

**FOUR (VMoPro)** **thymidine\_04.FOUR**

HKL (hkl I sigl)

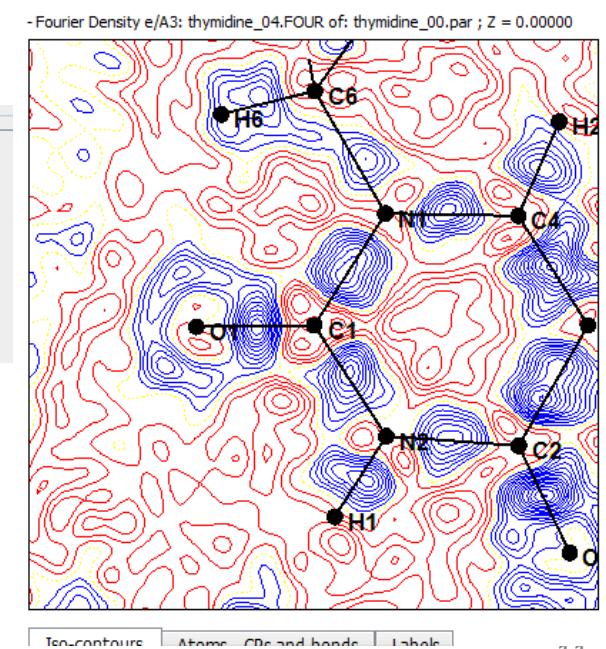
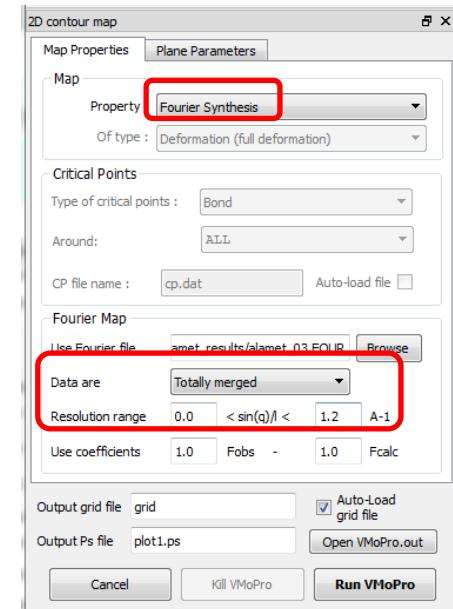
FCAL (VMoPro)

**Static Uij = 0**  Dynamic  Binary

FDEF (VMoPro)

**RESO 0.25 900.**  
**WRIT FOUR**

Slightly Stronger residual electron density visible on covalent bonds

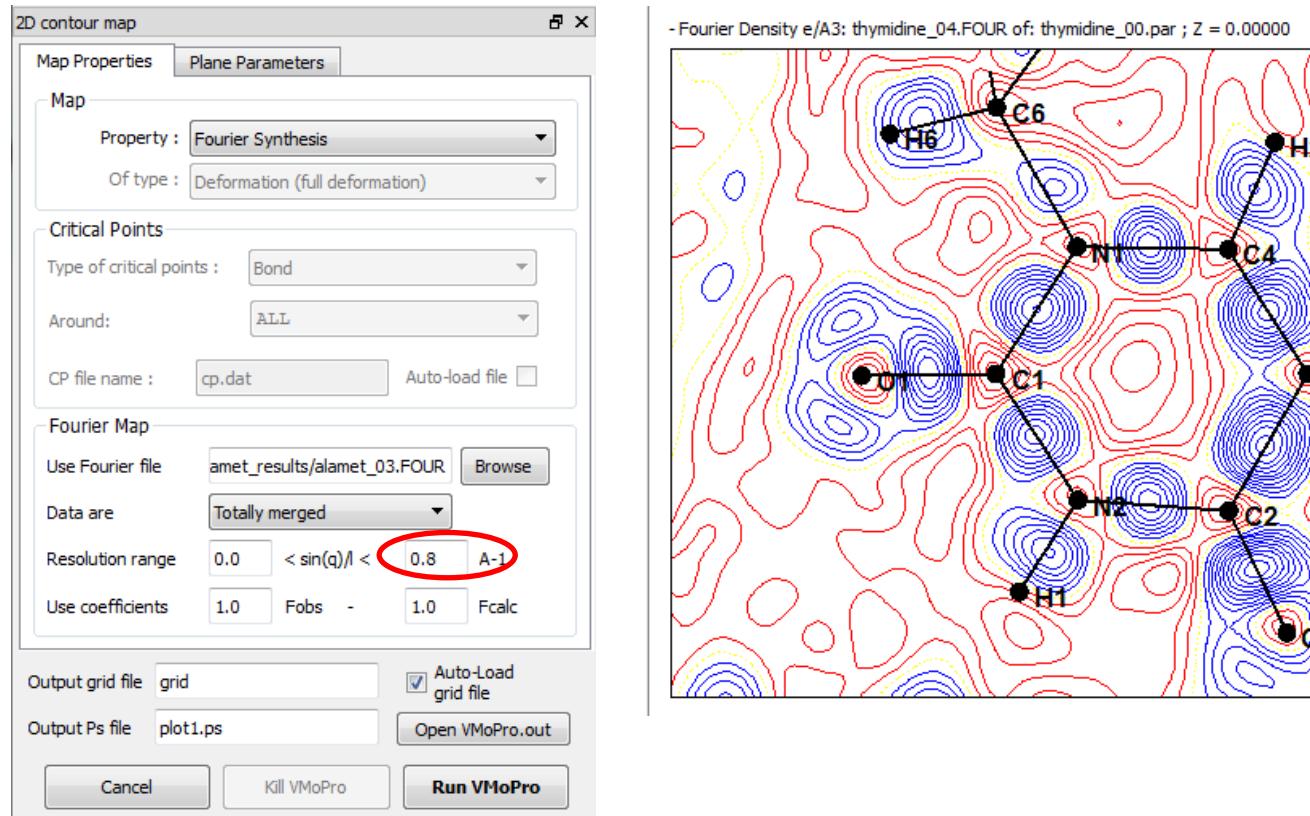


## Step 11 Compute a Fourier Residual map at LOW resolution after High-Order refinement

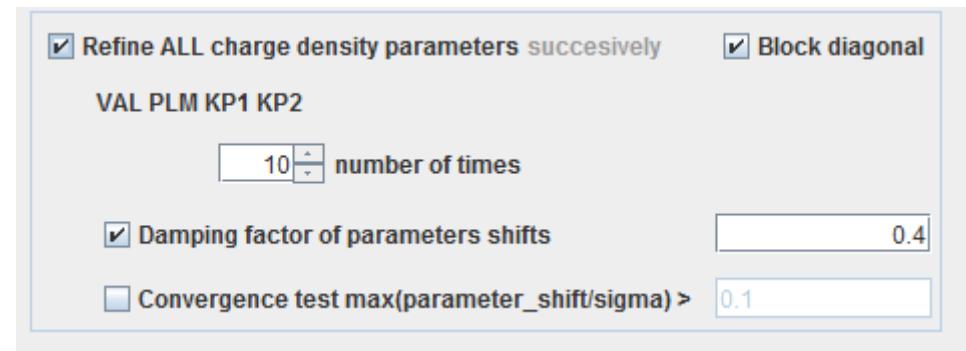
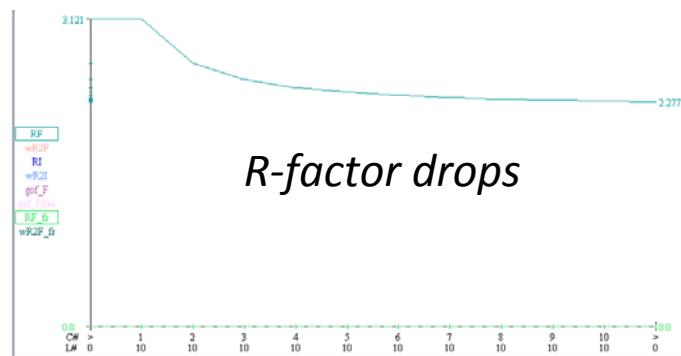
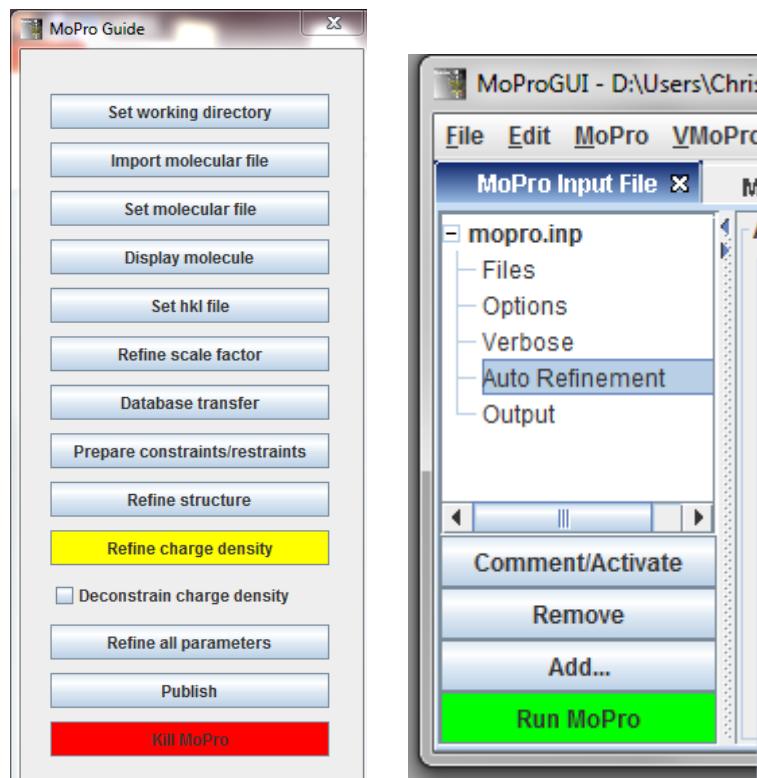
$$\sin \theta / \lambda < 0.8 \text{ \AA}^{-1}$$

resolution  
 $d > 0.6 \text{ \AA}$

Bonding  
Electron  
Density  
is clearly  
visible



## Step 12 Refinement of charge density

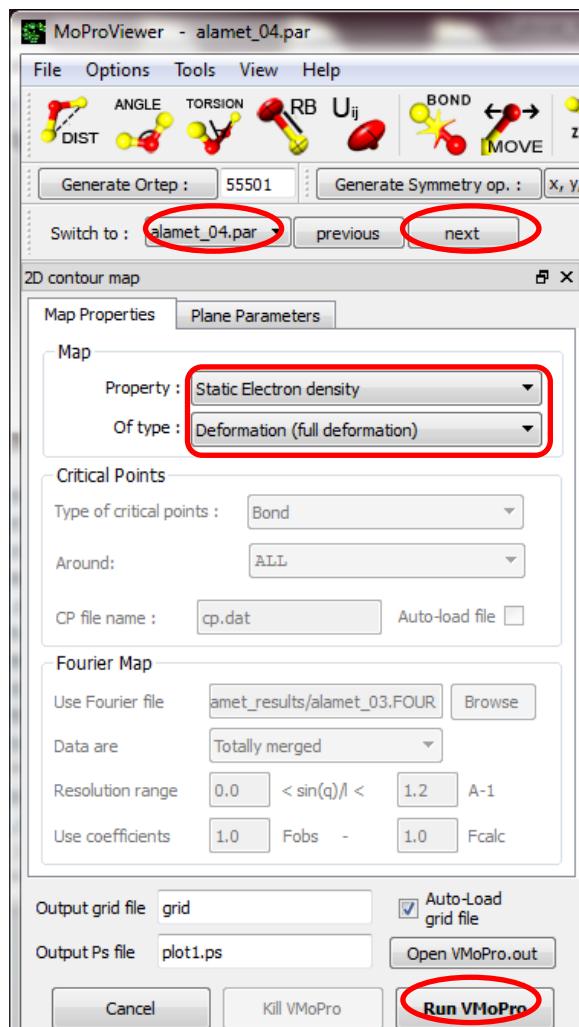


- \* Block diagonal: variables are decorrelated and can be refined together
- \* Damping to avoid divergence

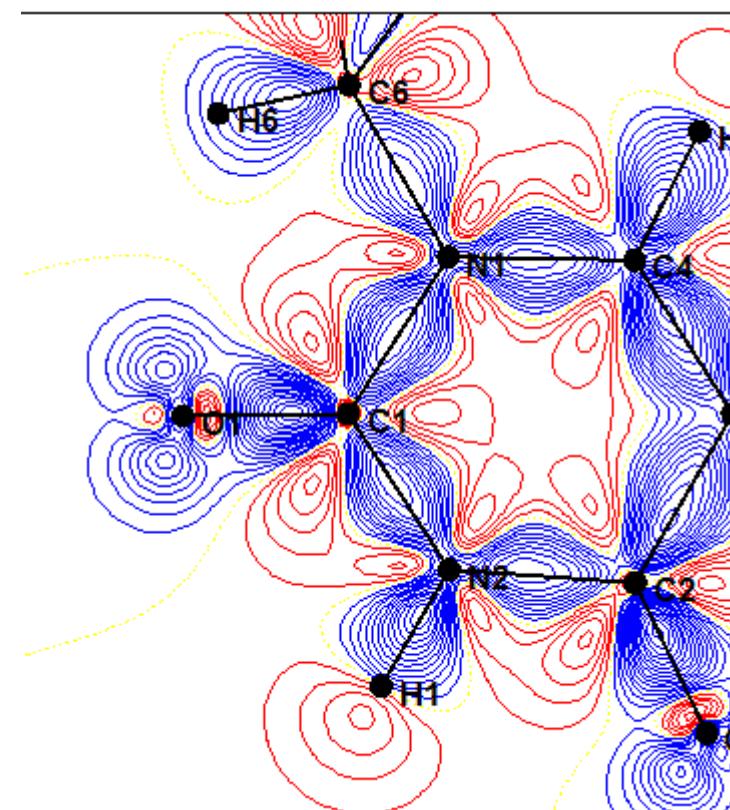
Have a look at resulting molecular .par file

```
ATOMS 31
ATOM 1 O1 thy 1 -0.274124 0.489775 0.825512 1.0000 1 O
XY C1 N1 OCT K1 V0 M0 Q0
UANI 0.011241 0.010160 0.007127 0.004751 0.000810 -.000807
6.14170 0. -.044 0. 0. -.052 0. 0. -.043 0.
0. 0.006 0. 0. 0. 0.027 0.
ATOMS 30
XYZ Pval =valence Plm = multipole populations
```

## Step 13 Compute a Static Deformation Electron Density map



Choose appropriate (last) molecular file



## Step 14 Refinement of all parameters

The screenshot shows the MoProGUI interface. On the left, the MoPro Guide panel lists various refinement steps. The 'Refine all parameters' button is highlighted with a red box. The main window shows the MoPro Input File tab selected, displaying a configuration for 'Automatic Refinement'. It includes options for refining all parameters successively (checked) or block-diagonally (checked), setting a damping factor of 0.3, and specifying a convergence test threshold of 0.1. Below this, a graph plots the R-factor (y-axis, ranging from 0.000 to 2.000) against the number of refinement cycles (x-axis, ranging from 1 to 10+). The R-factor starts at approximately 2.277 and drops sharply to around 1.2035 by cycle 10.

- Block diagonal & damp : refine all parameters together

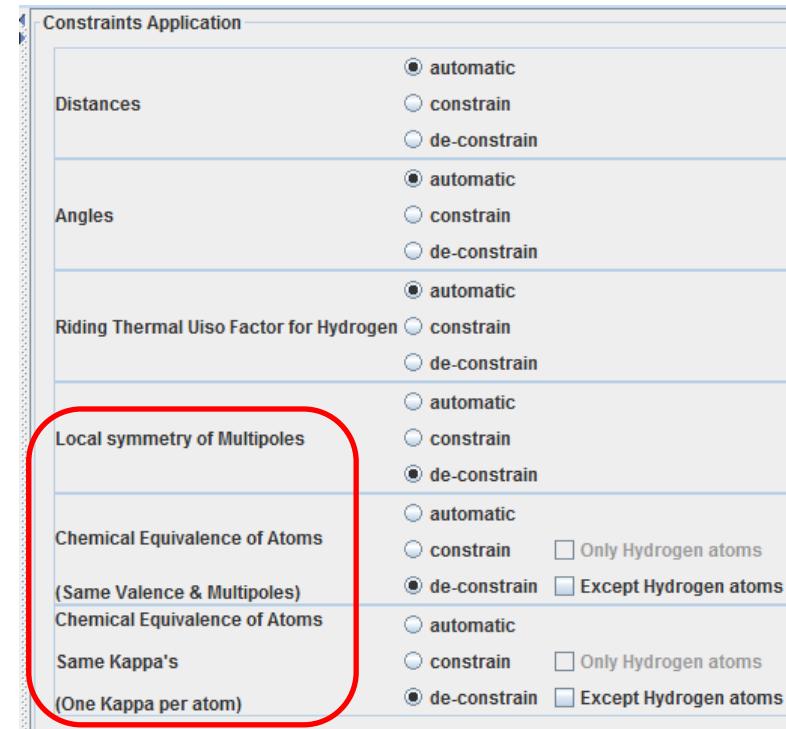
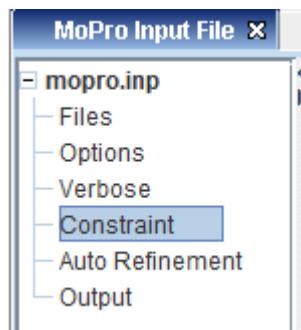
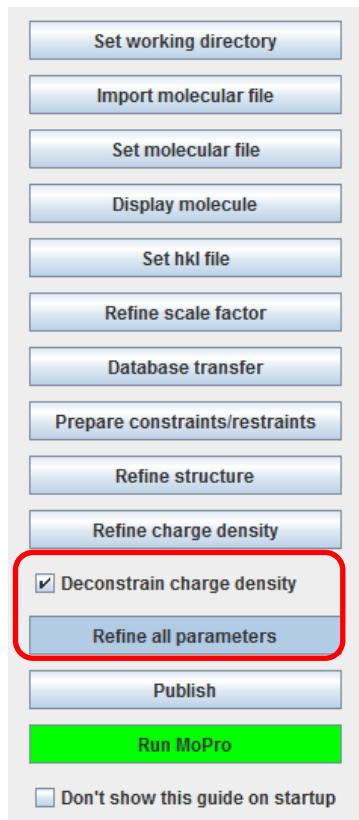
- Else : refine them successively

Further *R*-factor drop

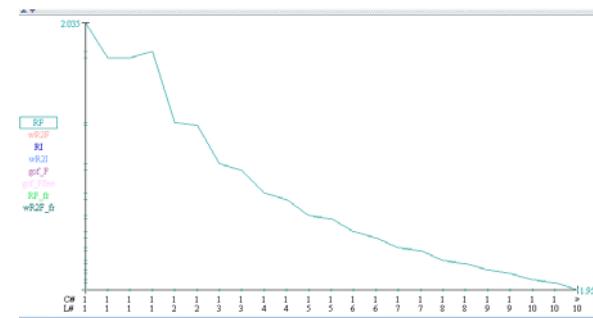
## Step 15 Deconstrain charge density

Removes

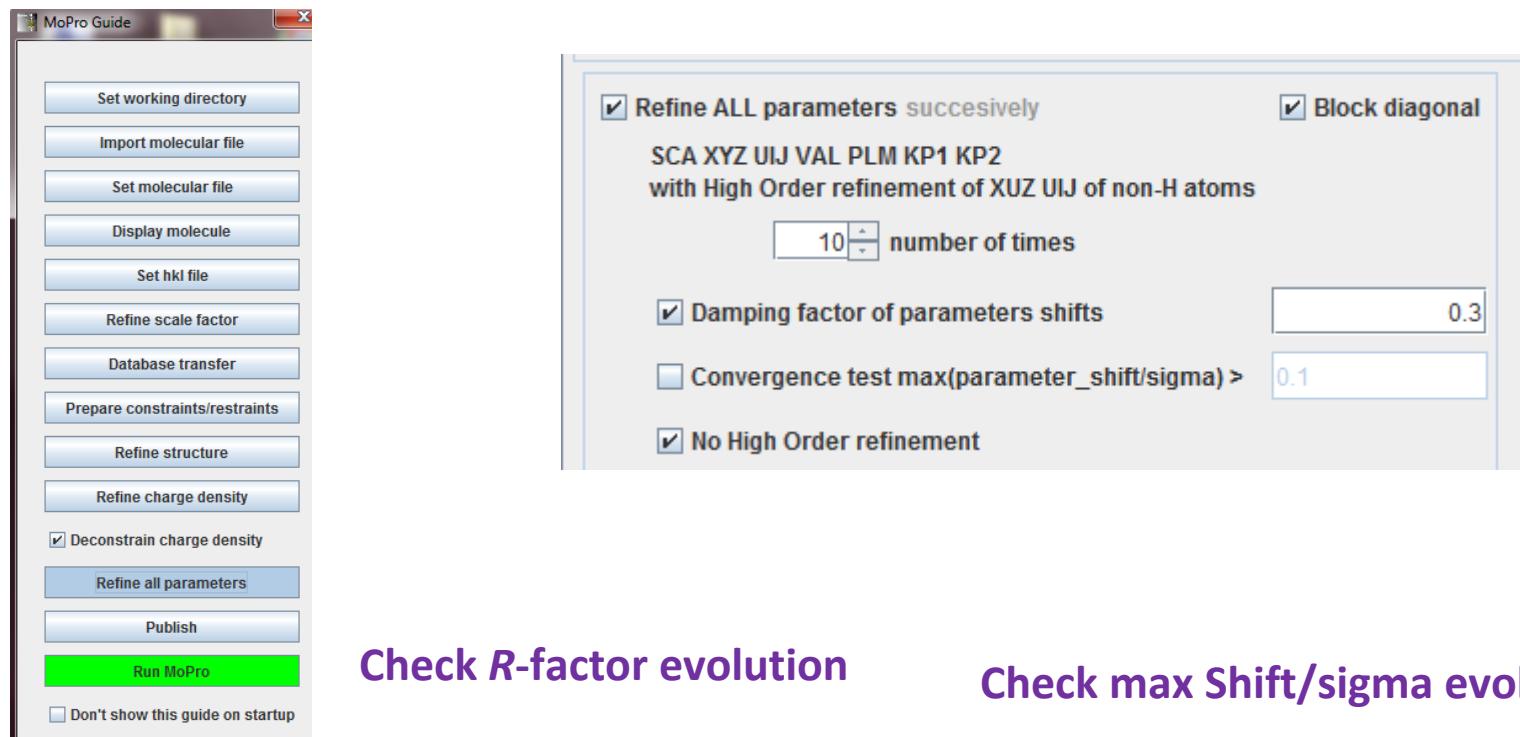
- Atoms equivalencies : similar atoms have same charge density
- Local symmetry of multipoles



More variables  
=>  
R-factor drop

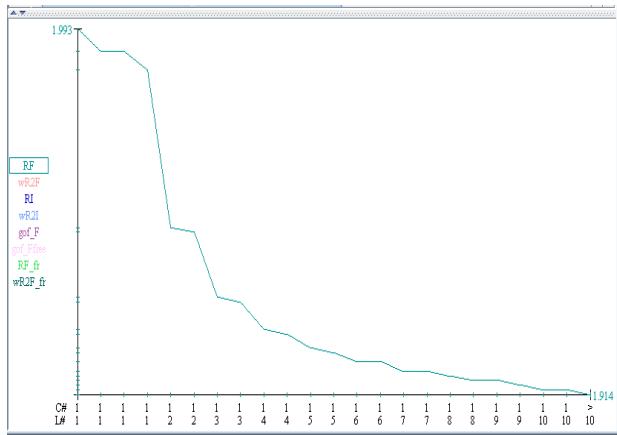


## Step 16 Refinement of all parameters till convergence



Check R-factor evolution

Check max Shift/sigma evolution

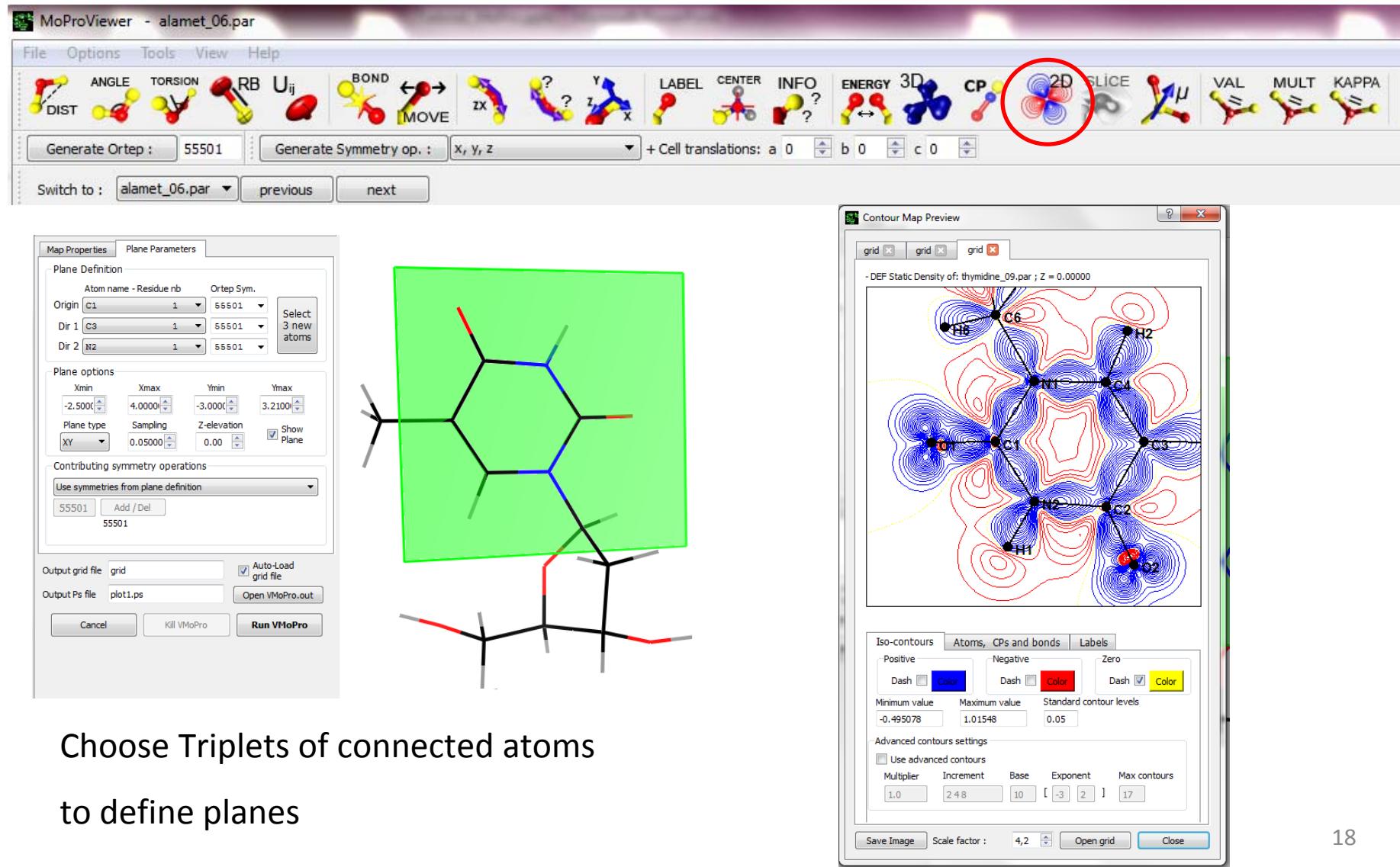


MoPro Log									
8/ 10 0/ 0 0 3.8583 6295 210 -0.759 Scale 1									
8/ 10 0/ 0 0 3.8560 6295 361 0.402 MONOP_1 1 04									
9/ 10 0/ 0 0 3.8533 6295 210 -0.755 Scale 1									
9/ 10 0/ 0 0 3.8511 6295 361 0.393 MONOP_1 1 04									
10/ 10 0/ 0 0 3.8487 6295 210 -0.751 Scale 1									
10/ 10 0/ 0 0 3.8466 6295 361 0.383 MONOP_1 1 04									

MoPro job finished

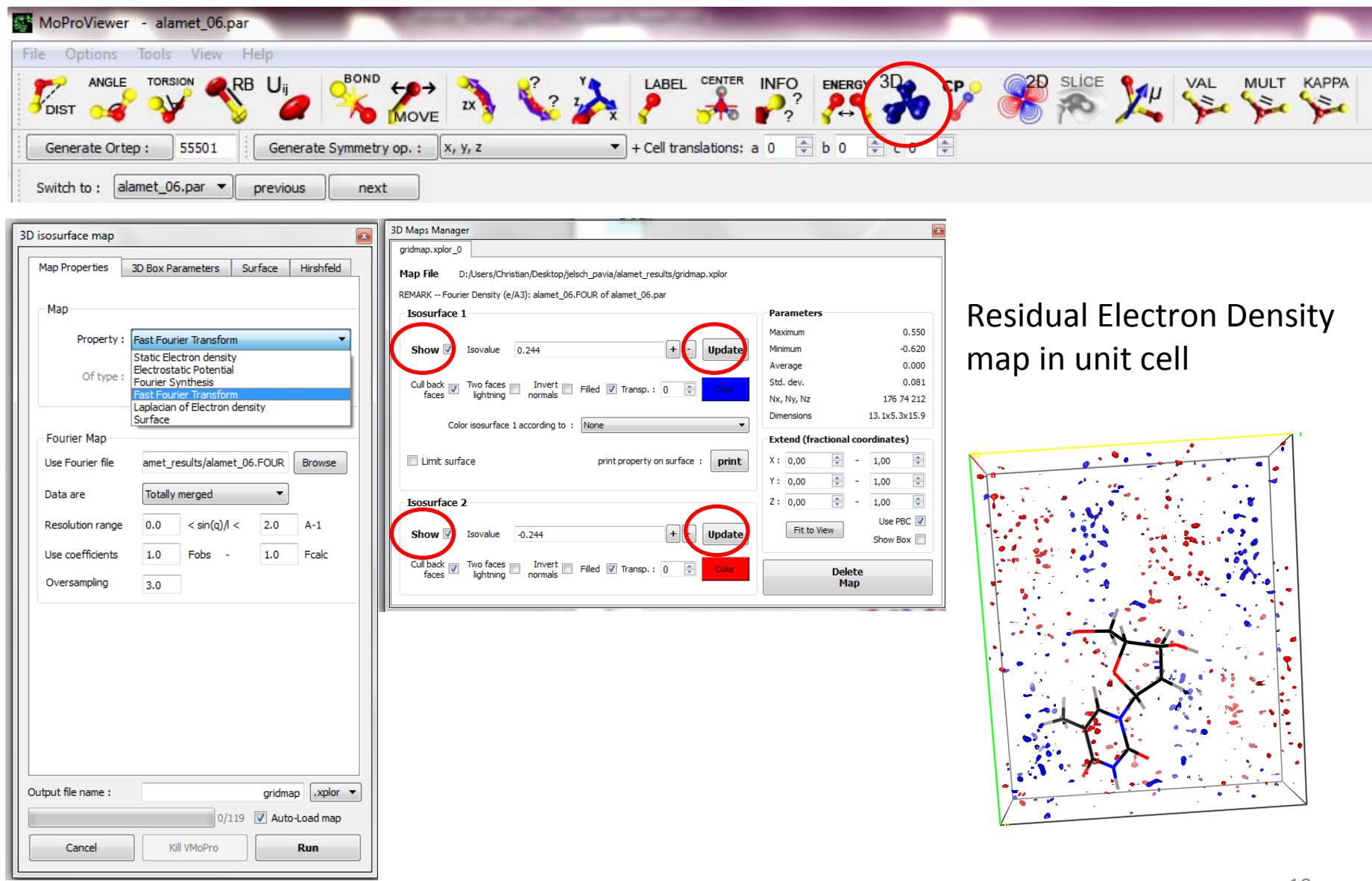
Validate & increment mol. file: 08->09      Cancel & restart from ver. 08

## Step 17 Check Static Deformation Electron Density 2D maps



Choose Triplets of connected atoms  
to define planes

## Step 18 Fast Fourier Transform 3D map



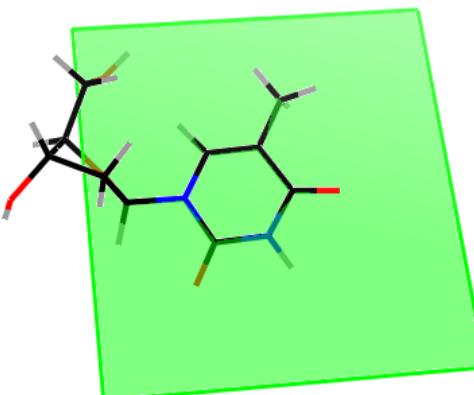
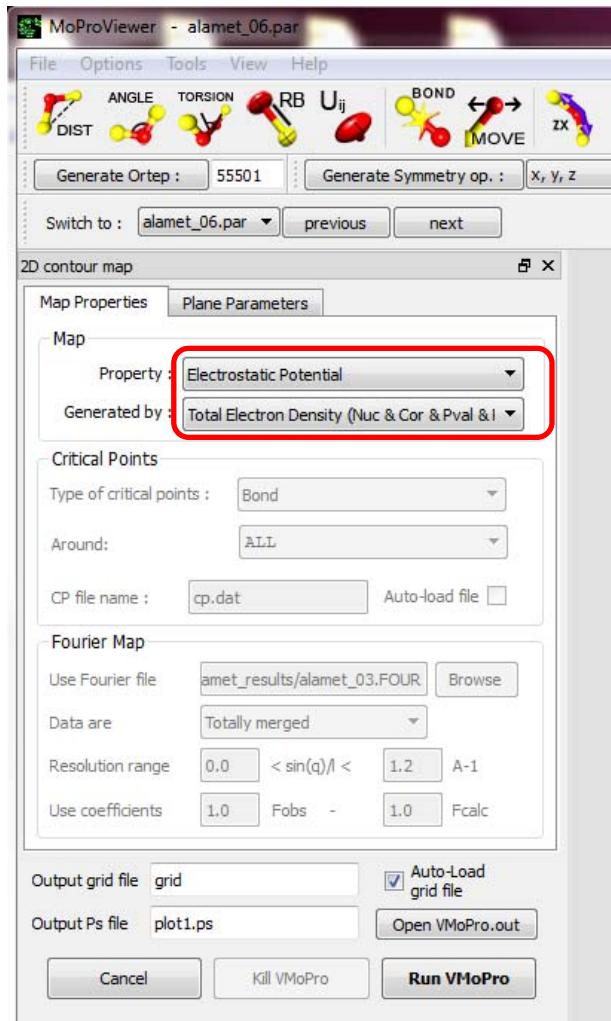
## Step 19 Stereochemical analysis in MoPro

The screenshot shows the MoProGUI software interface. The top window is titled "MoPro Input File" and displays the "Refinement" tab. It includes sections for "Refinement block name", "RESOLUTION SELECTION", "MANUAL SELECTION OF PARAMETERS TO REFINE" (with checkboxes for Scale factors, Occupation Factors, Valence Expansion/Contraction, Valence populations, XYZ, Anharmonicity, Spherical KP1, Multipole types All, DIP, QUA, OCT, and HEX), and "REFINEMENT OPTIONS" (with radio buttons for Full Matrix Inversion and Conjugate gradients, and checkboxes for Sparse Matrix Distance cutoff(A) set to 5, Diagonal Matrix, and Block diagonal). The bottom window is also titled "MoPro Input File" and displays the "Analysis" tab. It includes sections for "Molecular Geometry" (with checkboxes for Distances, Angles, Dihedral angles, Plane, and Chiral volumes, where "Distances" is highlighted with a red box) and "Molecular Connectivity". The "MoPro Output File" window at the bottom shows a table of refined atom coordinates:

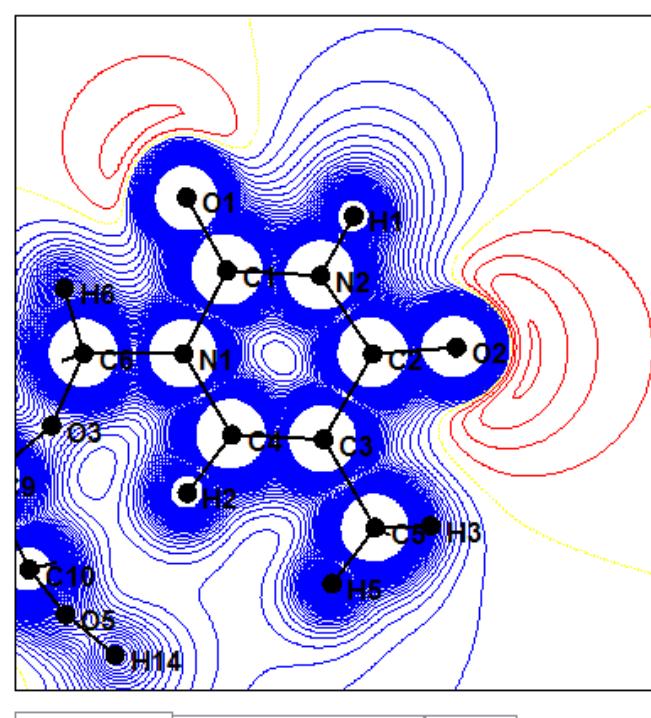
ATOM1	ATOM2	SYM2	DIST	sigDIST	xyz	xyz	
O1	thy	1 -- C1	thy	1	1.239082	0.000175	+++ +++
O2	thy	1 -- C2	thy	1	1.245673	0.000163	+++ +++
O3	thy	1 -- C6	thy	1	1.428634	0.000135	+++ +++
Etc....							

Refine  
at first  
Structure  
(LS)  
to obtain  
sigmas  
of distances

## Step 20 2D map of Electrostatic Potential

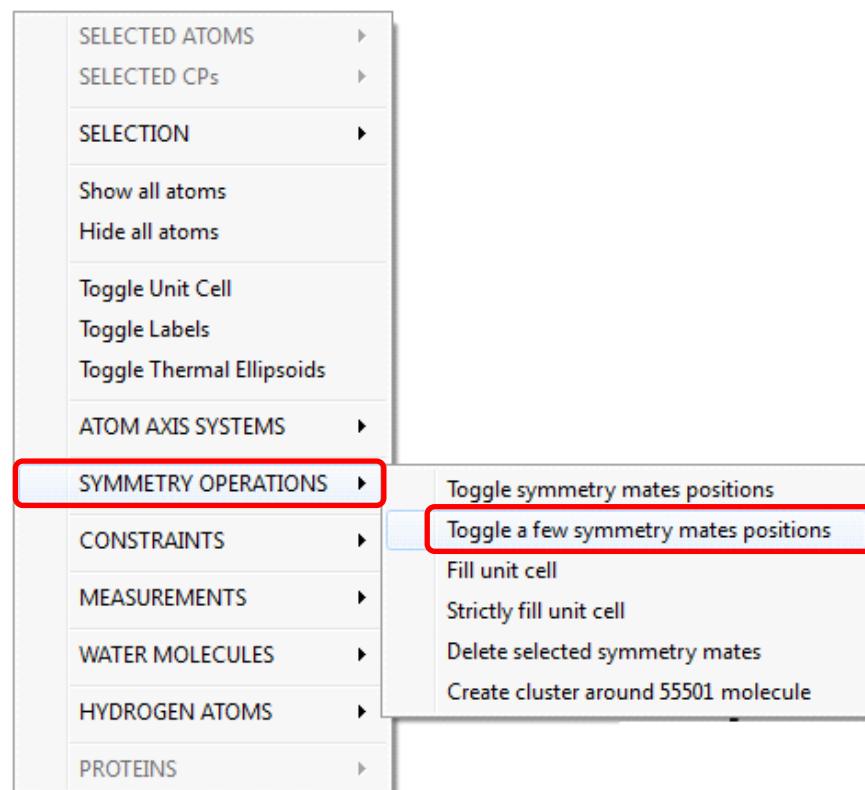


Augment dimensions  
of plane  
for a wider picture



## Step 21 Generate a dimer in MoProViewer

Click right on view



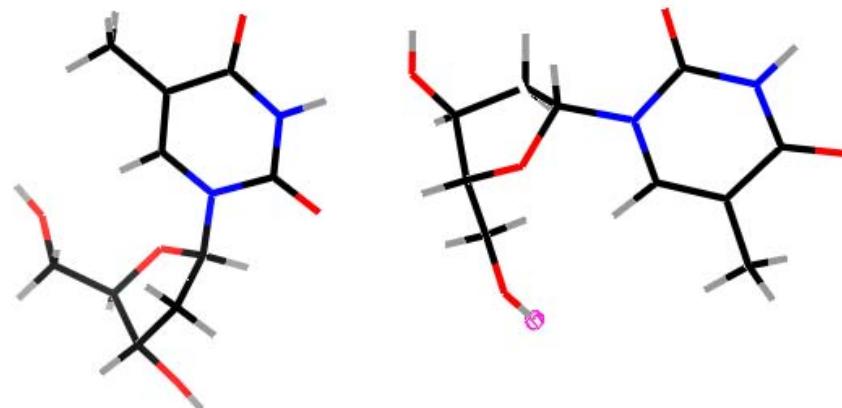
Keep a dimer like 55501 + 46502

p symmetry code

502

slation -1a + 1b + 0c & symmetry #02

1 6→+1 5→+0



## Step 22 Search Intermolecular critical points

MoProViewer - alamet\_06.par

File Options Tools View Help

DIST ANGLE TORSION RB U<sub>ij</sub> BOND MOVE ZX Y? X? LABEL CENTER INFO ENERGY 3D CP SLICE 2D SLICE

Critical Points Search

VMoPro MoProViewer

Critical Points Search using VMoPro

Property type

Property : Static Electron density

Of type : Total electron density (Cor & Pval & P00 & Plm)

Contributing symmetry operations

Use all currently active symmetric molecules

Add / Del : 55501 Generate Molecules

55501

Search options

Type of critical points : Intermolecular

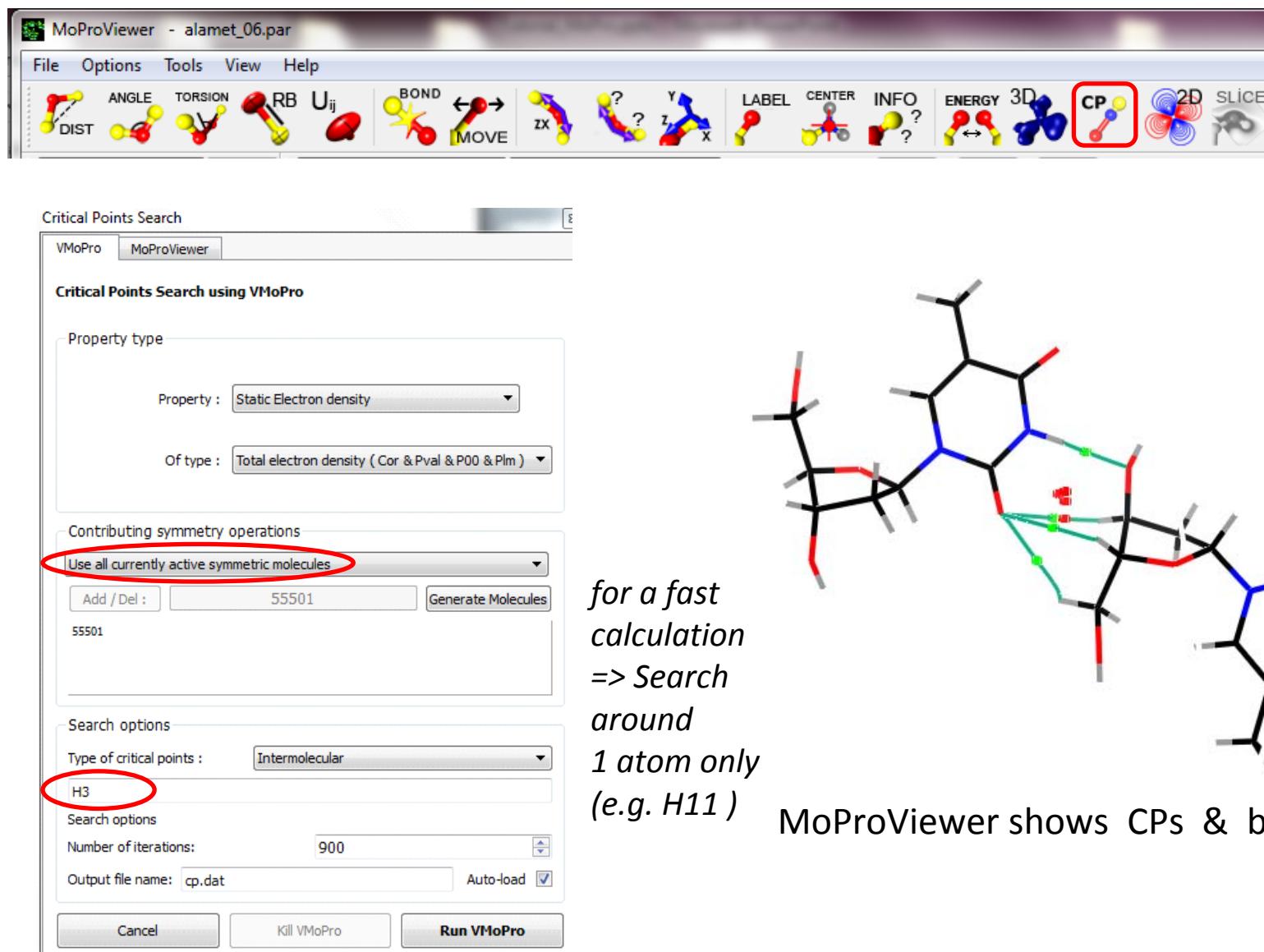
H3

Search options

Number of iterations: 900

Output file name: cp.dat Auto-load

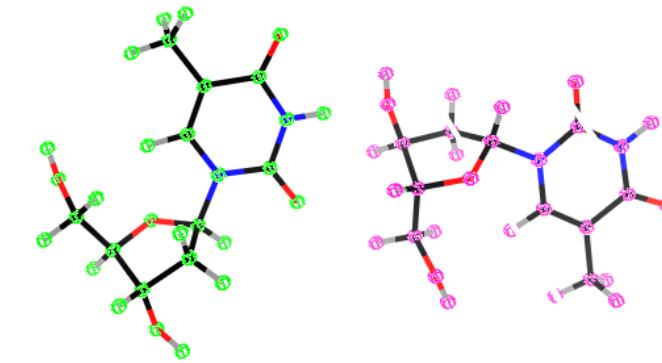
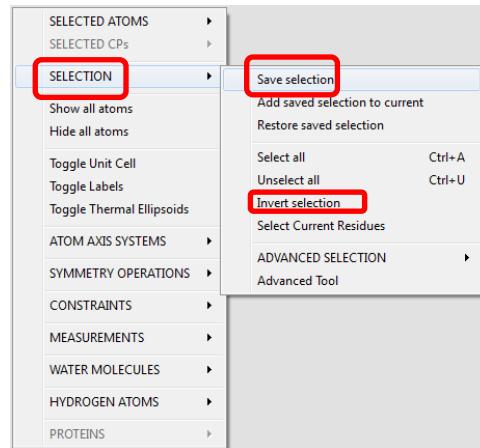
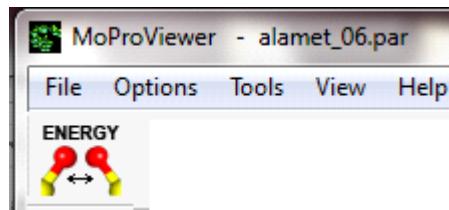
Cancel Kill VMoPro Run VMoPro



for a fast  
calculation  
=> Search  
around  
1 atom only  
(e.g. H11 )

MoProViewer shows CPs & bond paths

## Step 23 Compute electrostatic interaction energy of a dimer

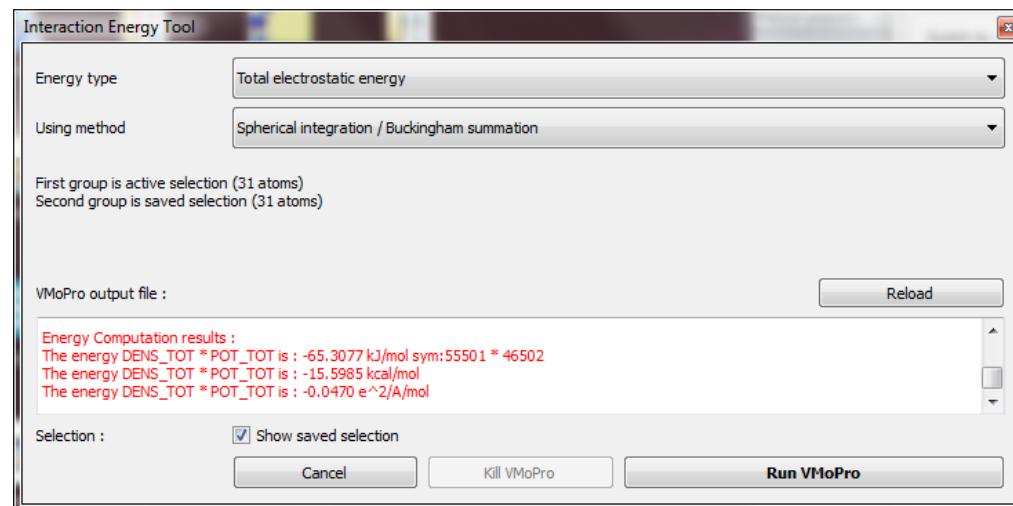


1) Click on **Energy** tool  
of MoProViewer

2) Select one molecule  
(shift+mouse)  
Right click, Selection / SAVE selection

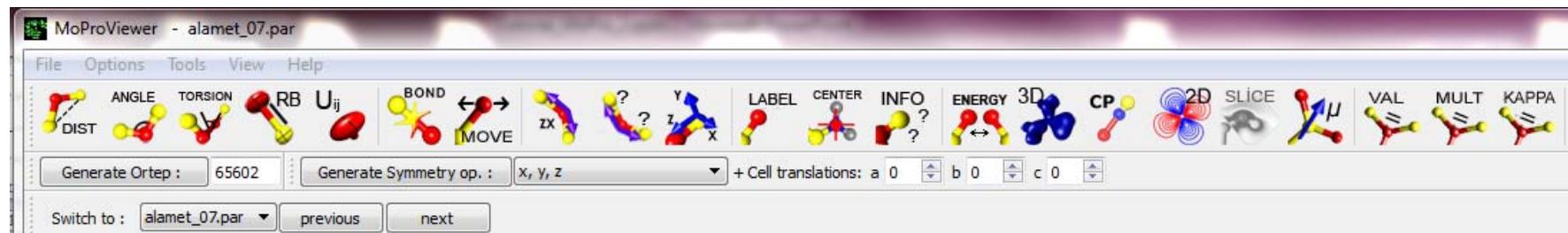
3) Invert Selection

4) Run VMoPro  
energy calculation



## Step 24 Discover the Tools of MoProViewer

$\mu$  Dipole  
moment



Stereo-  
chemistry

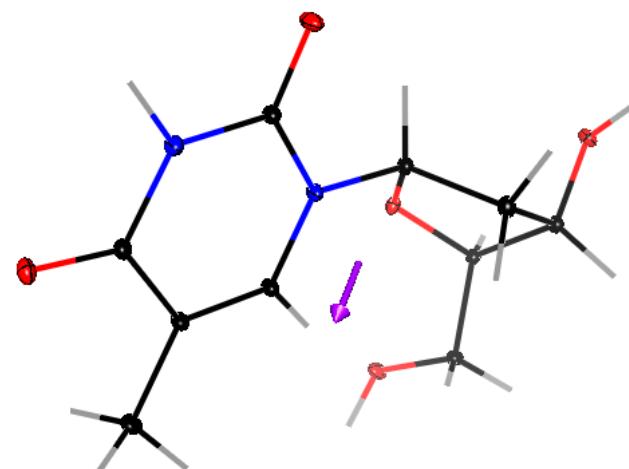
Move  
atoms

Show local  
axes system  
for multipoles  
orientation

Compute  
3D map      Compute  
2D map  
Critical  
points

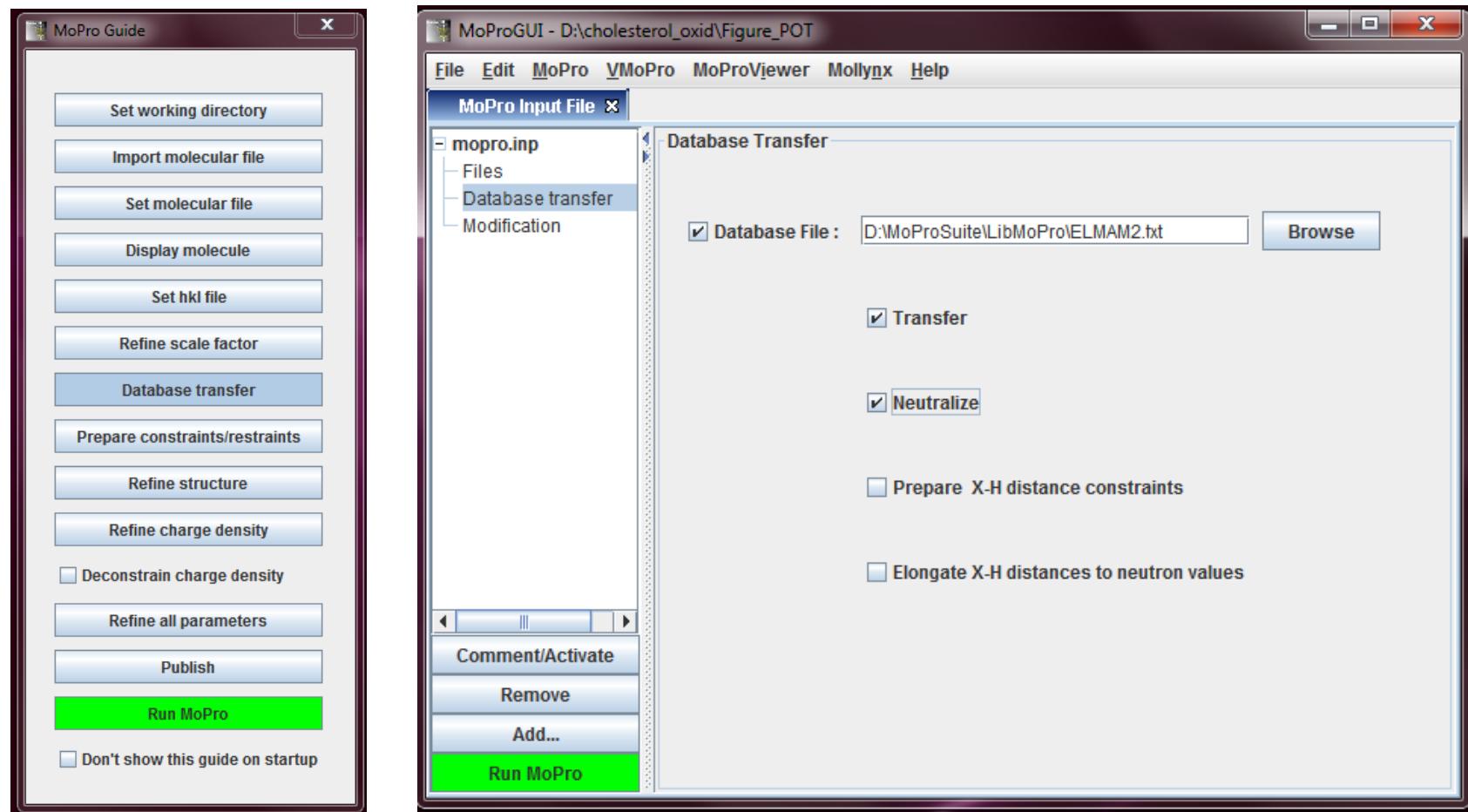
Equivalence  
Constraints  
of atomic  
charge  
density

U<sub>ij</sub>  
Thermal  
ellipsoids



## Step 25 ELMAM2 Database transfer

Useful for a protein or an organic molecule structure  
at usual atomic resolution  $d > 0.6 \text{ \AA}$  or  $s < 0.8 \text{ \AA}^{-1}$



Check the resulting Static Deformation Electron Density maps

## Step 25 Discover the MoPro Menus

Commands are classified and visible in menus

