Tutorial

MoProSuite : Crystallographic software for charge density refinement

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

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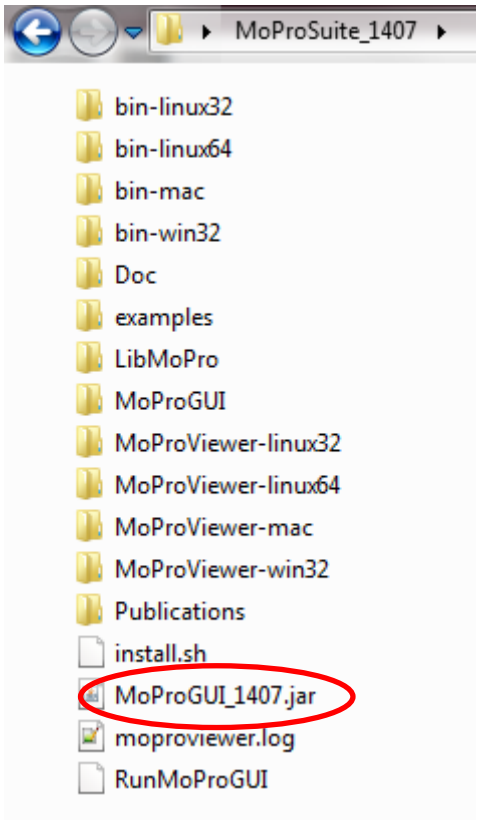
MoProSuite working under Windows, linux & mac.

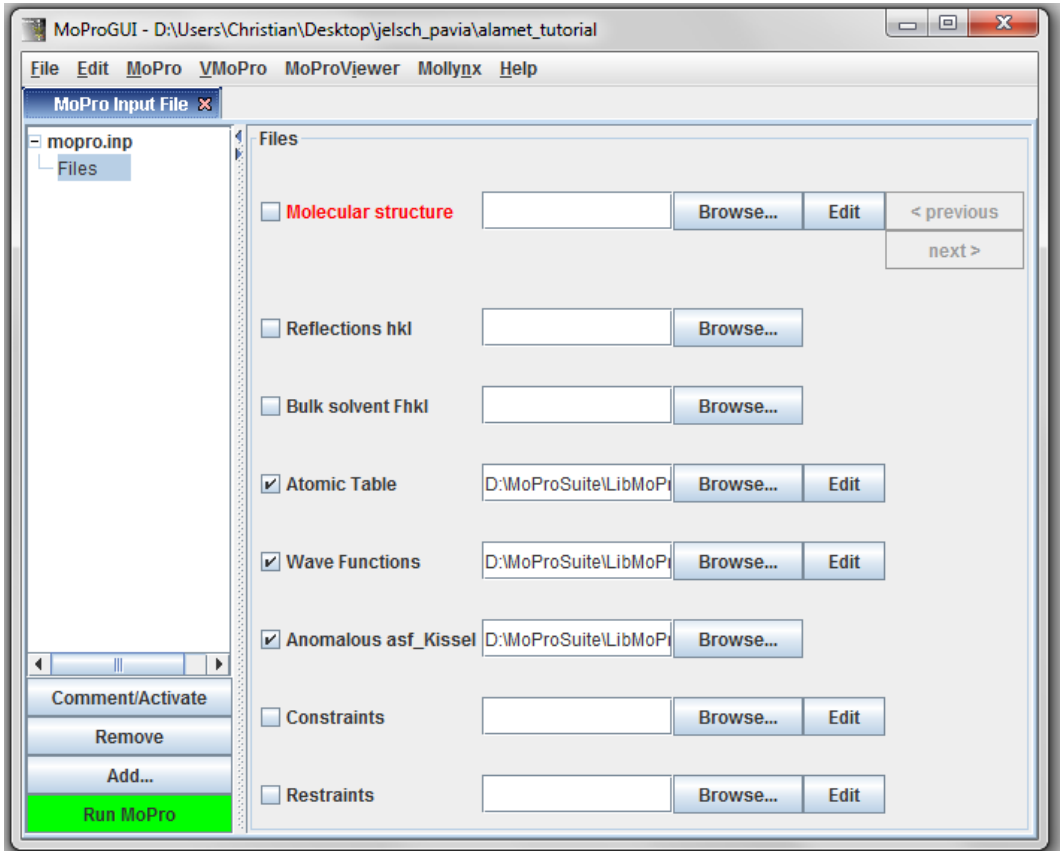
29th ECM
Crystallographic Computing School

Croatia, Rovinj 20th-21st August 2015

Step 1 Lauch MoProGUI

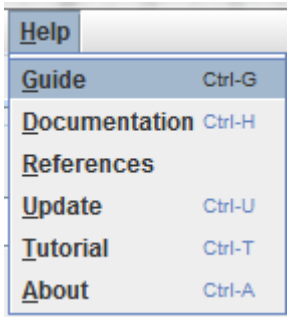
MoPro Graphical User Interface

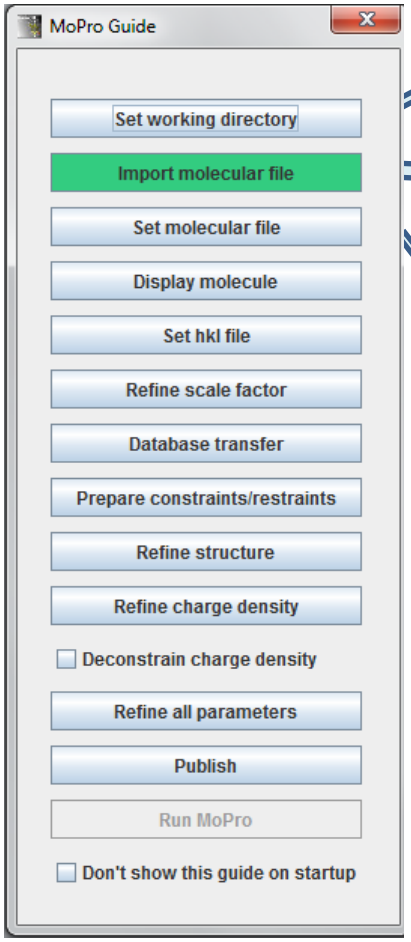


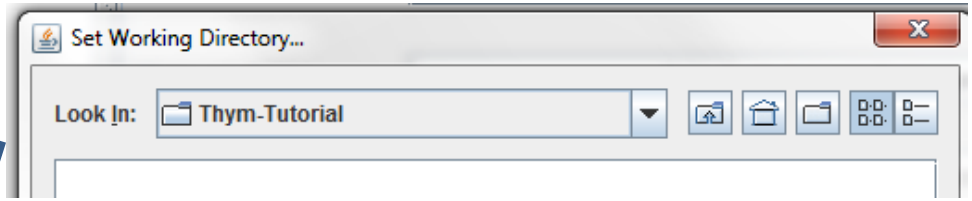


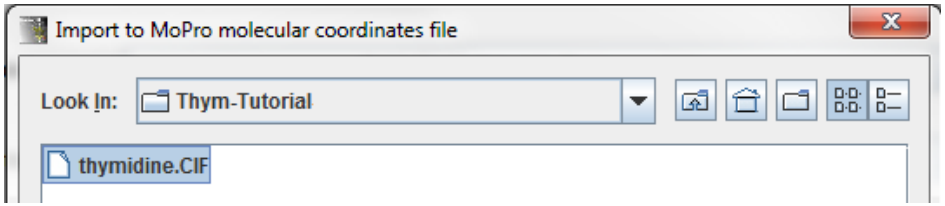
Requires JAVA, which can be downloaded at:
https://www.java.com/fr/download/

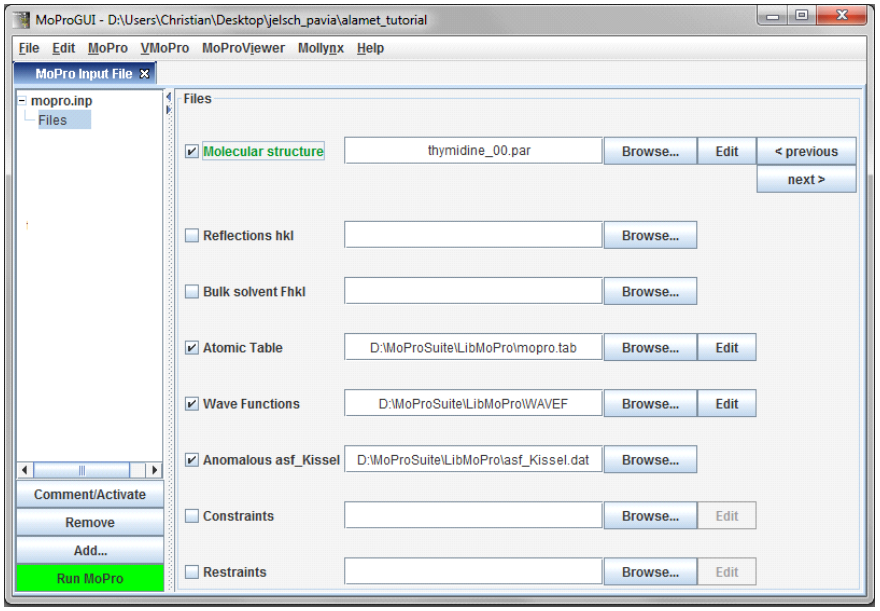
Step 2 initial steps : follow the GUIDE



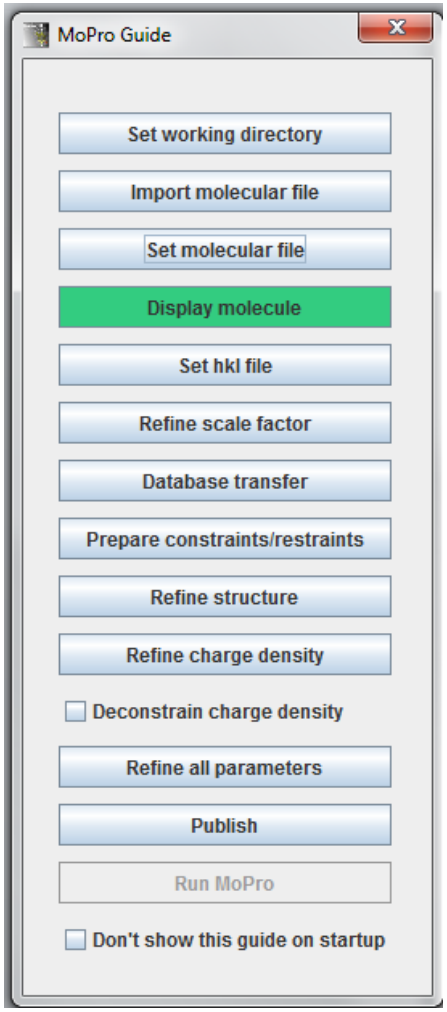


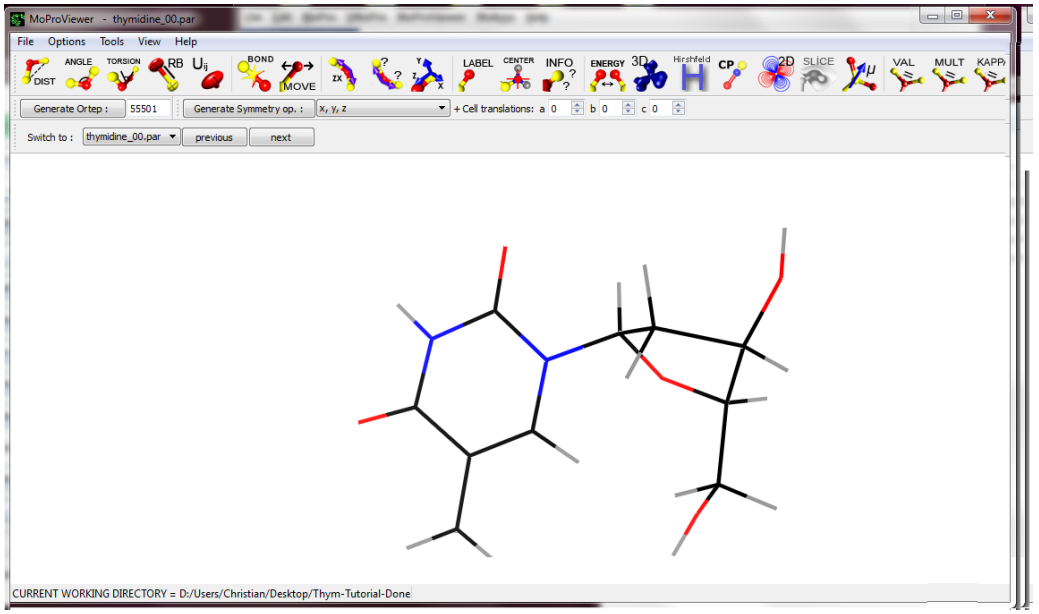




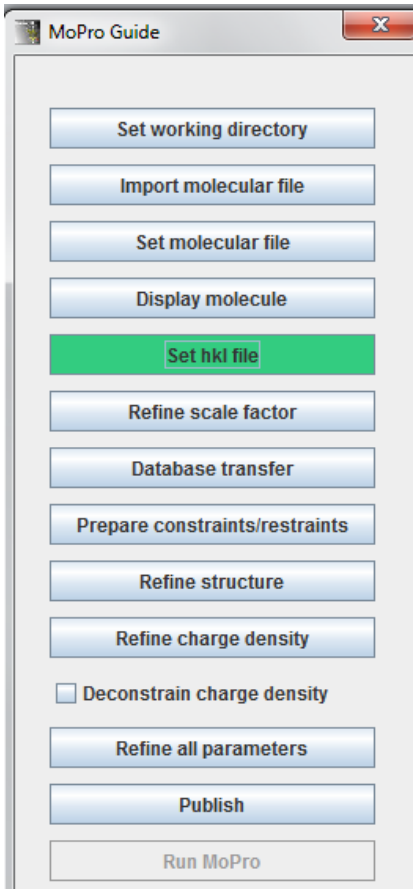


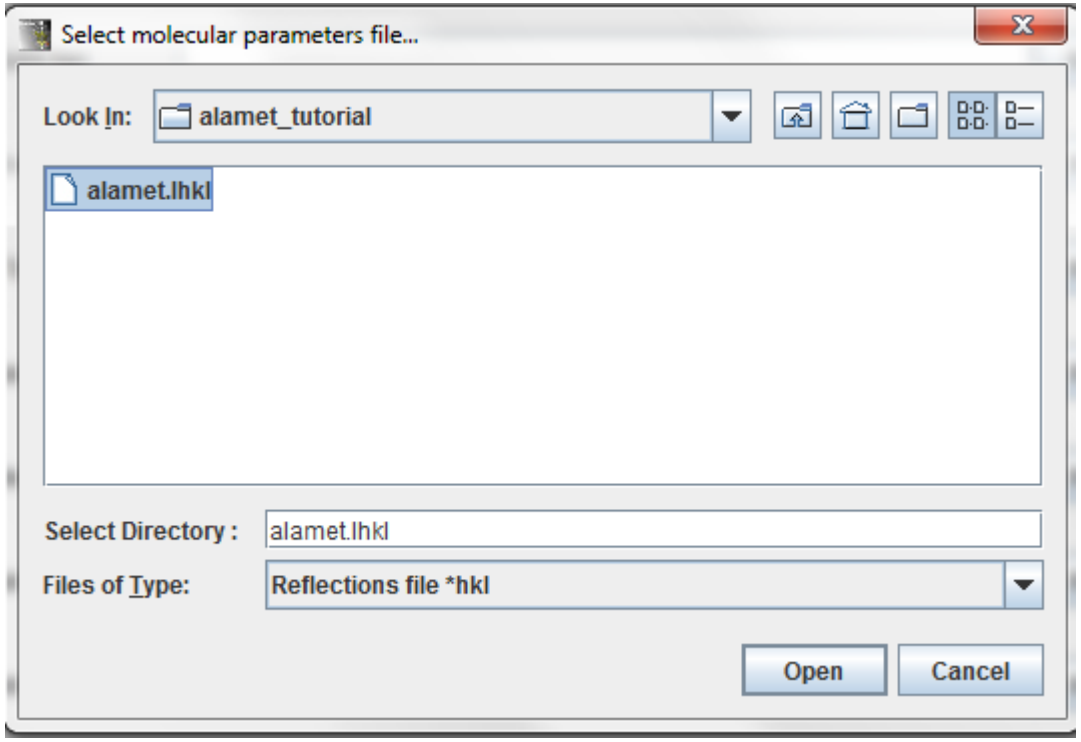
Step 3 Display molecule with MoProViewer





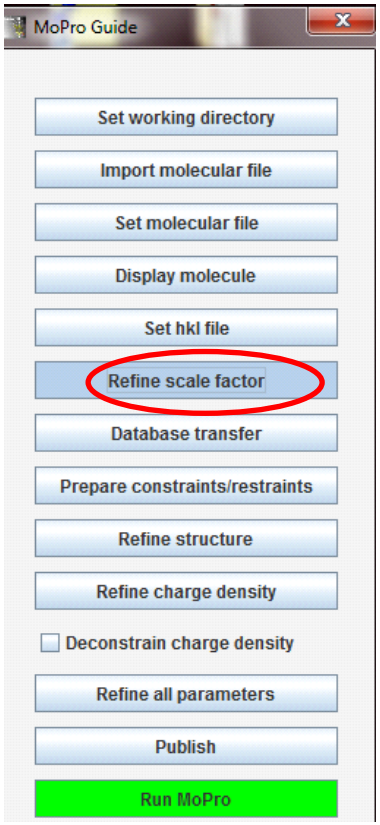
Step 4 Select reflections file



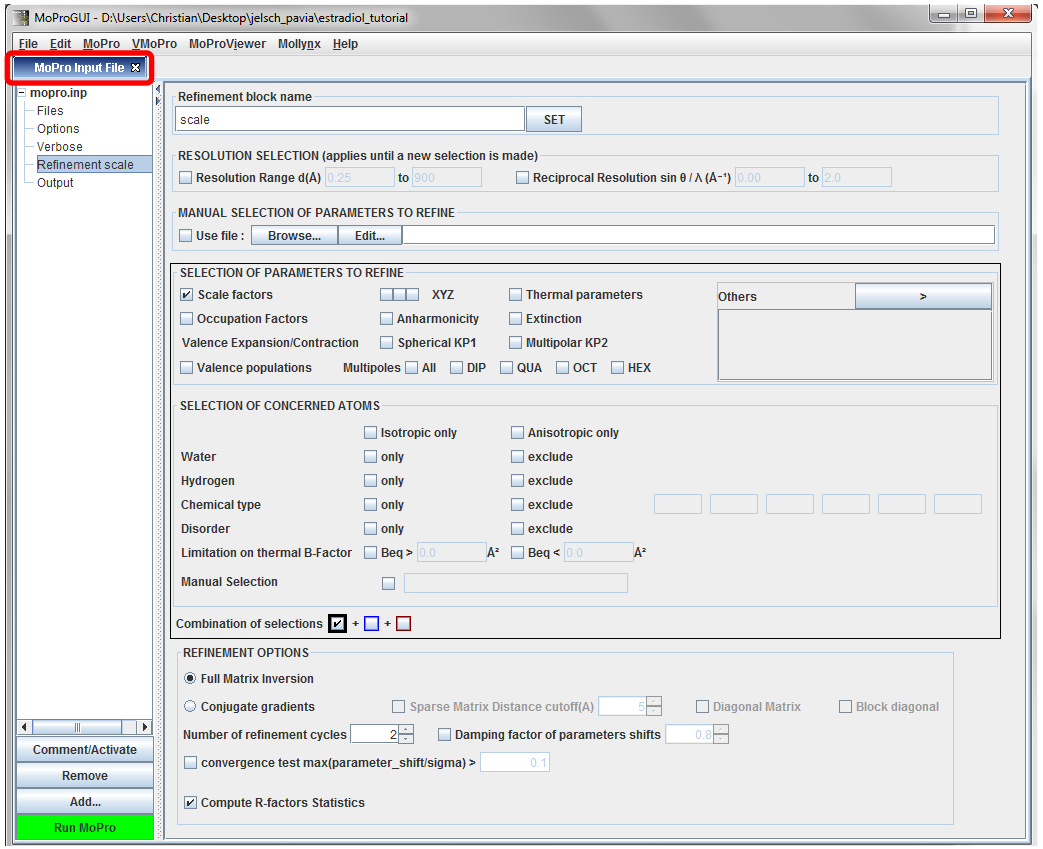


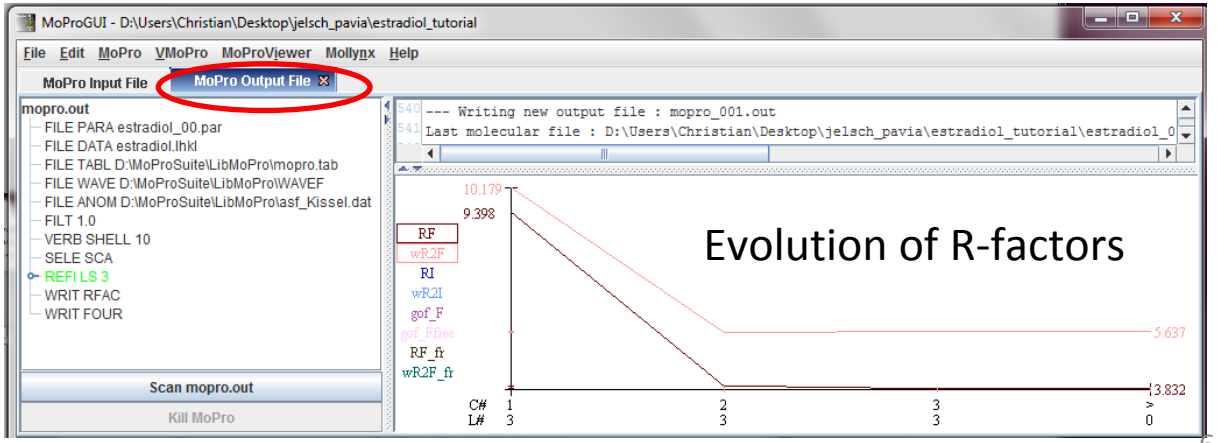
h k l Iobs sigma(Iobs)

Step 5 Refine SCAle factor



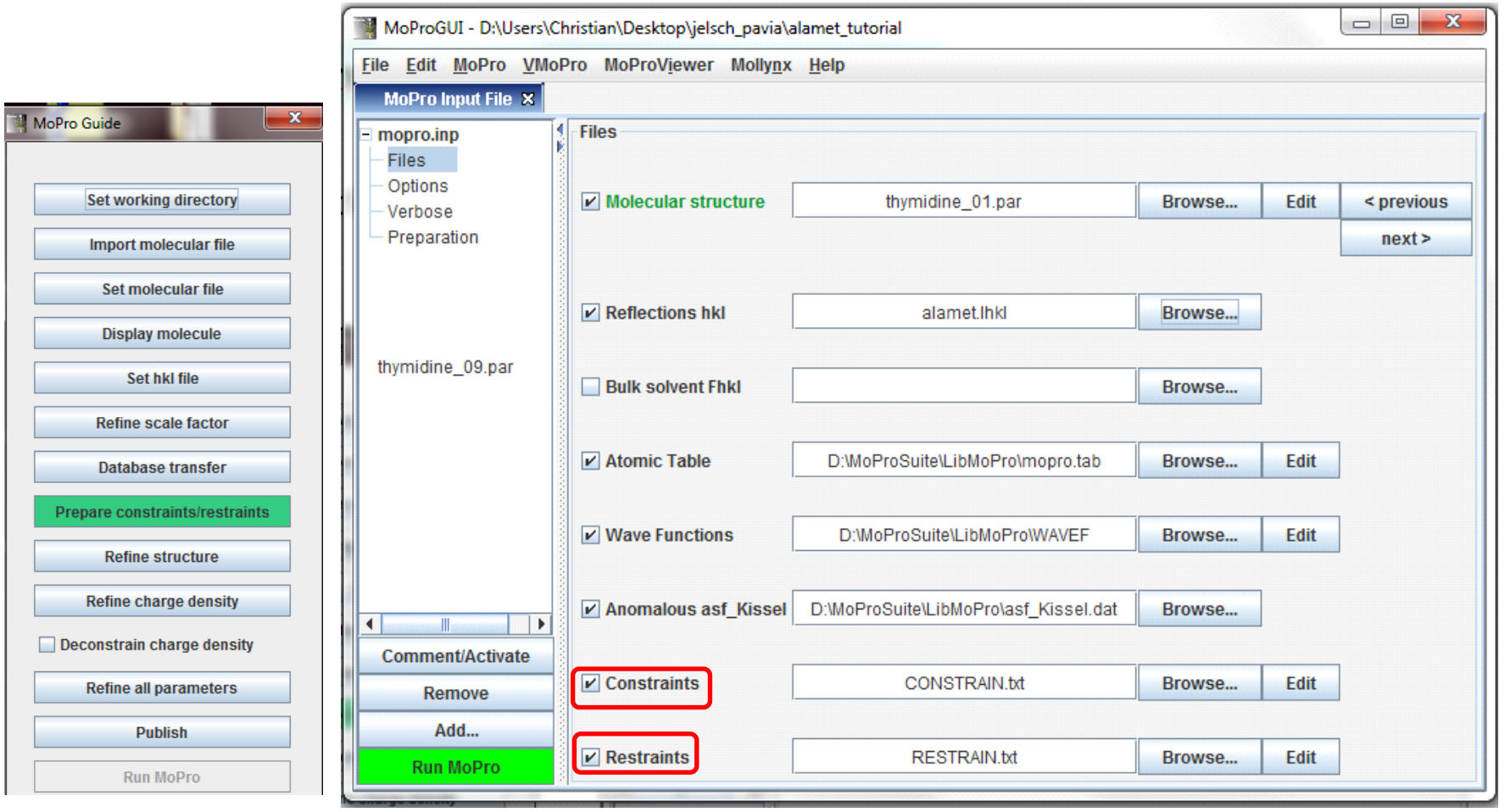
Click on
''mopro Input file''
&
''mopro Output file''





Step 6 Preparation of constraints & restraints

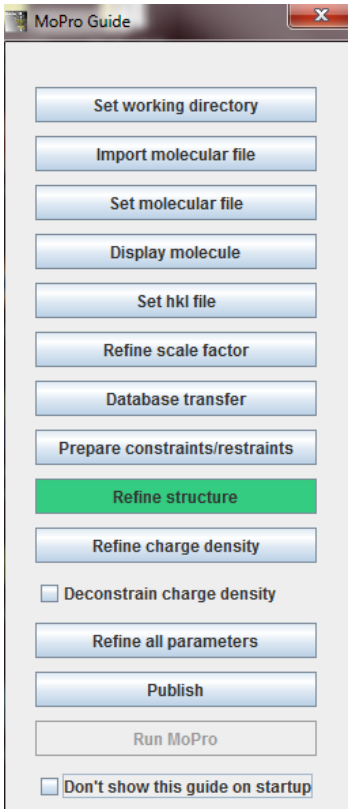
e.g. H-X distances for Hydrogen atoms

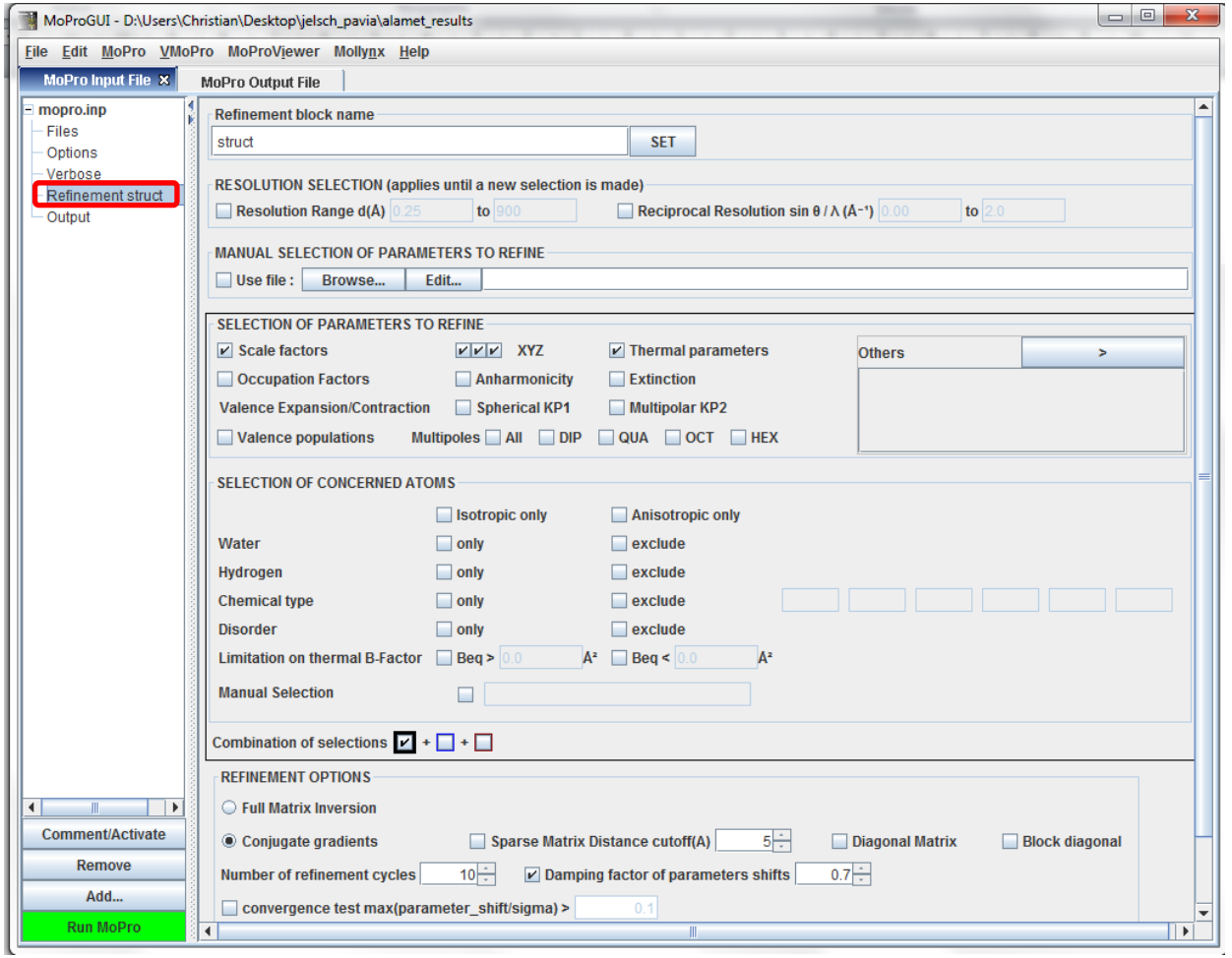


Edit and have a look at the generated CONSTRAIN.txt & RESTRAIN.txt files

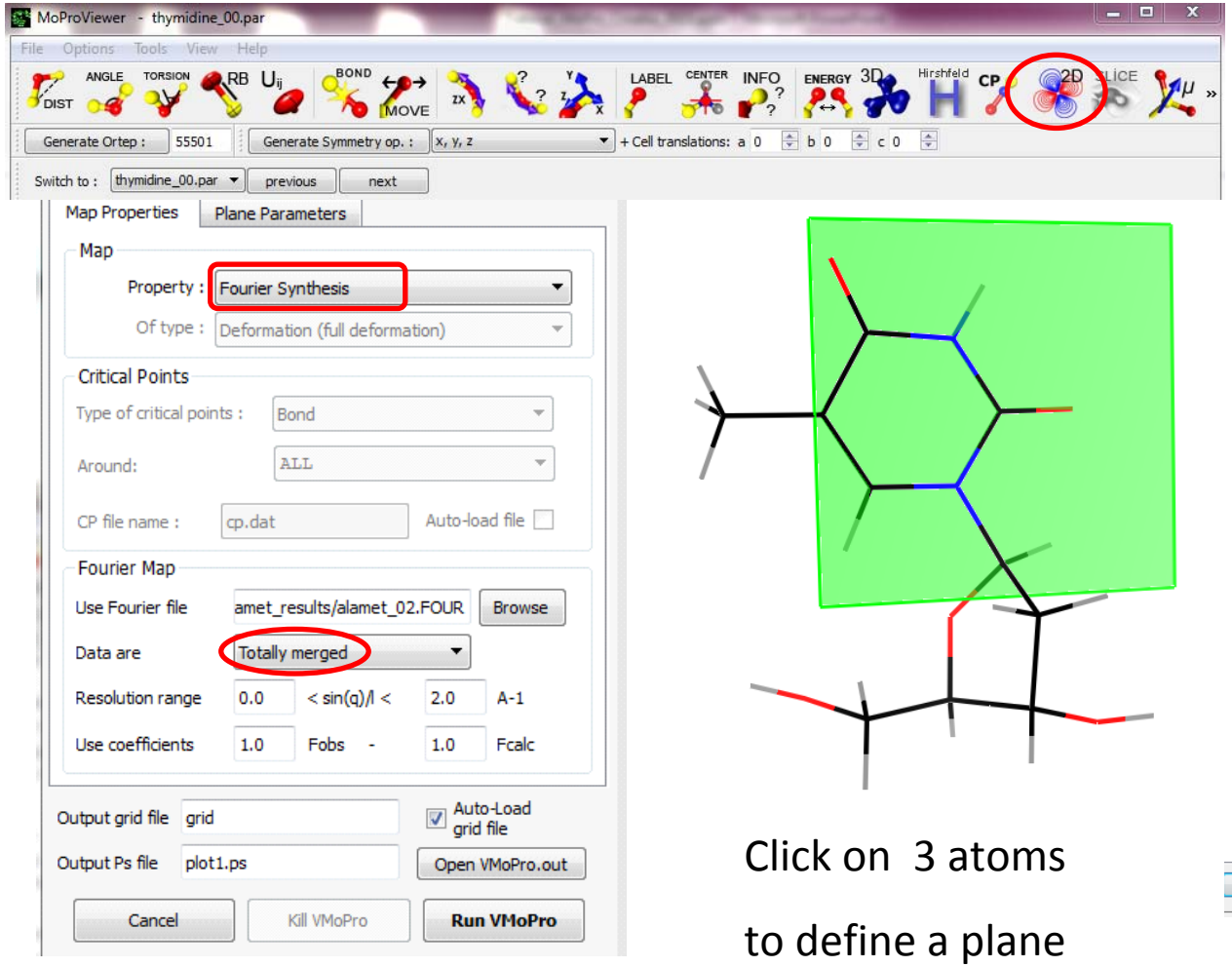
Step 7 Refine structure

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



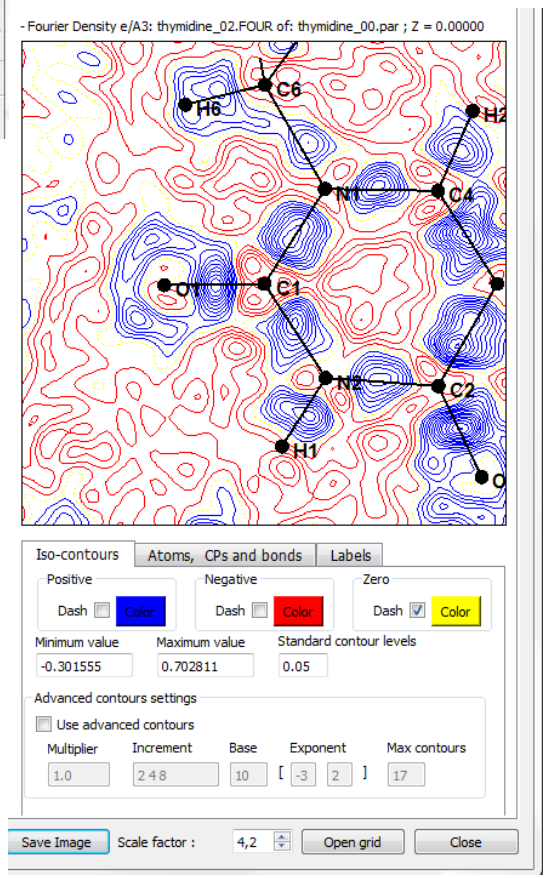


Step 8 Compute a Fourier Residual Electron Density 2D map



Click on 3 atoms

to define a plane



2D map:

Select Map Property : Fourier Synthesis

Select Fourier file : alamet_02.FOUR

Data are Merged

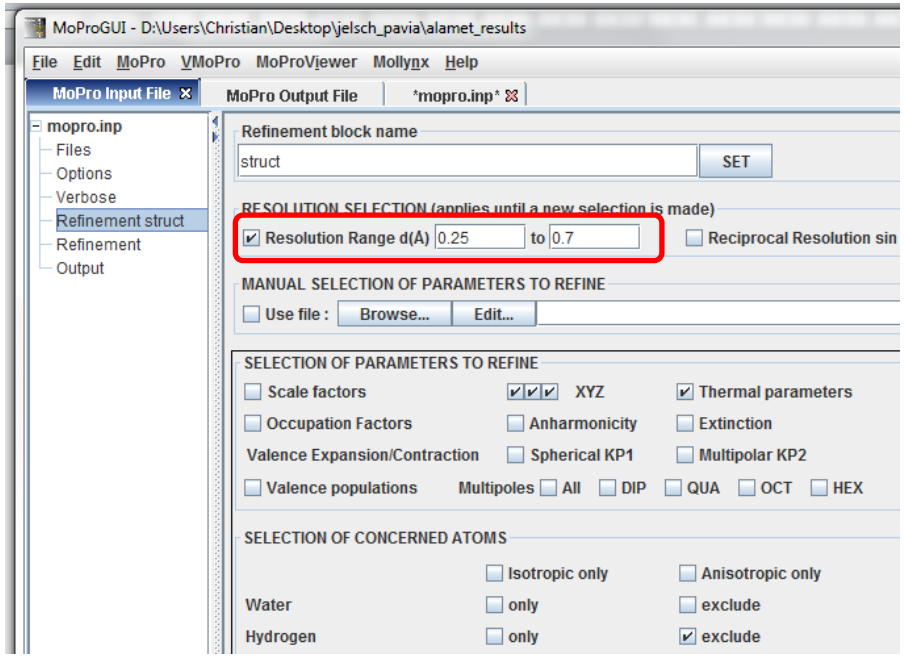
Click on ''Run VMoPro'' to start calculation

Step 9 HIGH ORDER refinement of structure

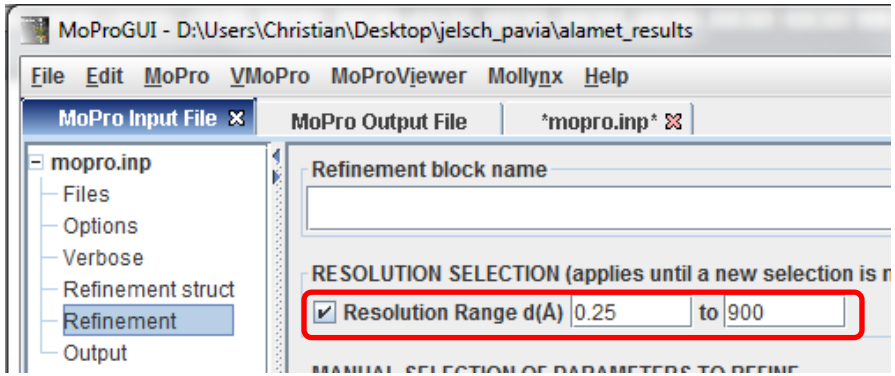
High resolution data $d < 0.7$ Å ,
Hydrogen not refined

The MoPro commands

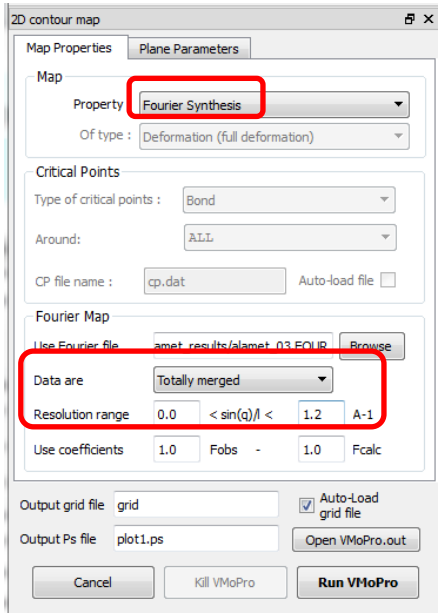
```
! <refinement> structural
RESO   0.25   0.7
SELE  XYZ UIJ  NOH
REFI   CG 10  DAMP 0.7
WRIT RFAC
```

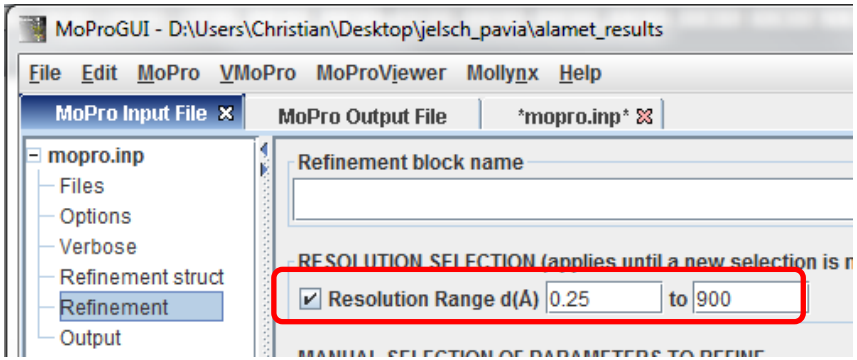


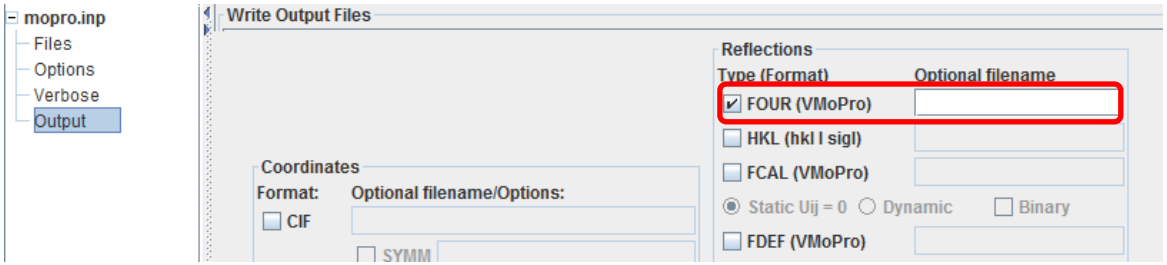
Write a Fourier reflections file
for all resolution



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

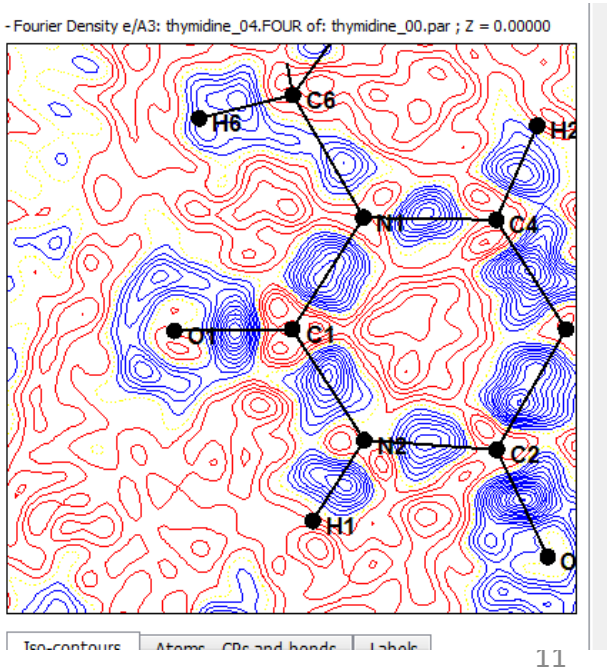




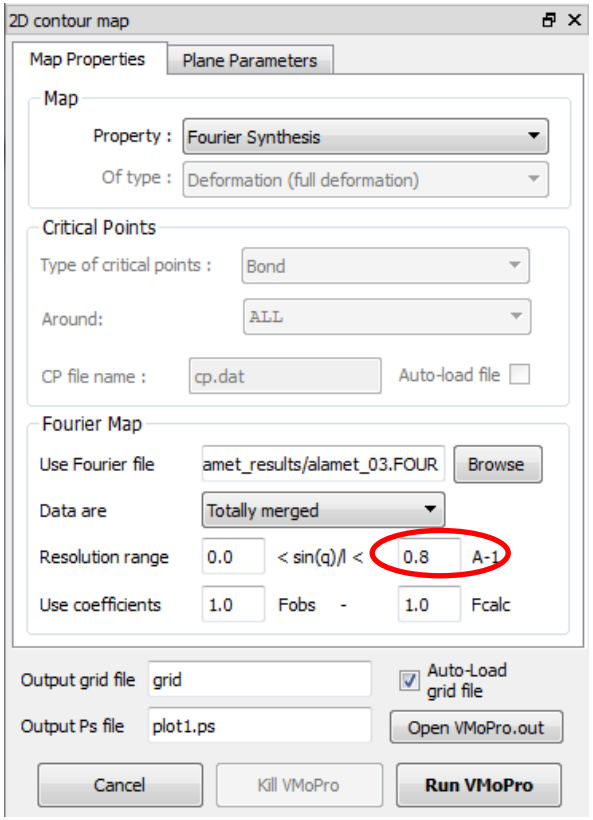


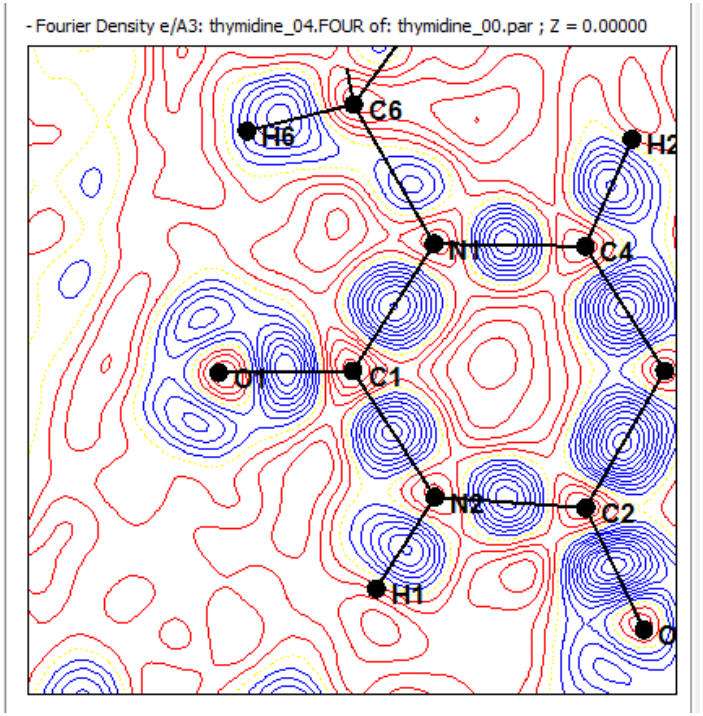
RESO 0.25 900.
WRIT FOUR

Slightly Stronger residual electron density visible on covalent bonds



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



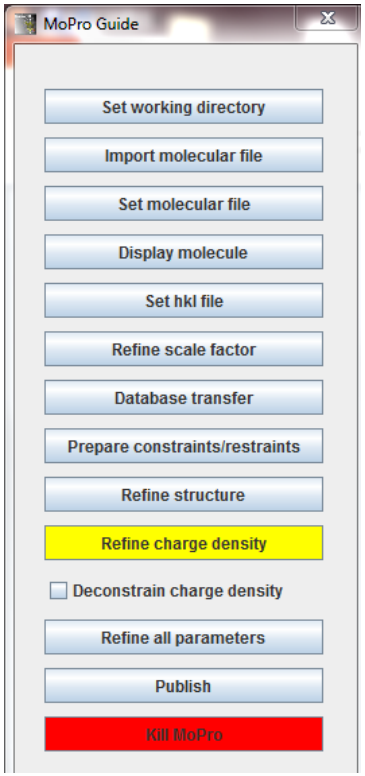


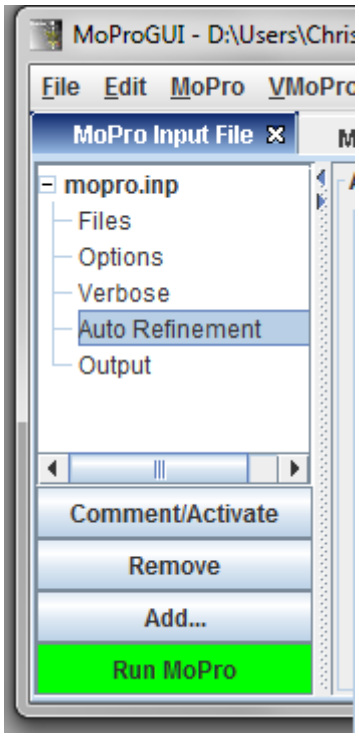
$\sin\theta/\lambda < 0.8$ Å^{-1}

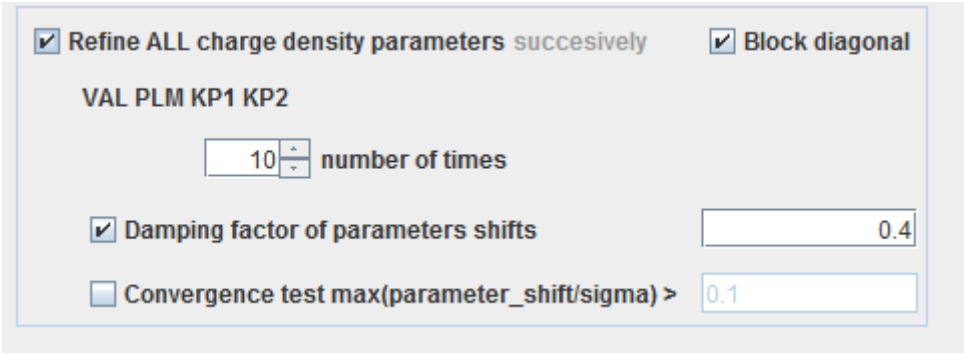
resolution
$d > 0.6$ Å

Bonding Electron Density is clearly visible

Step 12 Refinement of charge density

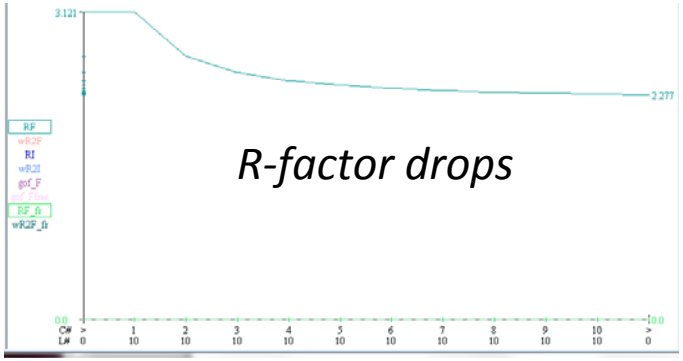






* Block diagonal: variables are decorrelated and can be refined together

* Damping to avoid divergence

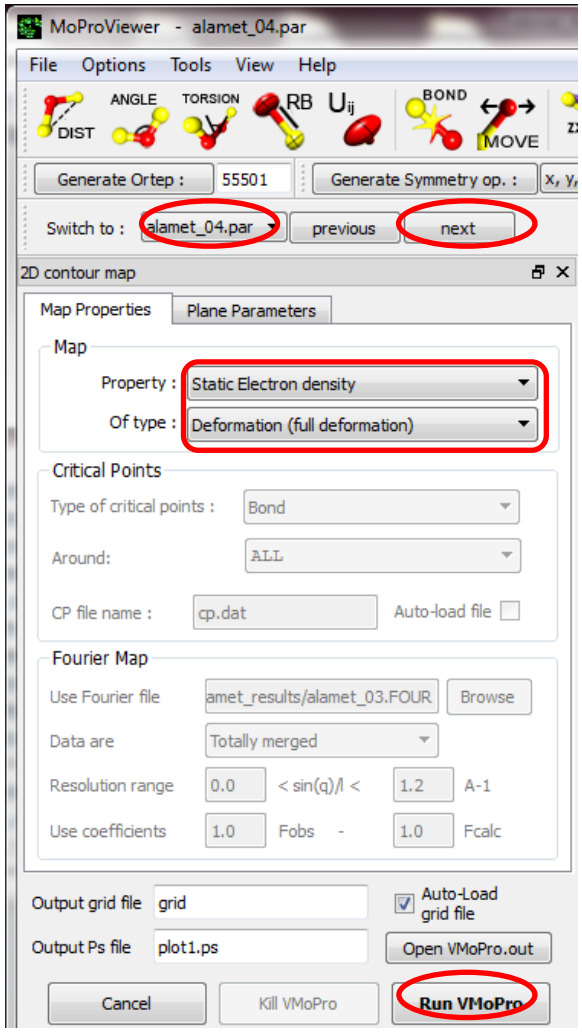


Have a look at resulting molecular .par file

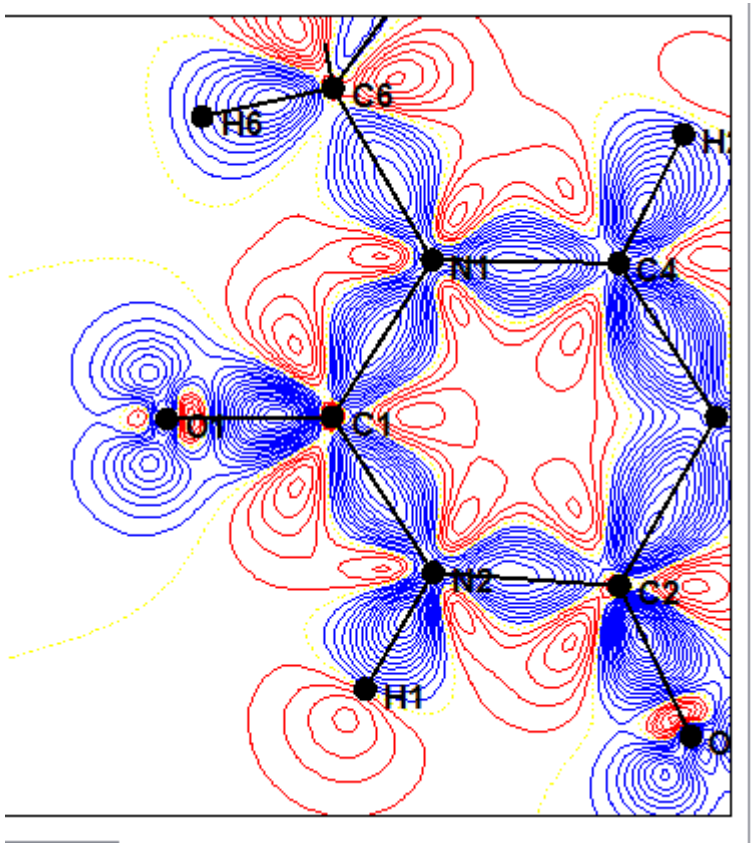
```
ATOMS    31

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

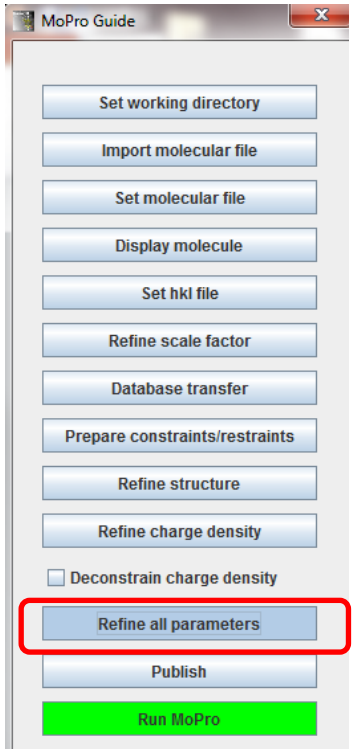
Step 13 Compute a Static Deformation Electron Density map

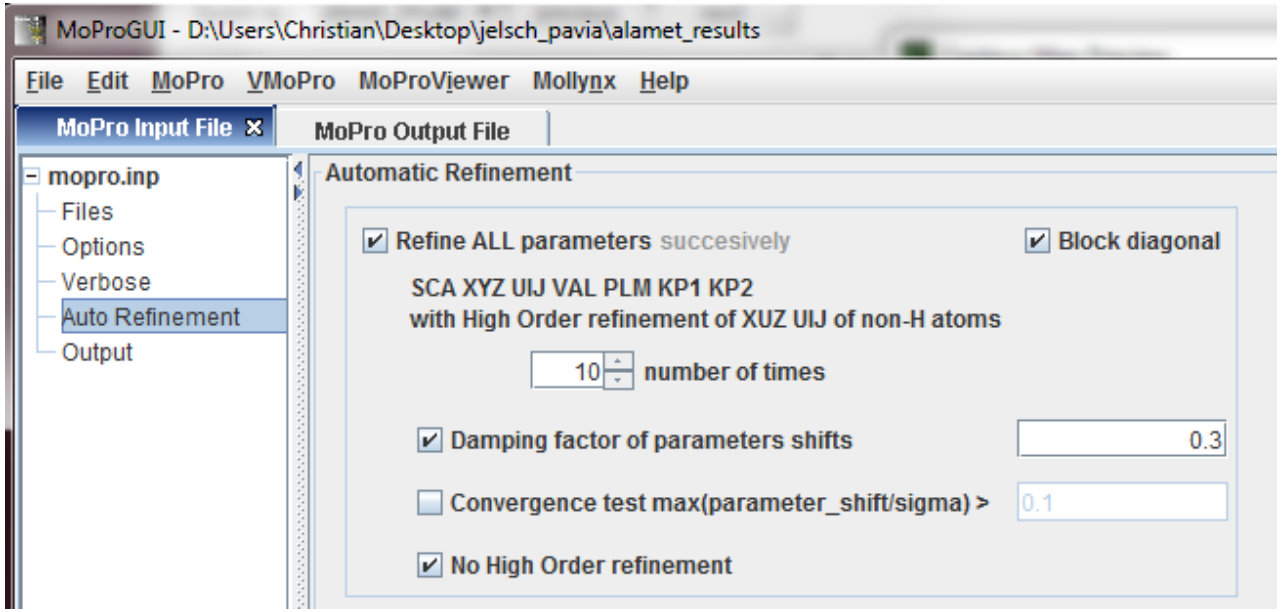


Choose appropriate (last) molecular file



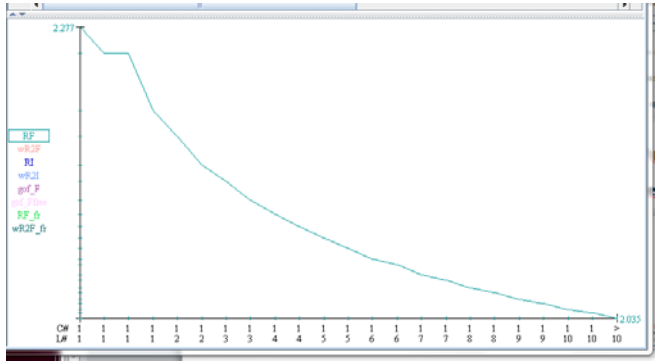
Step 14 Refinement of all parameters





- Block diagonal & damp : refine all parameters together

- Else : refine them successively

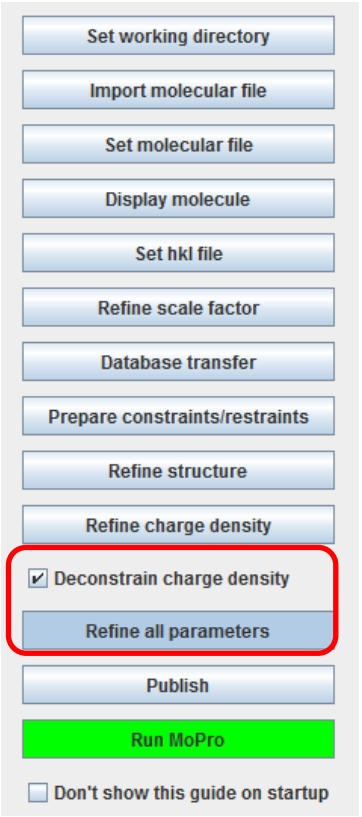


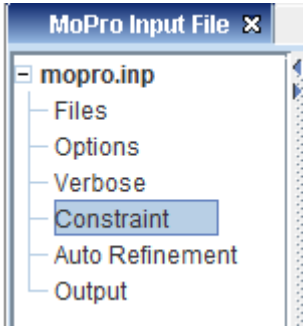
Further *R*-factor drop

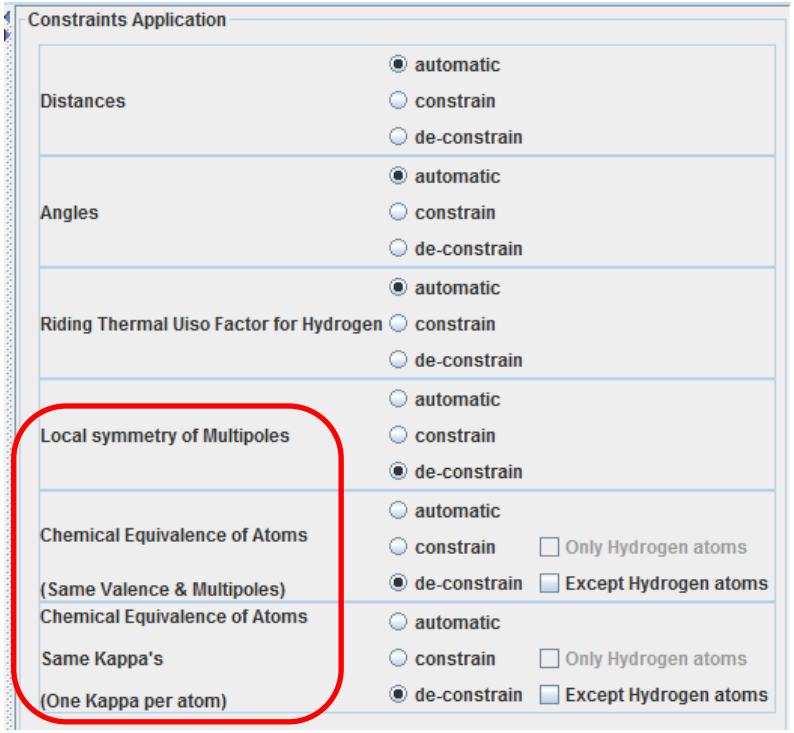
Step 15 Deconstrain charge density

Removes

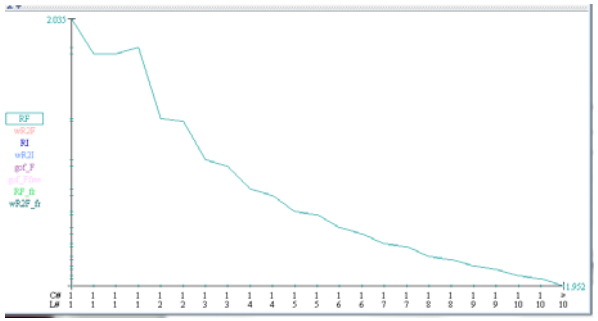
- Atoms equivalencies : similar atoms have same charge density
- Local symmetry of multipoles



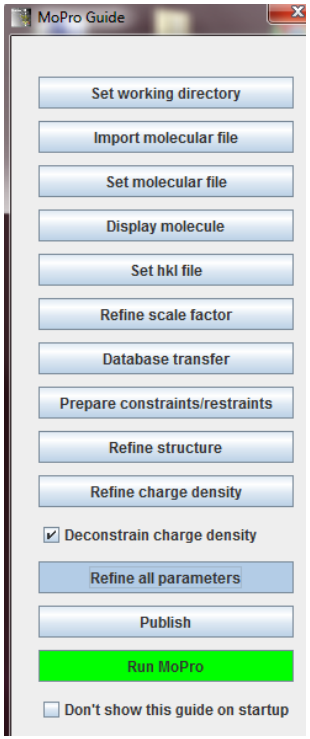


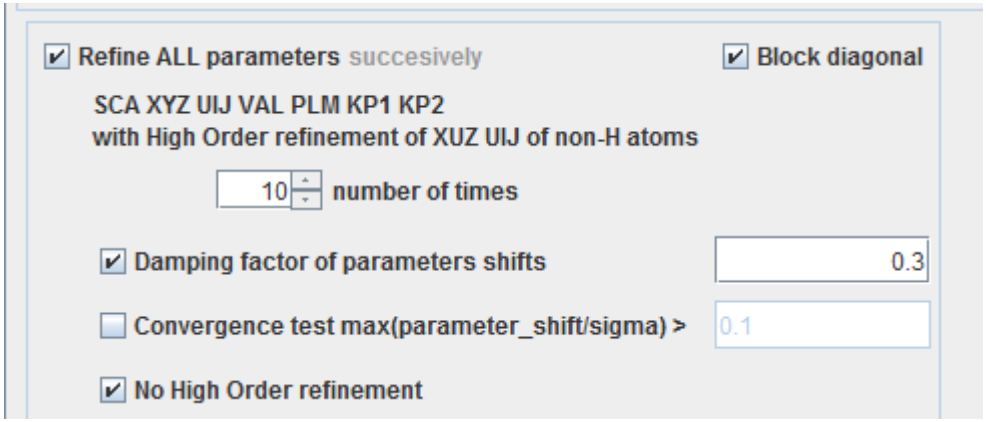


More variables
=>
R-factor drop

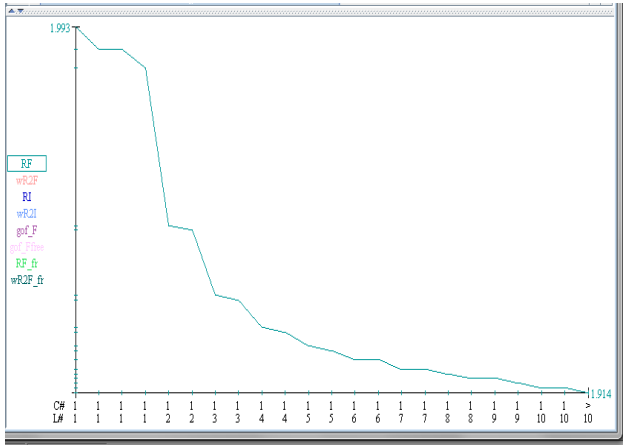


Step 16 Refinement of all parameters till convergence

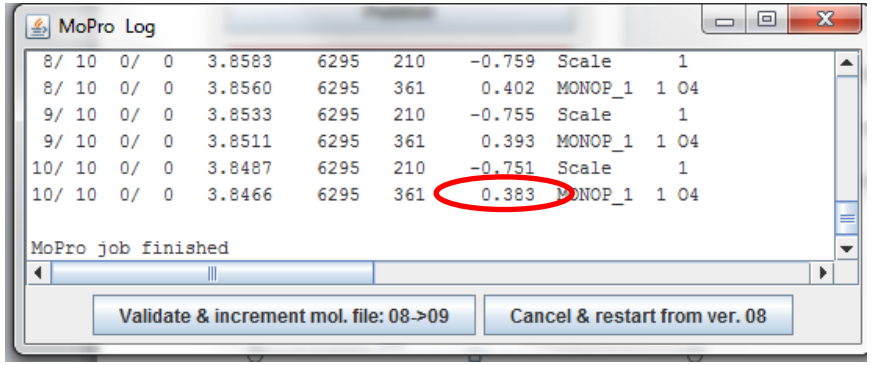




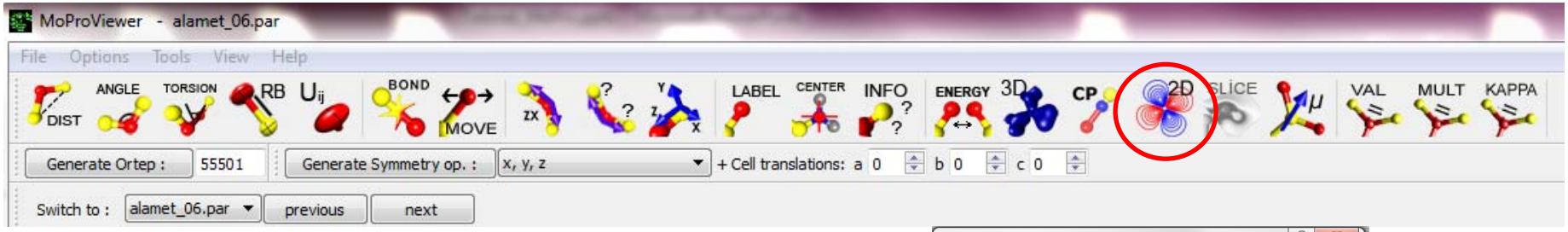
Check *R*-factor evolution

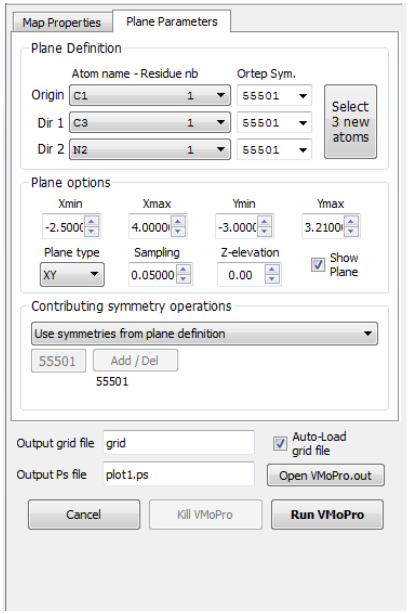


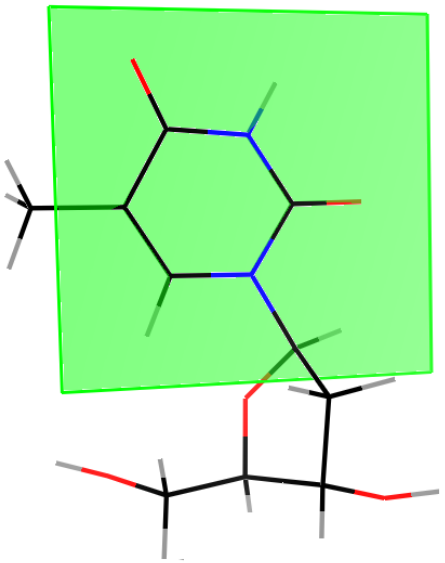
Check max Shift/sigma evolution

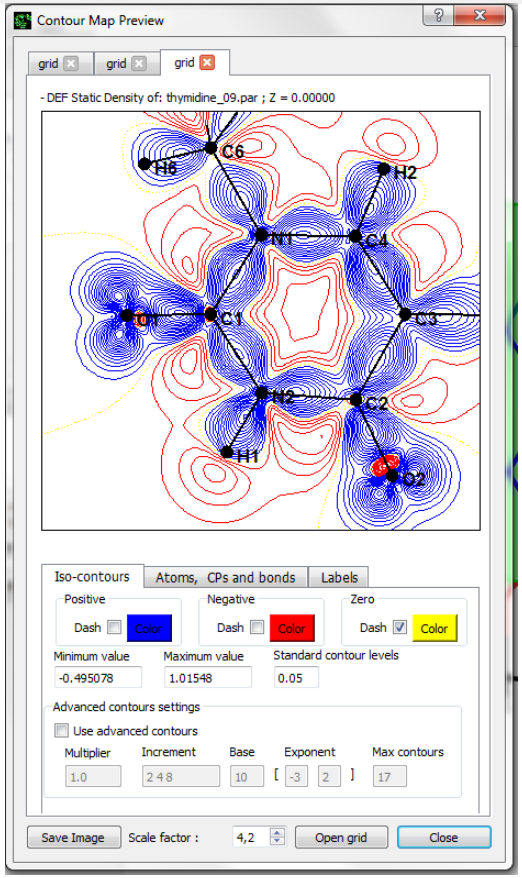


Step 17 Check Static Deformation Electron Density 2D maps





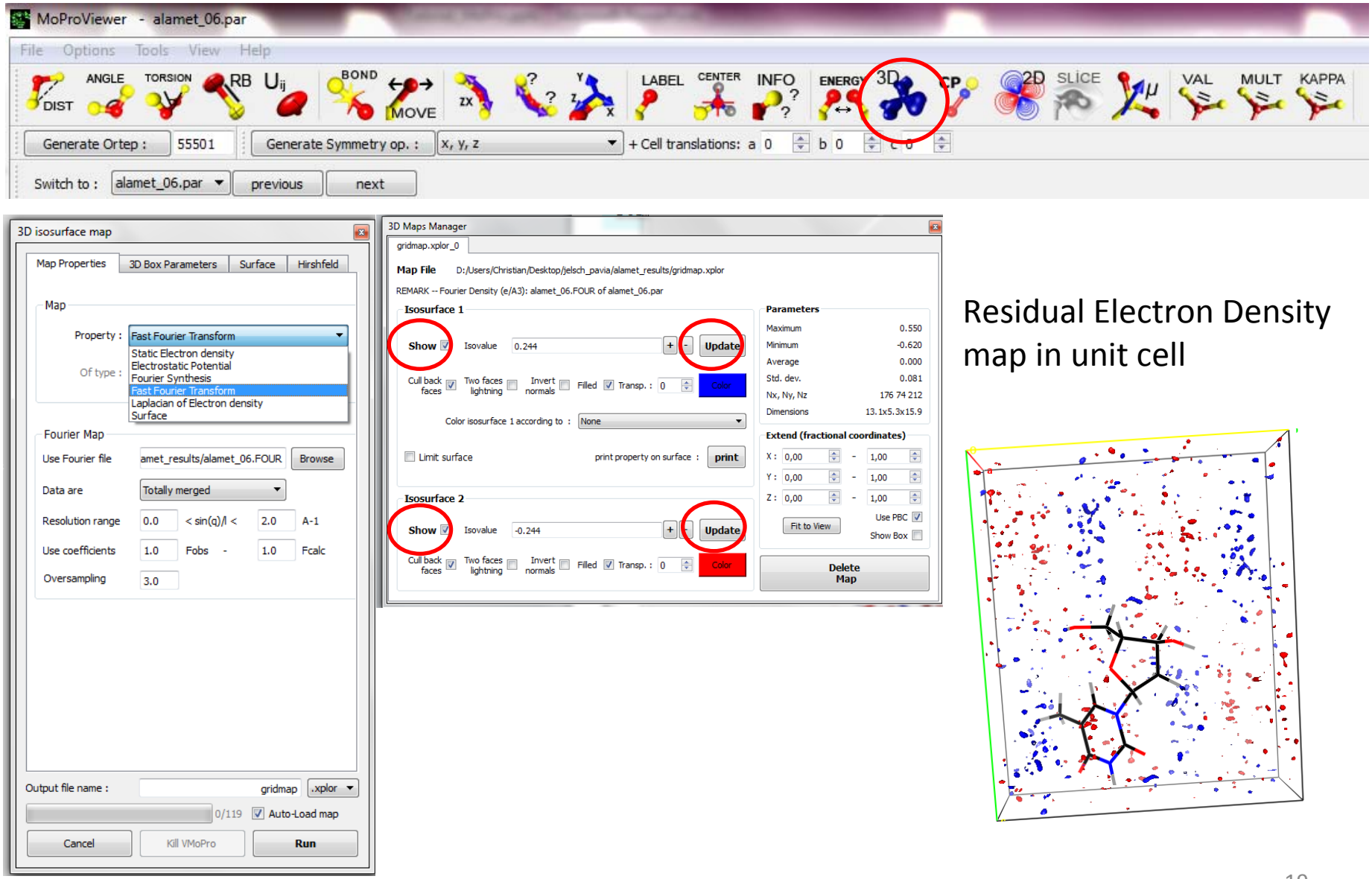




Choose Triplets of connected atoms

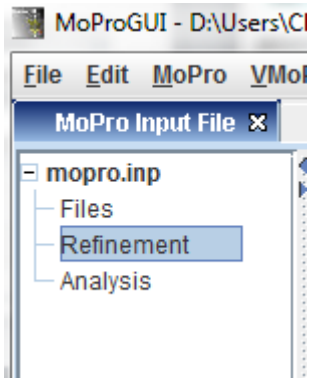
to define planes

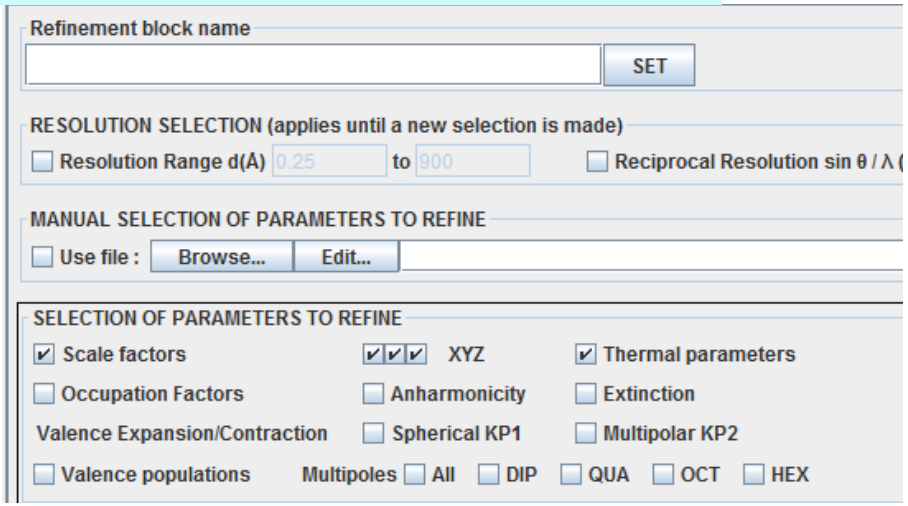
Step 18 Fast Fourier Transform 3D map



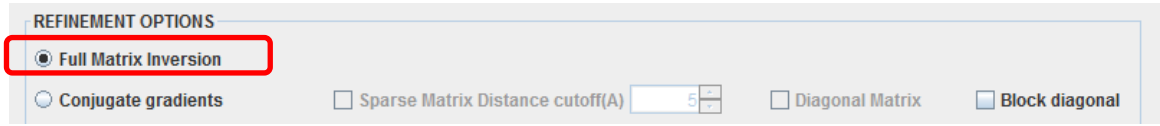
Residual Electron Density map in unit cell

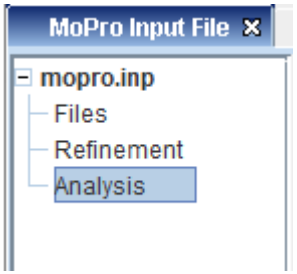
Step 19 Stereochemical analysis in MoPro

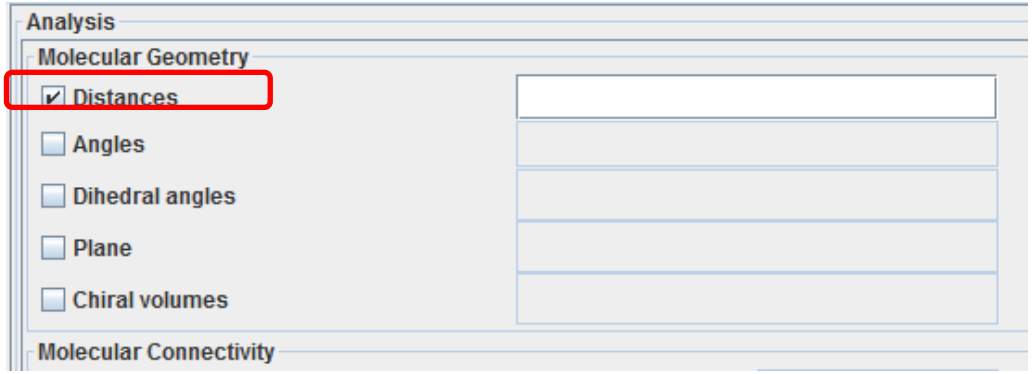




Refine
at first
Structure
(LS)
to obtain
sigmas
of distances



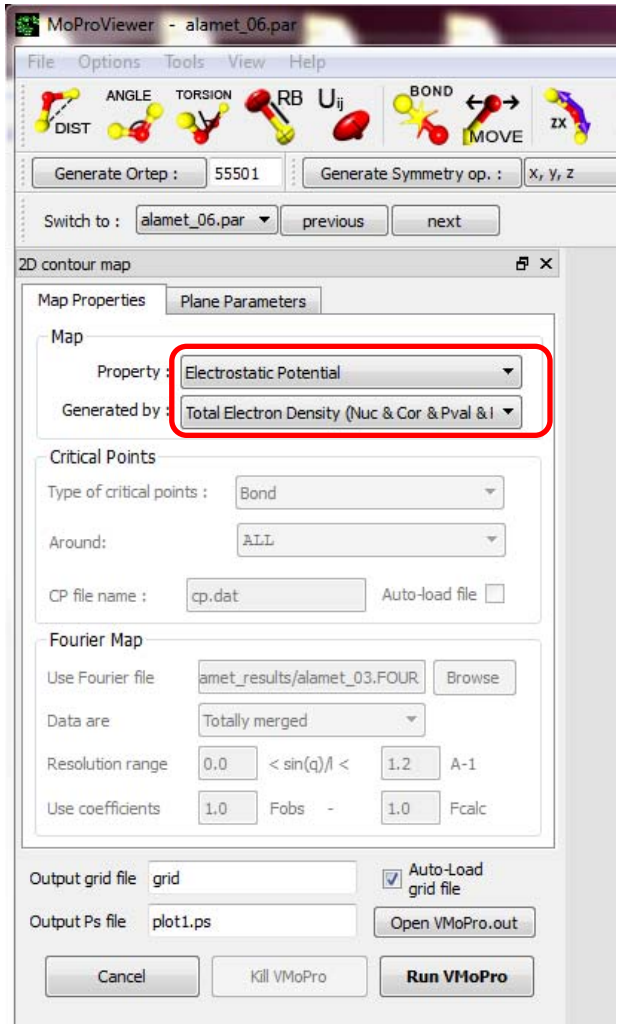


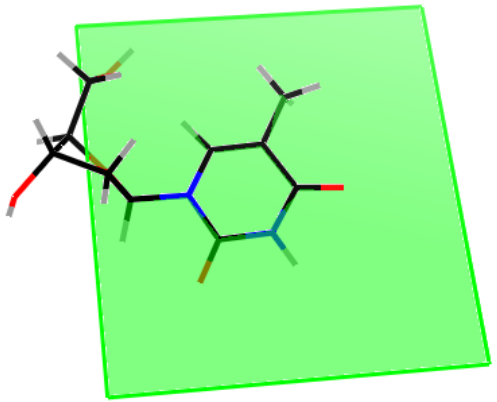


									refined	
ATOM1				ATOM2		SYM2	DIST	sigDIST	xyz	xyz
O1	thy	1	--	C1	thy	1	1.239082	0.000175	+++	+++
O2	thy	1	--	C2	thy	1	1.245673	0.000163	+++	+++
O3	thy	1	--	C6	thy	1	1.428634	0.000135	+++	+++

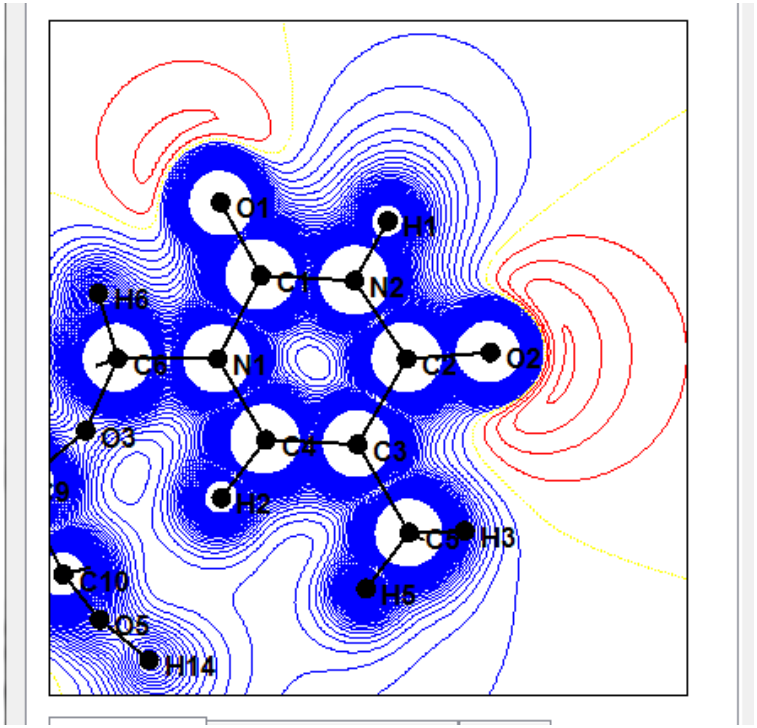
Etc….

Step 20 2D map of Electrostatic Potential



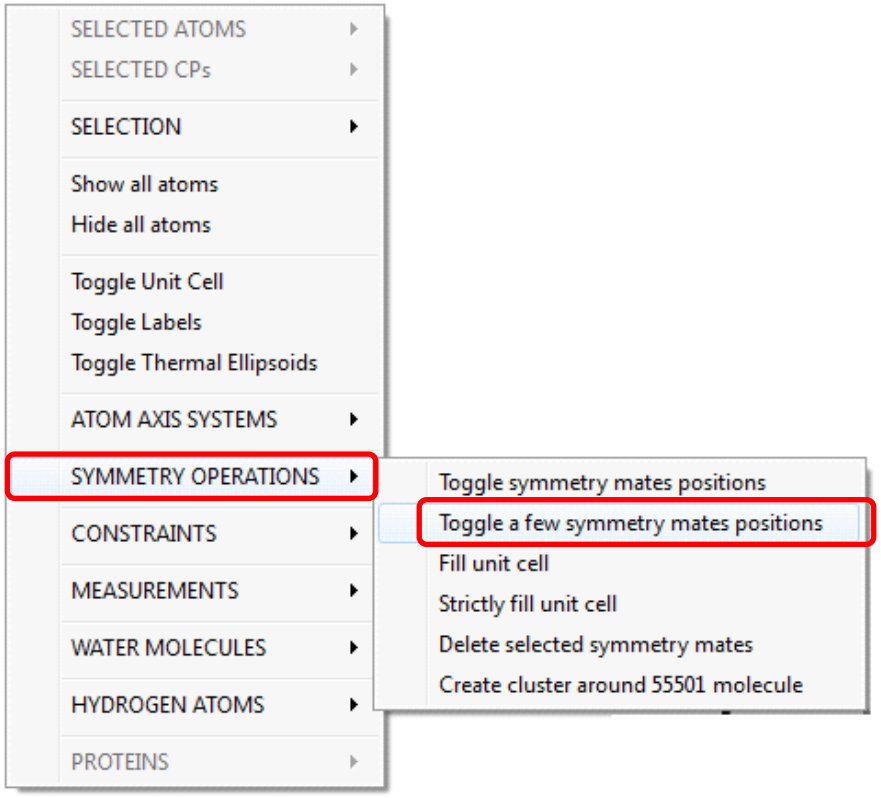


Augment dimensions
of plane
for a wider picture



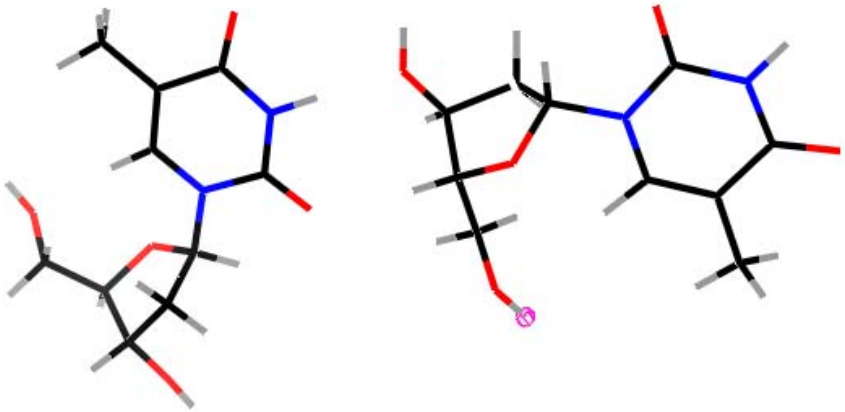
Step 21 Generate a dimer in MoProViewer

Click right on view

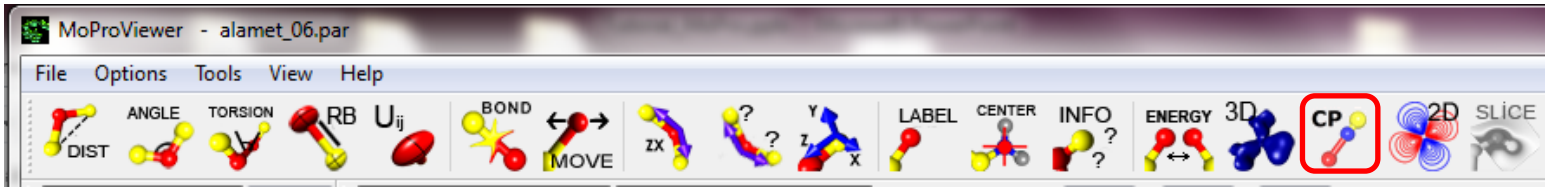


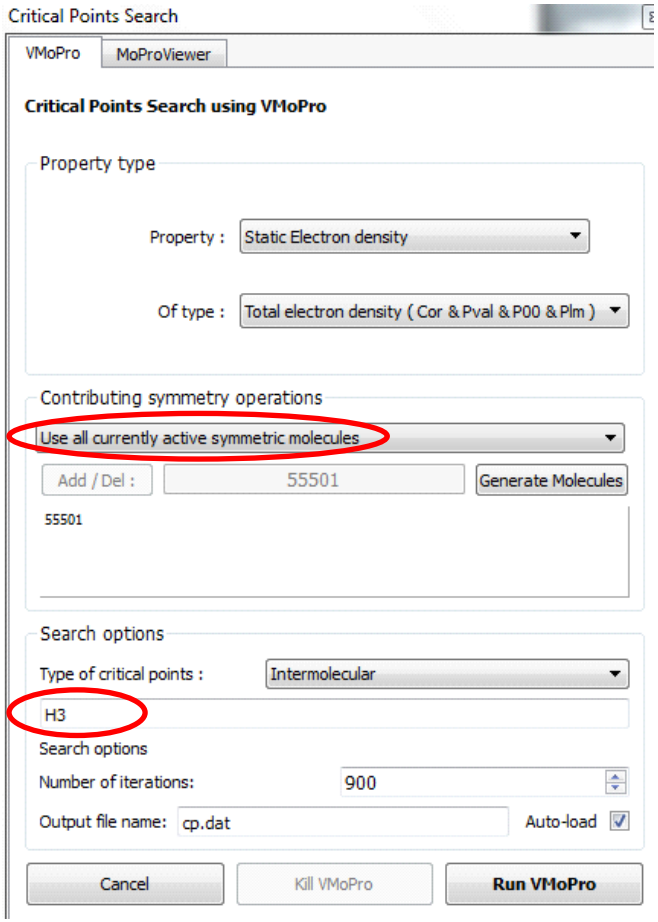
Keep a dimer like 55501 + 46502

p symmetry code
502
slation -1**a** + 1**b** + 0**c** & symmetry #02
1 6⟶+1 5⟶+0

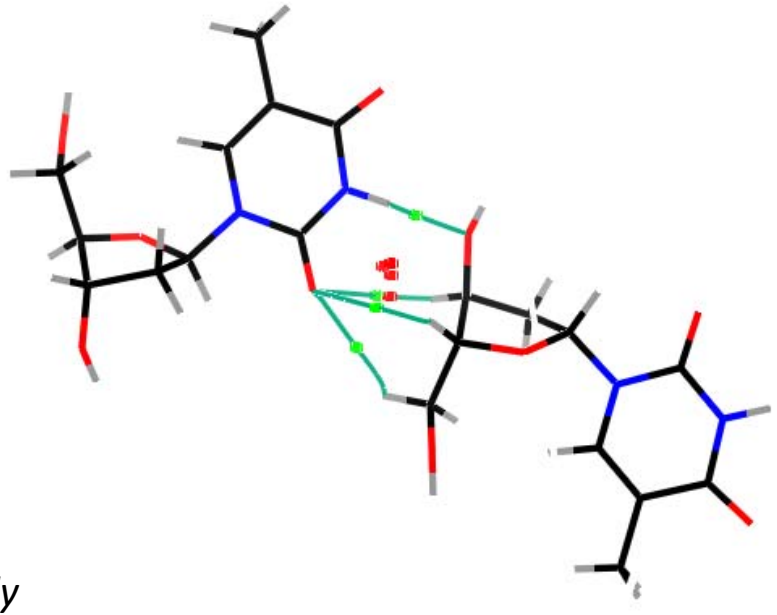


Step 22 Search Intermolecular critical points



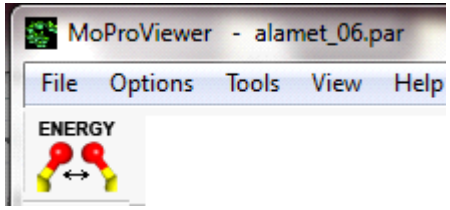


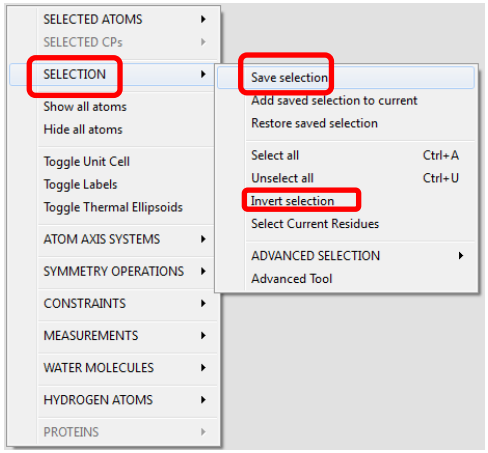
for a fast calculation => Search around 1 atom only (e.g. H11)

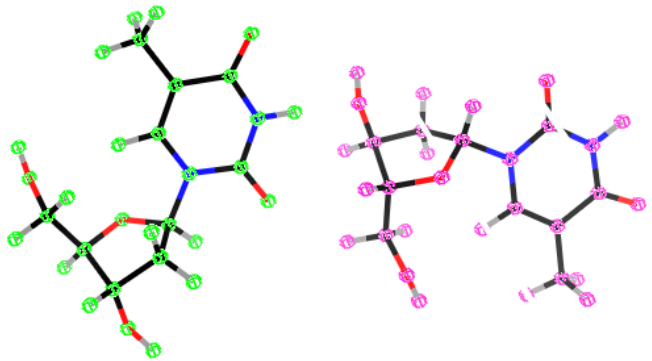


MoProViewer shows CPs & bond paths

Step 23 Compute electrostatic interaction energy of a dimer







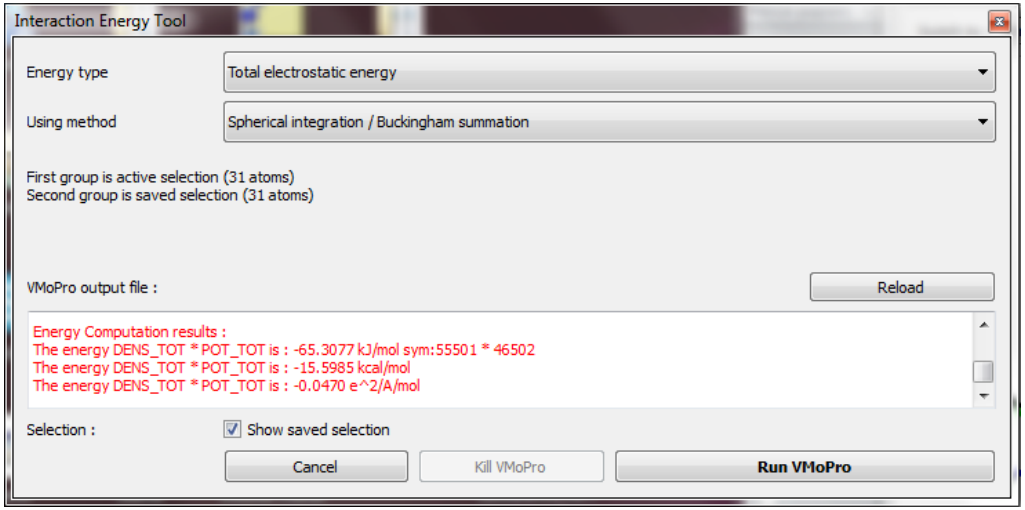
1) Click on ***Energy*** tool of MoProViewer

2) Select one molecule (shift+mouse)

Right click, Selection / SAVE selection

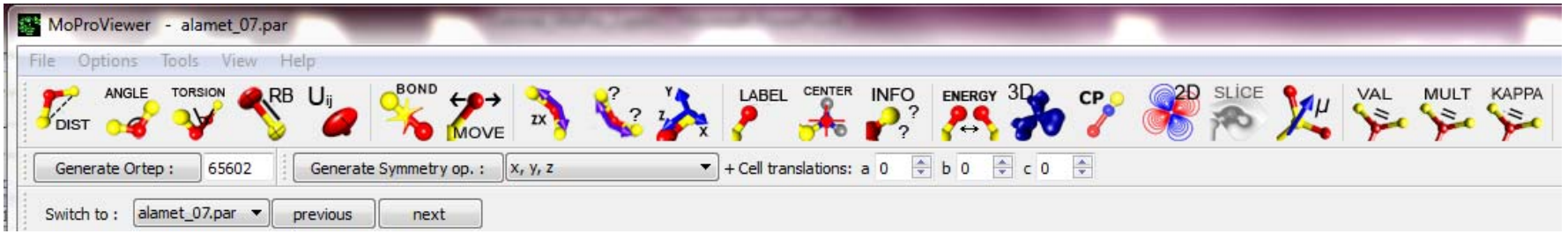
3) Invert Selection

4) Run VMoPro energy calculation



Step 24 Discover the Tools of MoProViewer

μ Dipole moment



Stereo-chemistry

Move atoms

Show local axes system for multipoles orientation

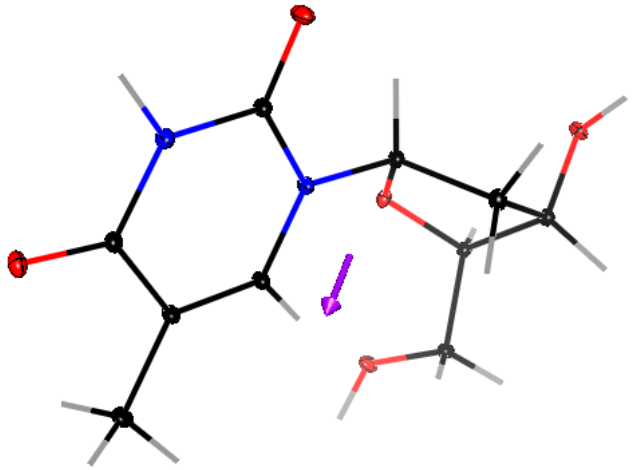
Compute 3D map

Compute 2D map

Critical points

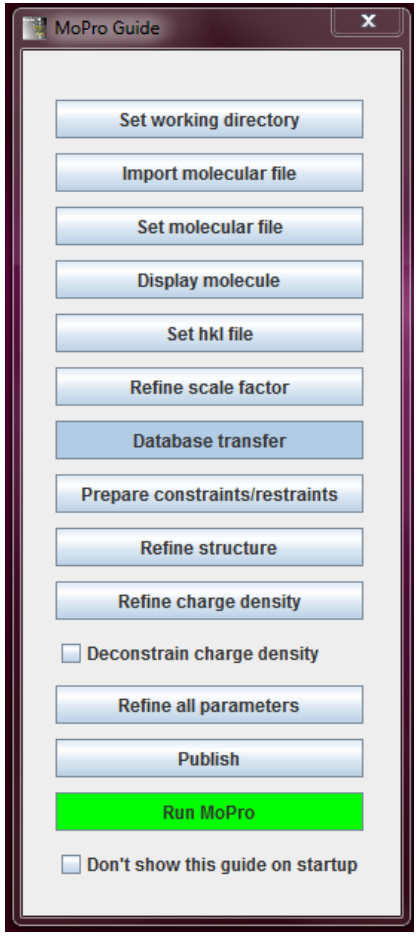
Equivalence Constraints of atomic charge density

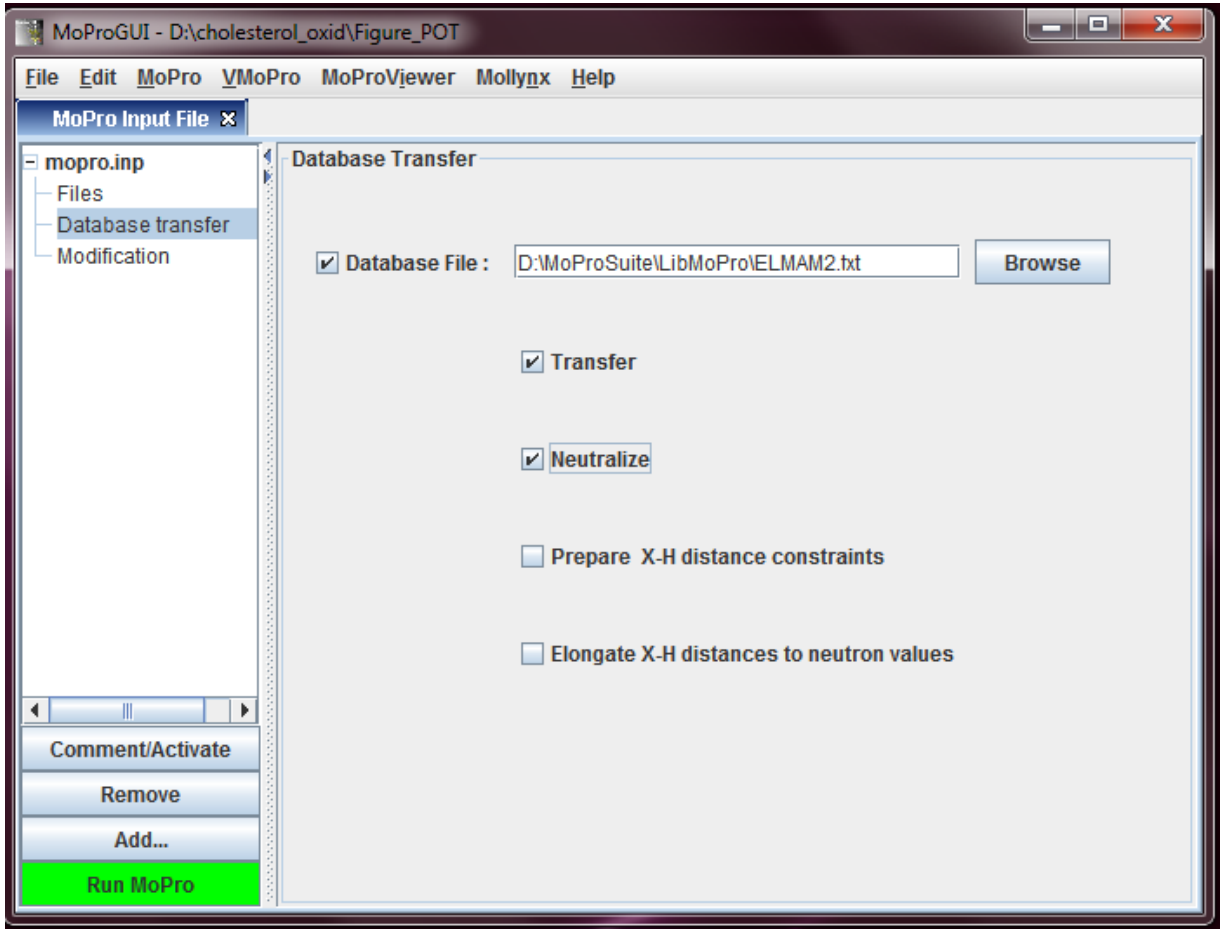
Uij Thermal ellipsoids



Step 25 ELMAM2 Database transfer

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





Check the resulting Static Deformation Electron Densiy maps

Step 25 Discover the MoPro Menus

Commands are classified and visible in menus