T u t o r i a l

MoProSuite :
Crystallographic software for charge density refinement

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

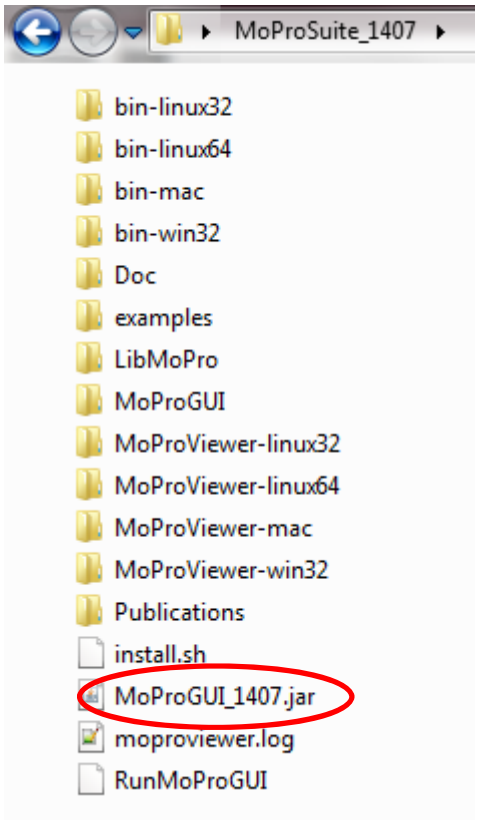
Christian Jelsch. CNRS. Université de Lorraine. France;

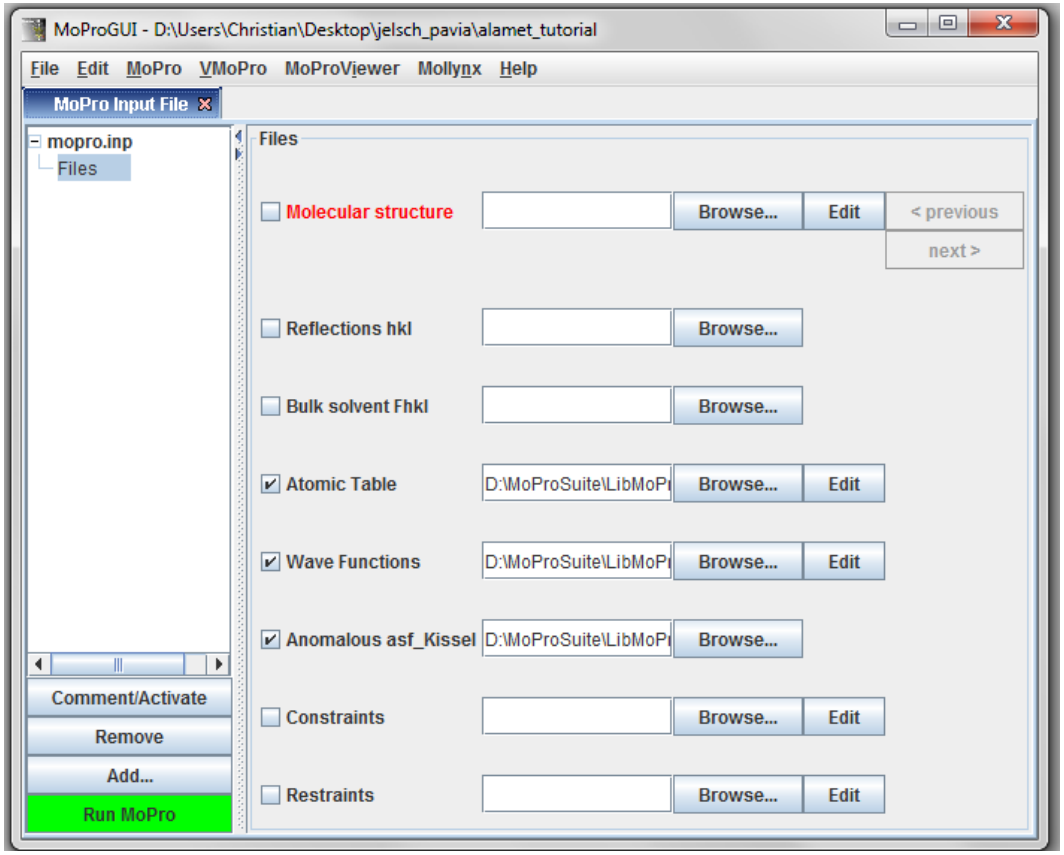
Available on windows, linux & mac.

July 2014

Step 1 Lauch MoProGUI

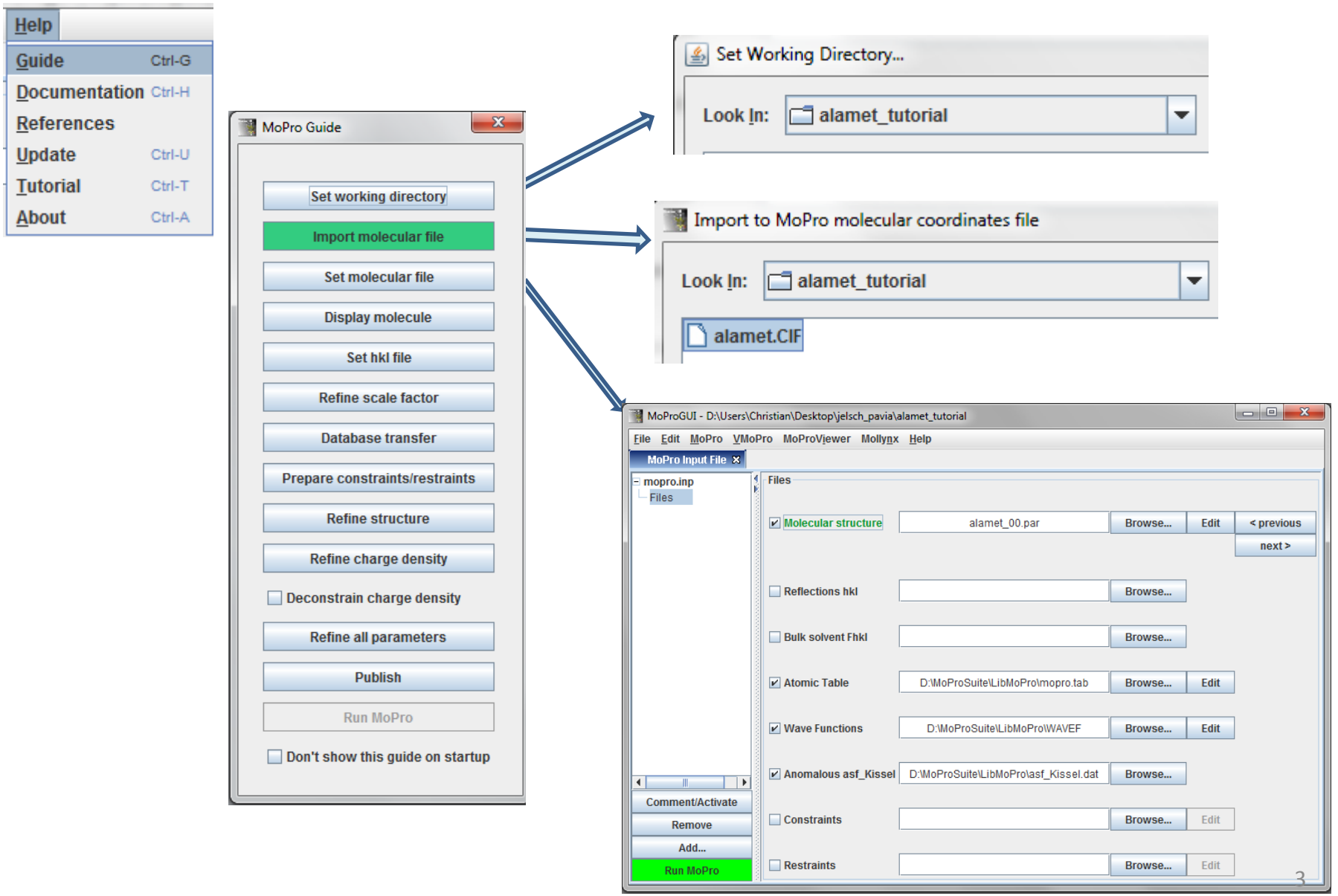
MoPro Graphical User Interface



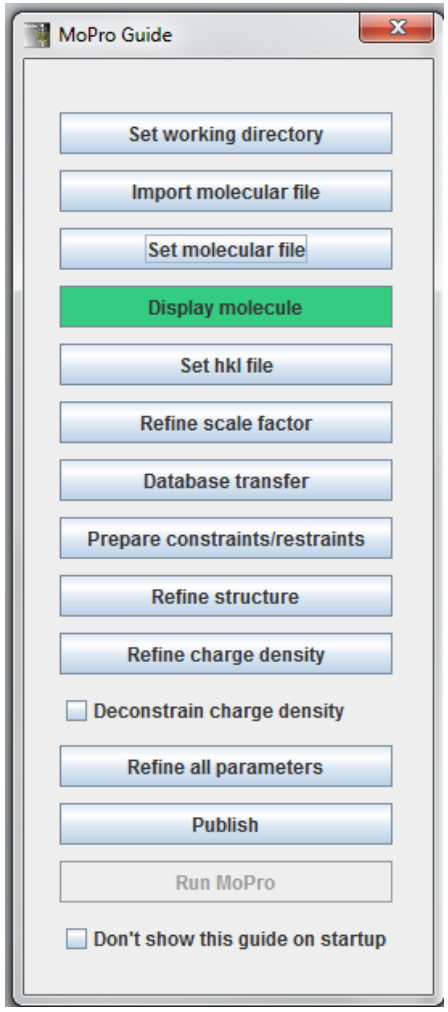


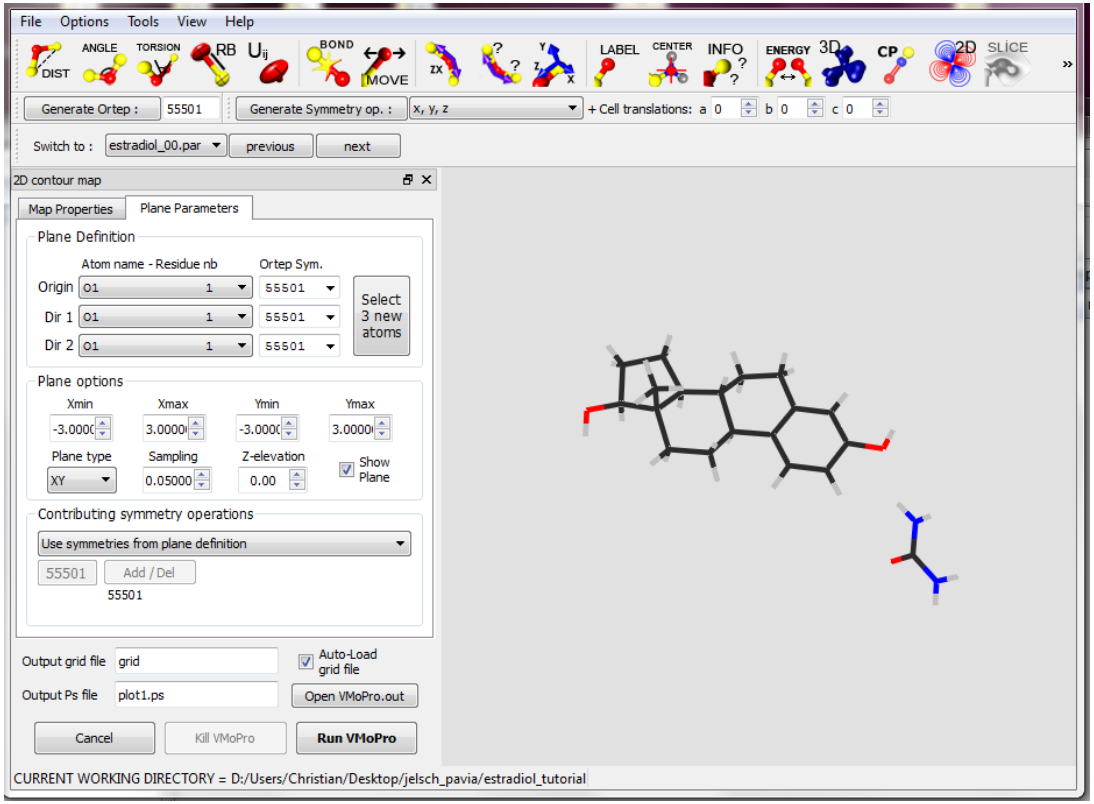
Requires JAVA, which can be downloaded at:
https://www.java.com/fr/download/

Step 2 initial steps : follow the GUIDE

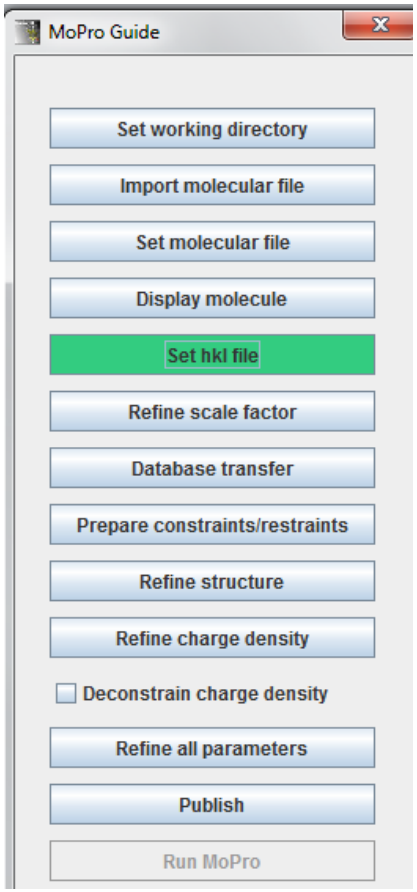


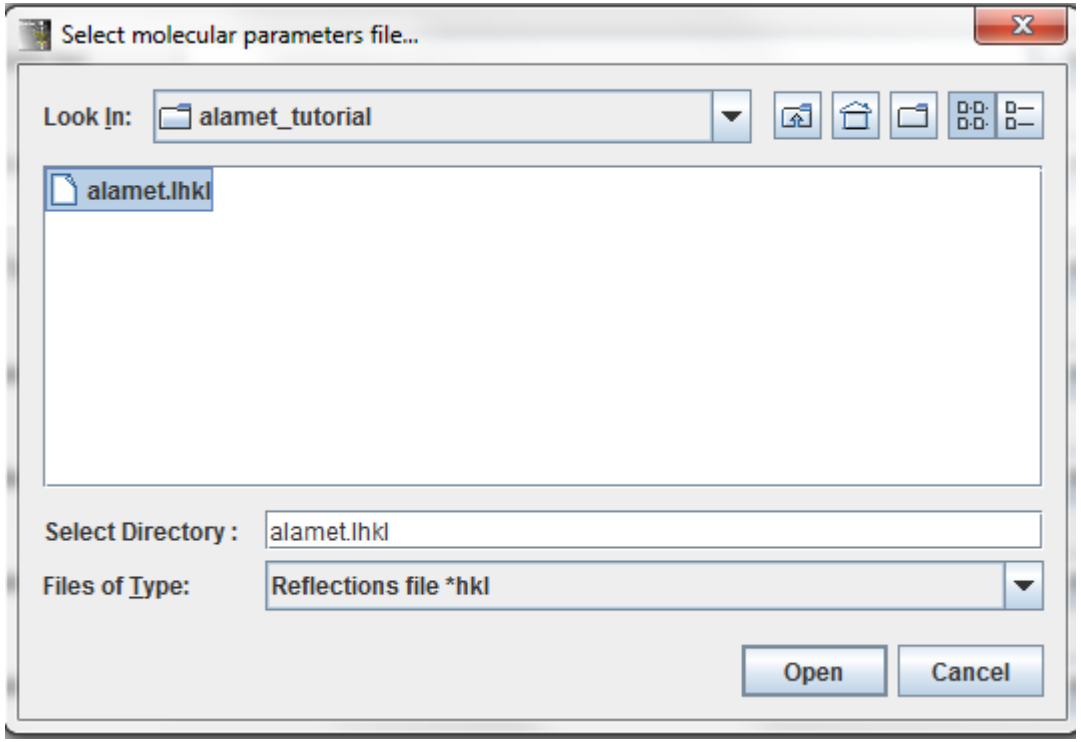
Step 3 Display molecule with MoProViewer





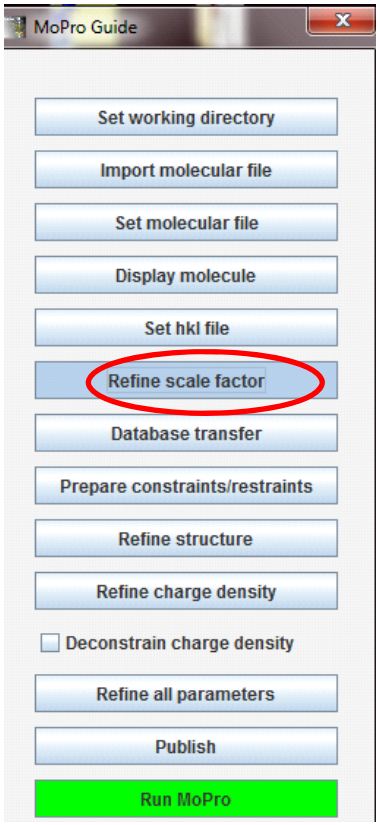
Step 4 Select reflections file



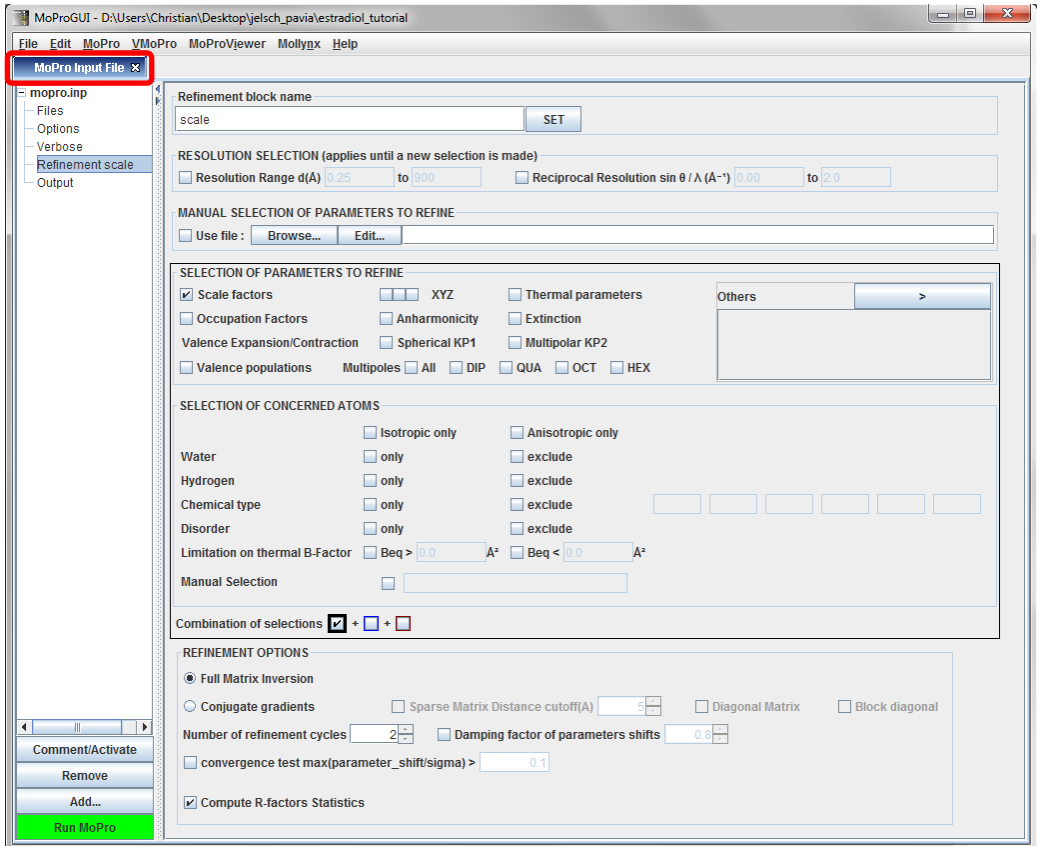


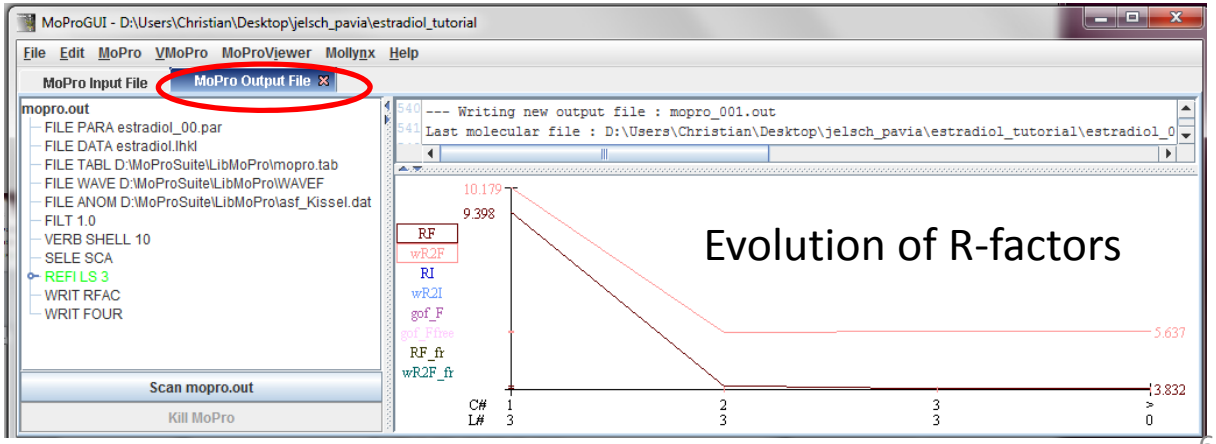
h k l Iobs sigma(Iobs)

Step 5 Refine SCAle factor



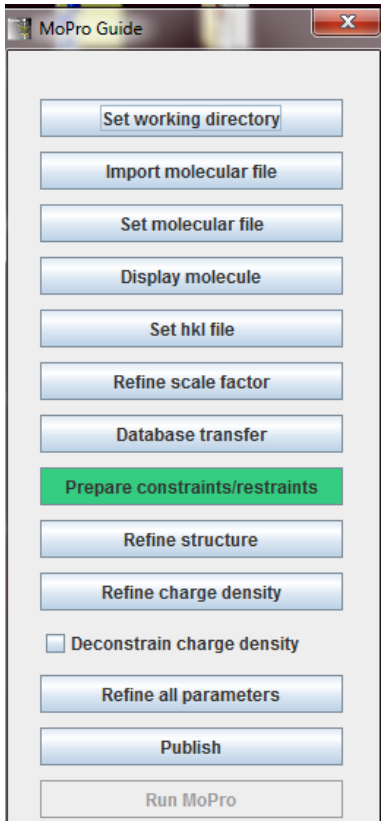
Click on
''mopro Input file''
&
''mopro Output file''

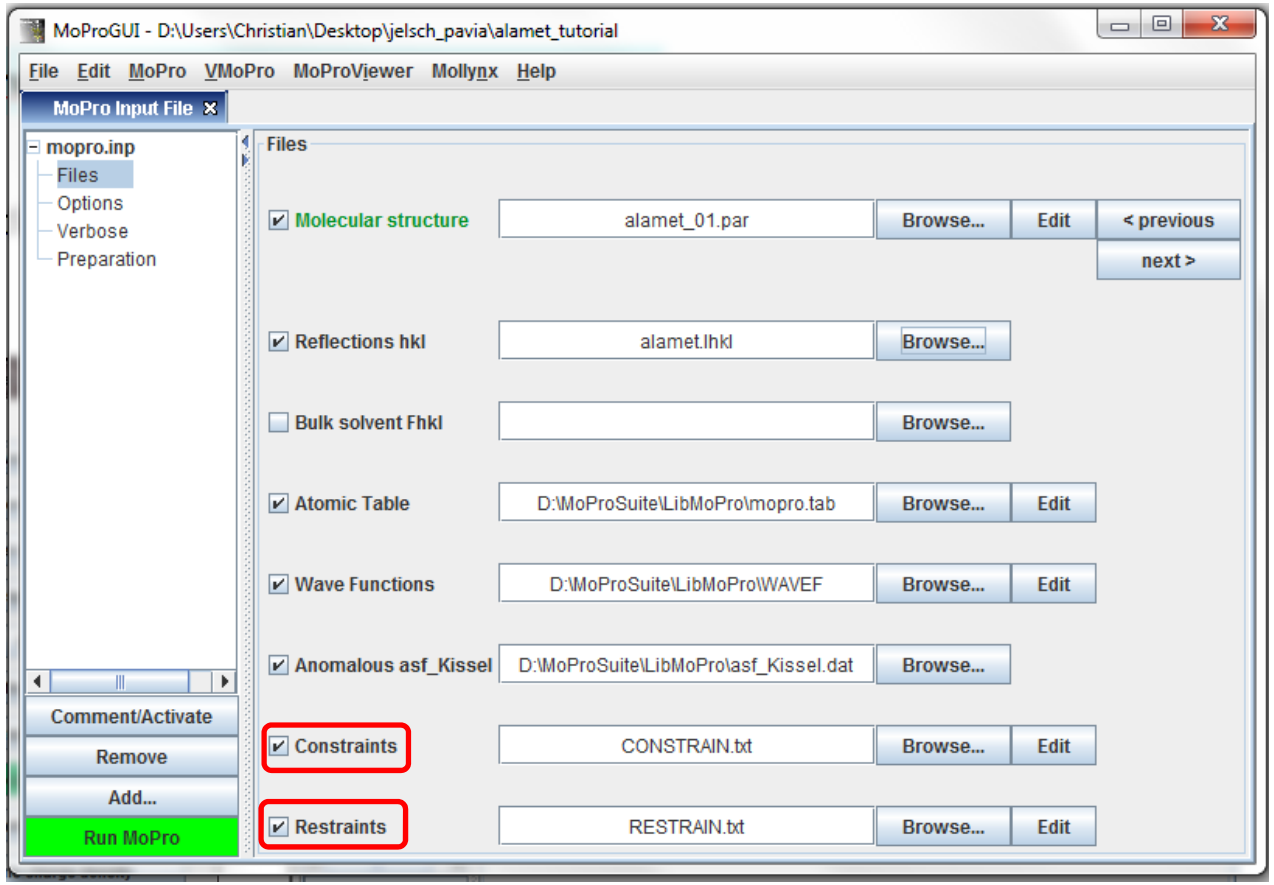




Step 6 Preparation of constraints & restraints

e.g. H-X distances for Hydrogen atoms

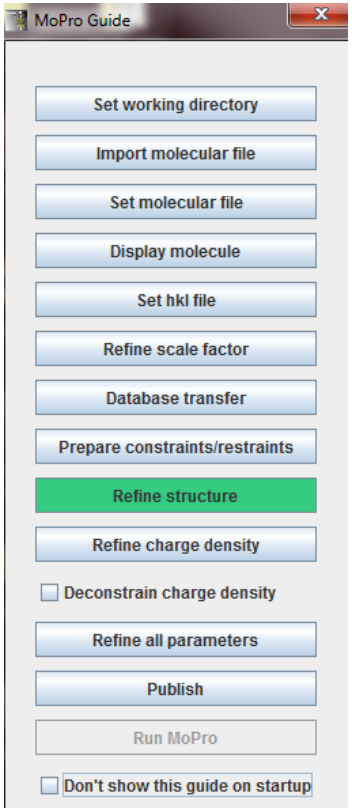


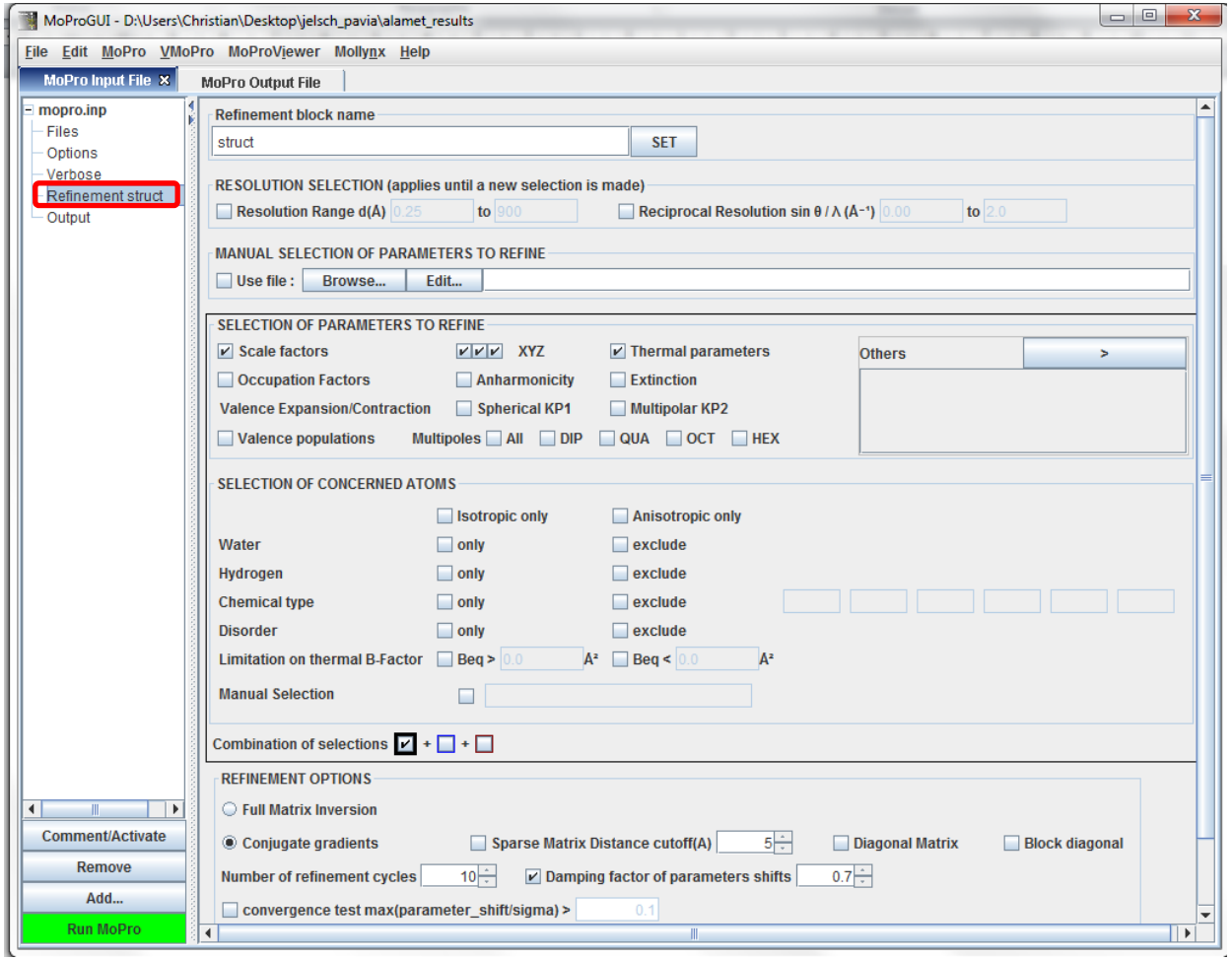


Edit and have a look at the generated CONSTRAIN.txt & RESTRAIN.txt files

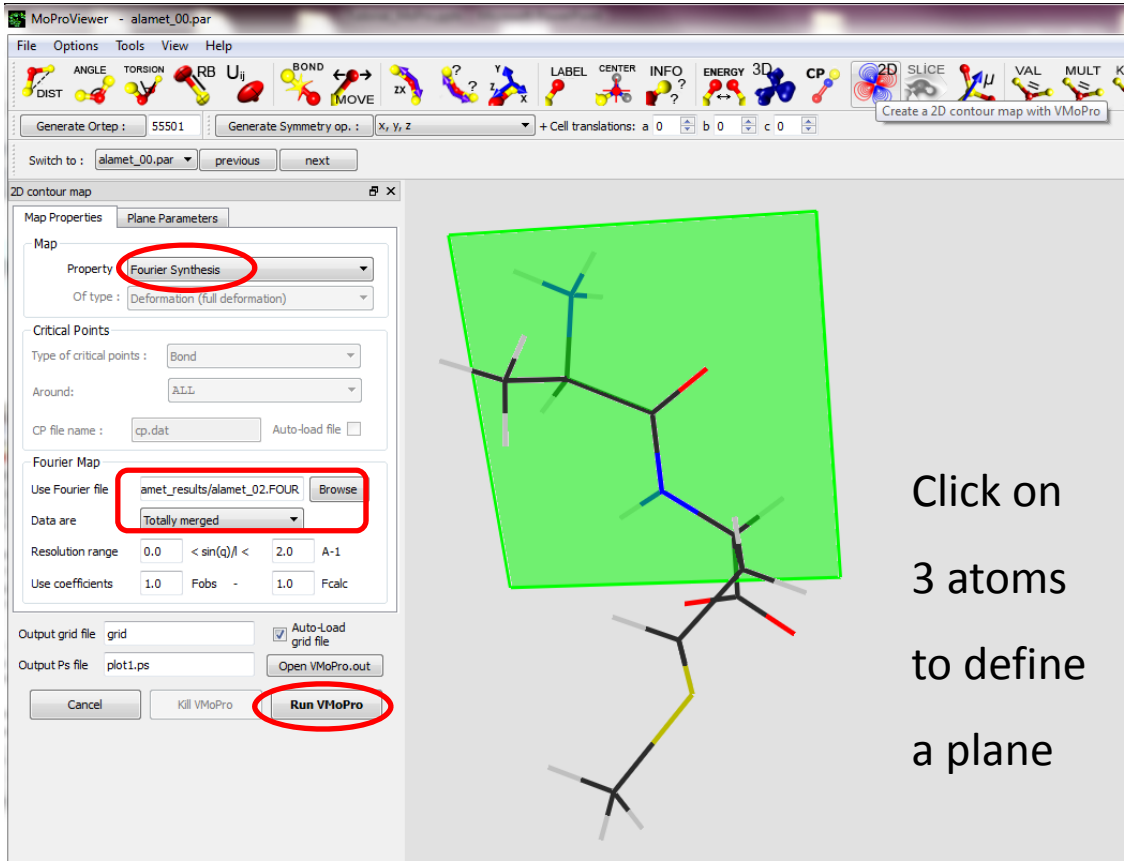
Step 7 Refine structure

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





Step 8 Compute a Fourier Residual Electron Density 2D map

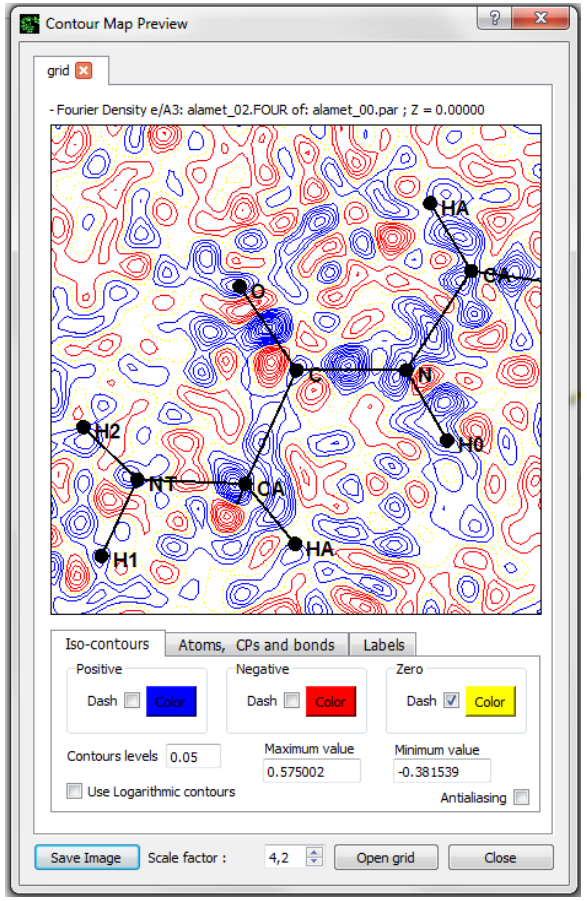


Click on

3 atoms

to define

a plane



2D map:

Select Map Property : Fourier Synthesis

Select Fourier file : alamet_02.FOUR

Data are Merged

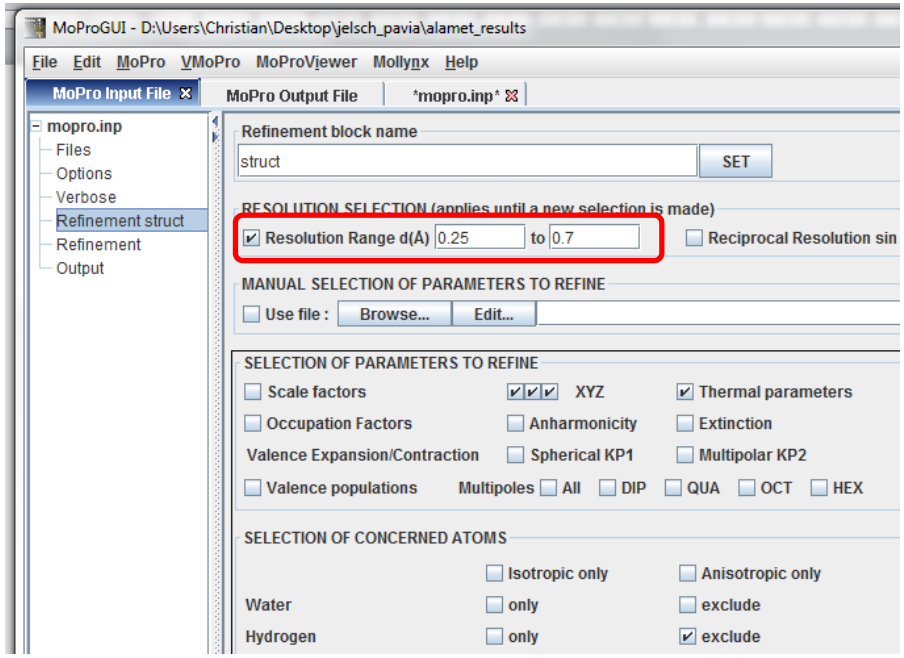
Click on ''Run VMoPro'' to start calculation

Step 9 HIGH ORDER refinement of structure

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

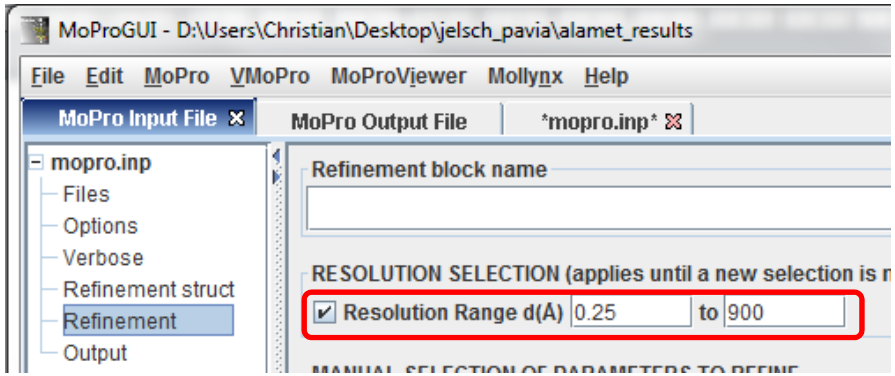
The MoPro commands

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

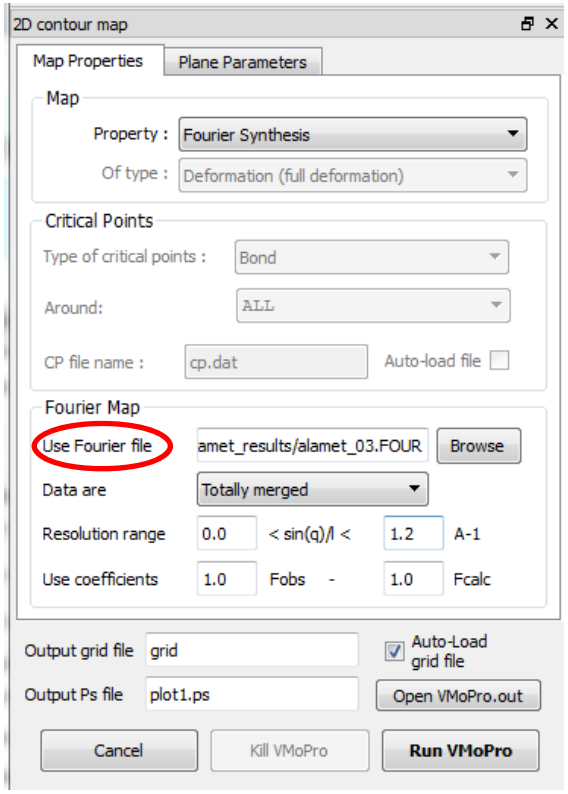


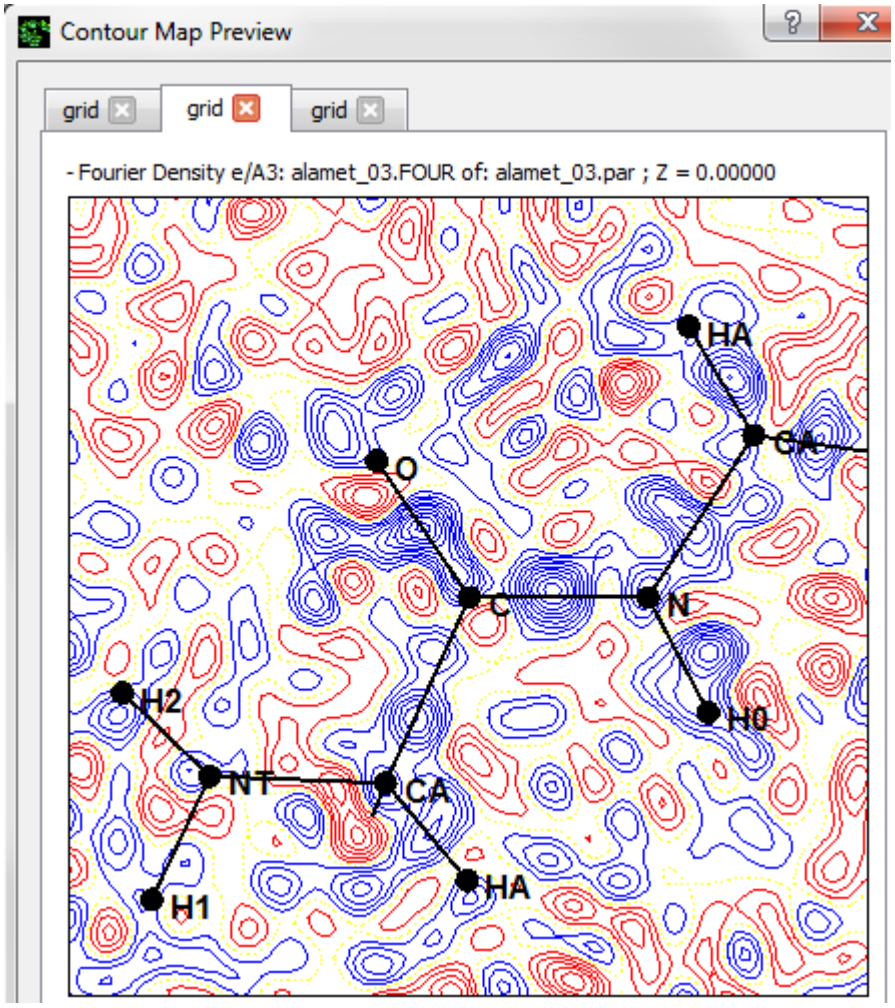

```
RESO  0.25 900
WRIT FOUR
```

Write a Fourier reflections file
for all resolution



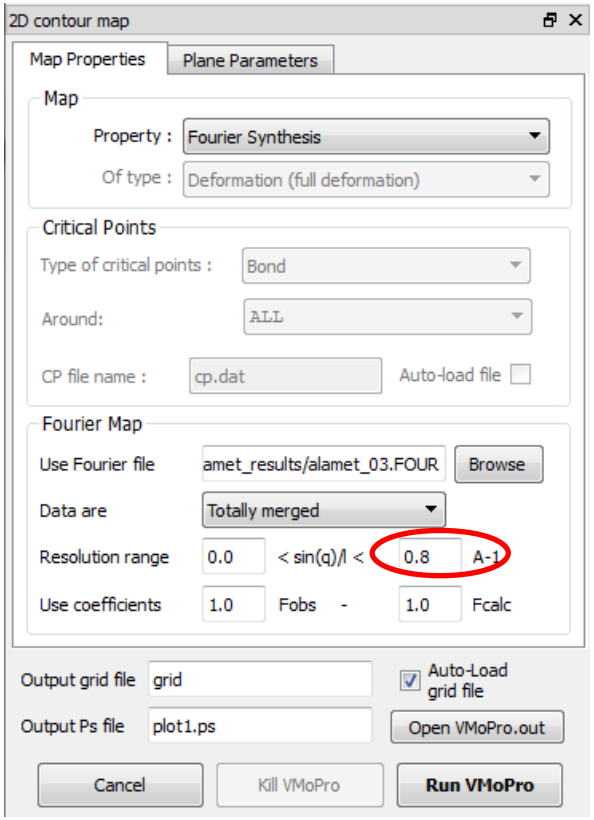
Step 10 Compute a Fourier Residual Electron Density after High-Order refinement

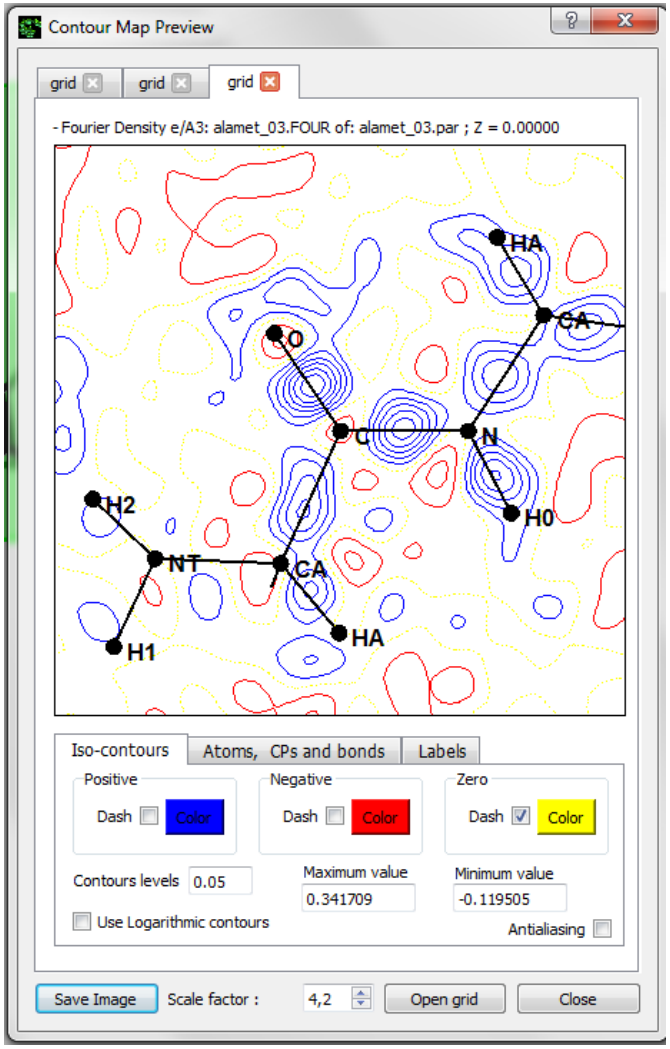




Stronger residual electron density visible on covalent bonds

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



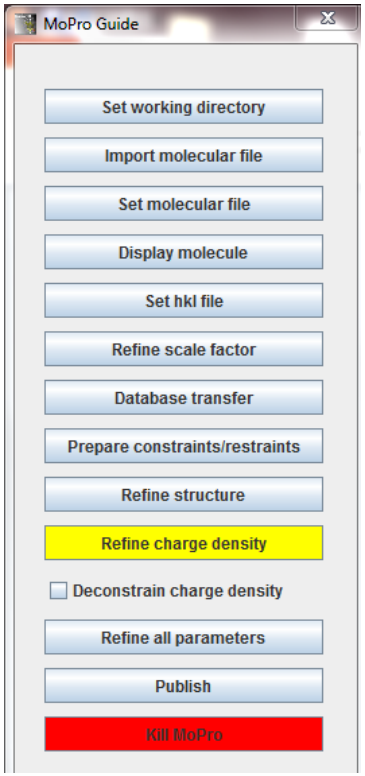


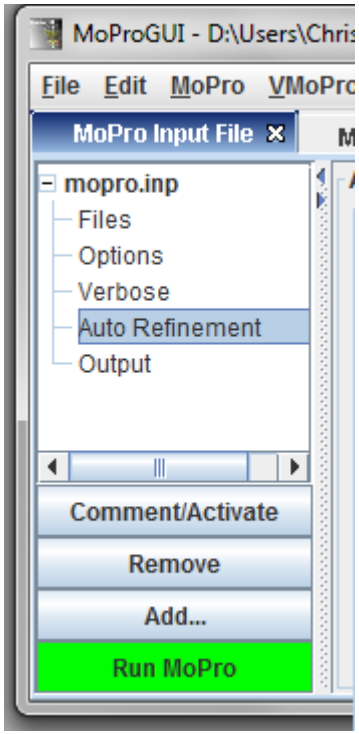
$\sin\theta/\lambda < 0.8$ Å^{-1}

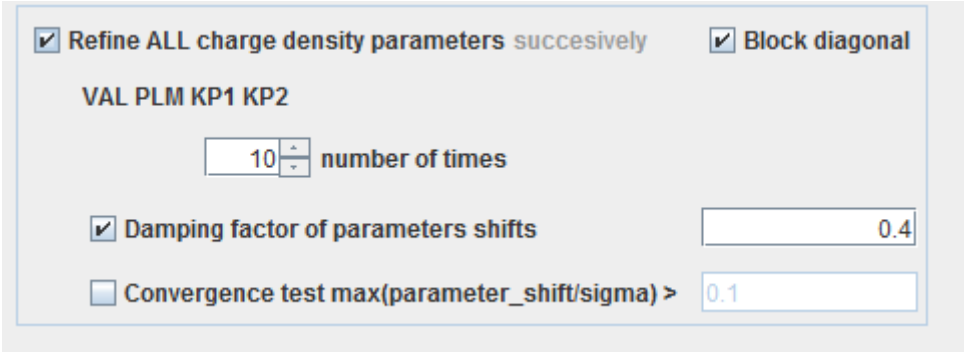
resolution
$d > 0.6$ Å

Bonding Electron Density is clearly visible

Step 12 Refinement of charge density

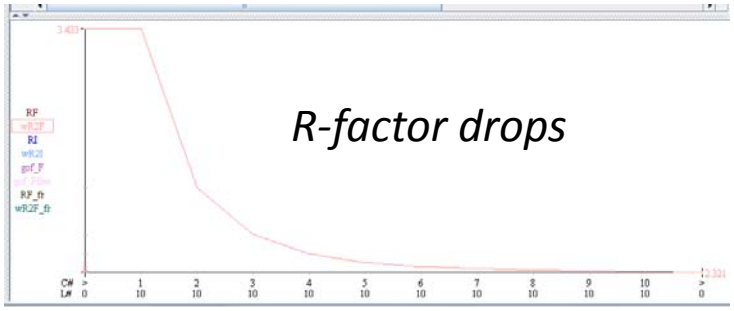






* Block diagonal: variables are decorrelated and can be refined together

* Damping to avoid divergence



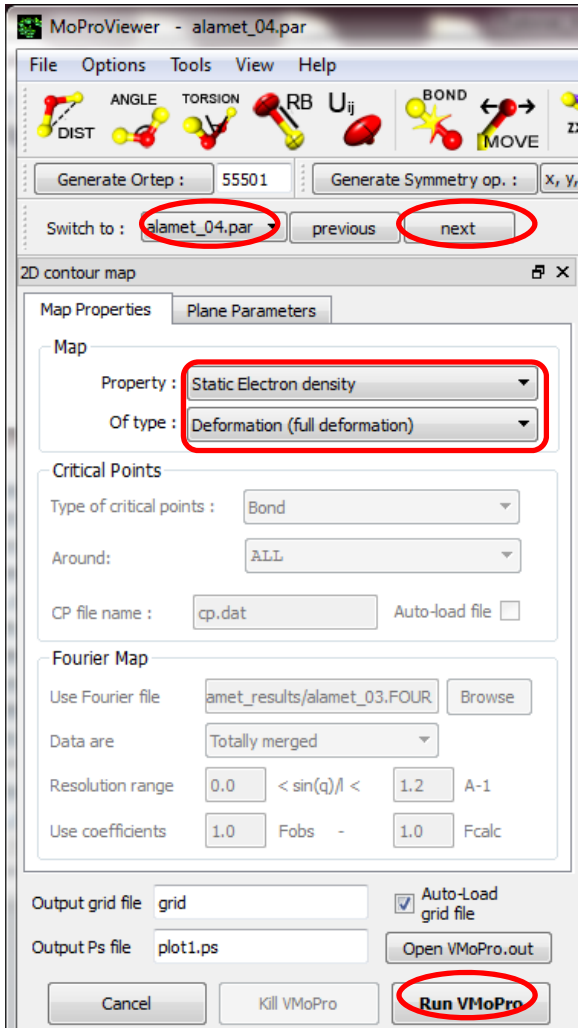
R-factor drops

Have a look at resulting molecular .par file

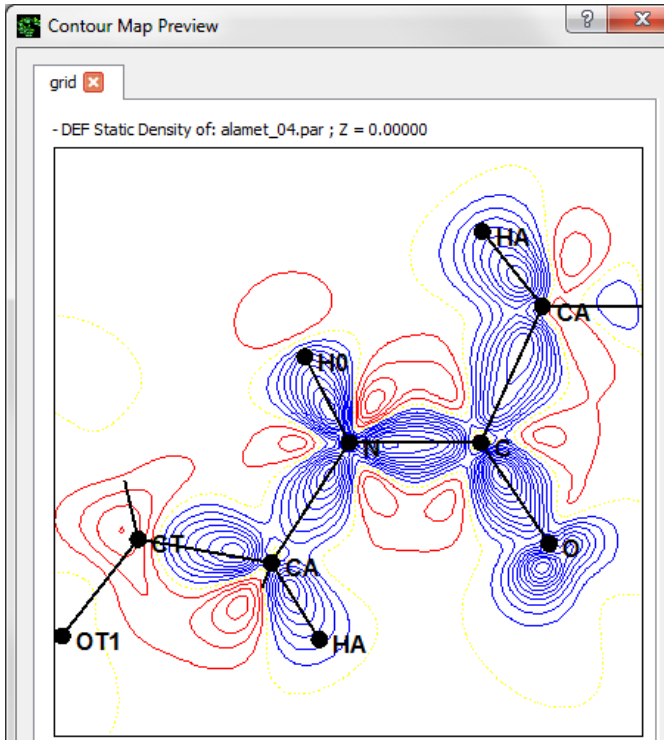
```
ATOMS    30

ATOM    1 NT   ala   1  0.427429  0.050030  0.613817 1.0000   1 N
 ZX CA      H1        OCT K1     V0   M0   Q0
UANI 0.013163  0.010518  0.009881  -.000244  0.005418  -.000507
 5.07251 0.     0.    0.    -.017   -.030 0.    0.    0.    0.
  0.173  0.    0.    0.    0.    0.128  0.
XYZ       Pval =valence       Plm = multipole populations
```

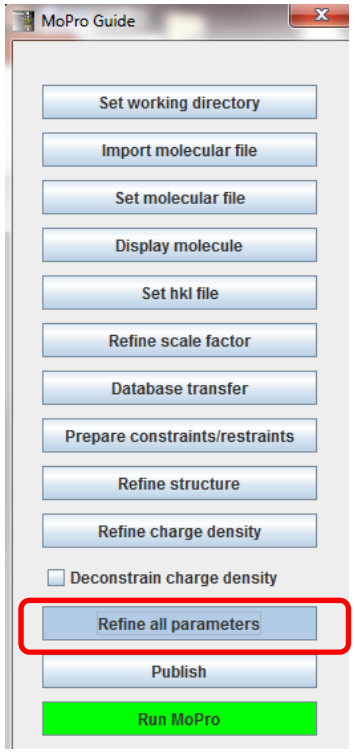
Step 13 Compute a Static Deformation Electron Density map

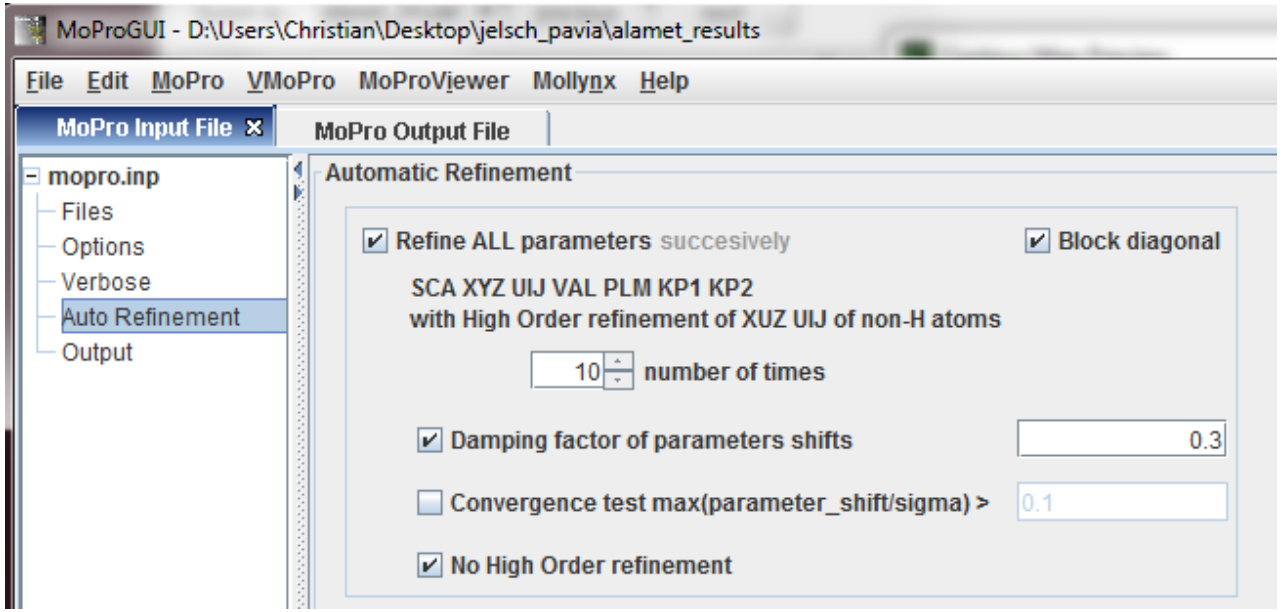


Choose appropriate molecular file



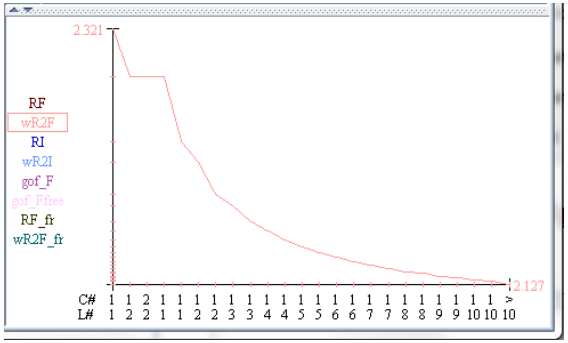
Step 14 Refinement of all parameters





- Block diagonal & damp : refine all parameters together

- Else : refine them successively

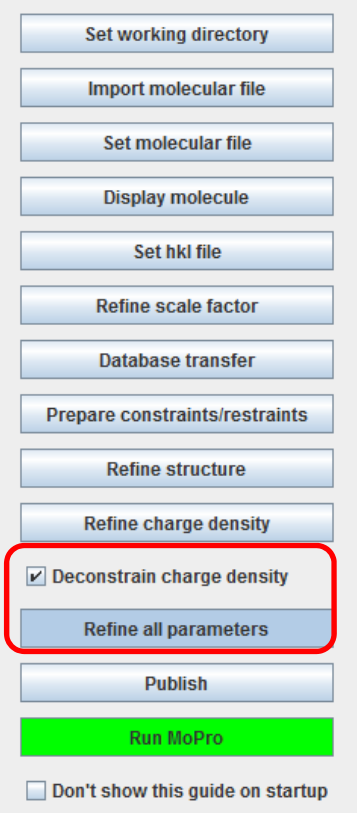


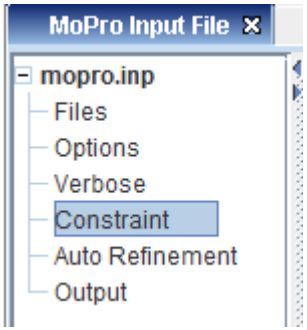
Further R-factor drop

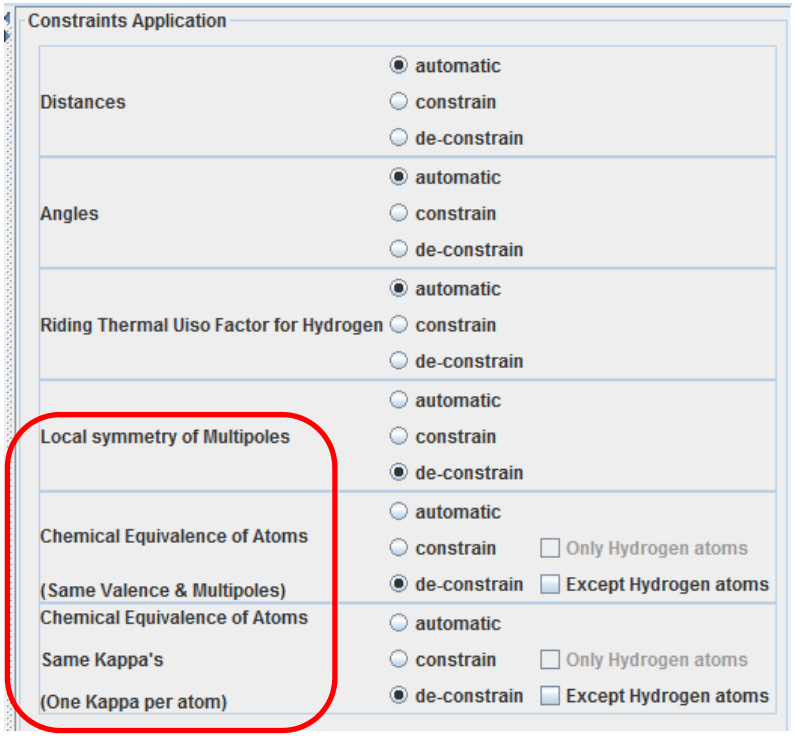
Step 15 Deconstrain charge density

Removes

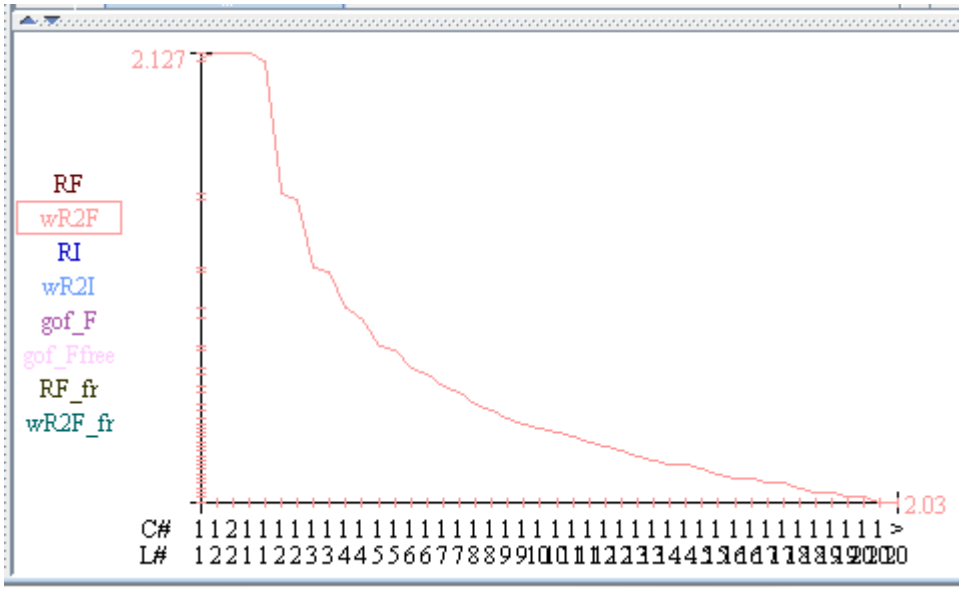
- Local symmetry of multipoles
- Atoms equivalencies : similar atoms have same charge density





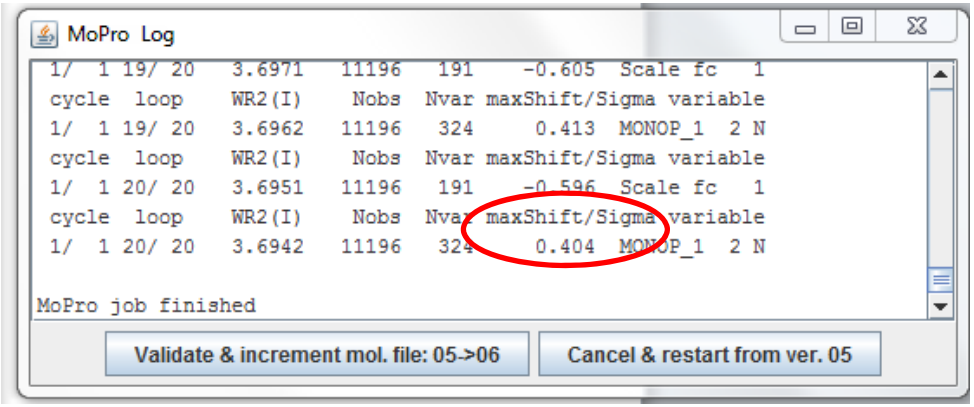


Step 16 Refinement of all parameters till convergence

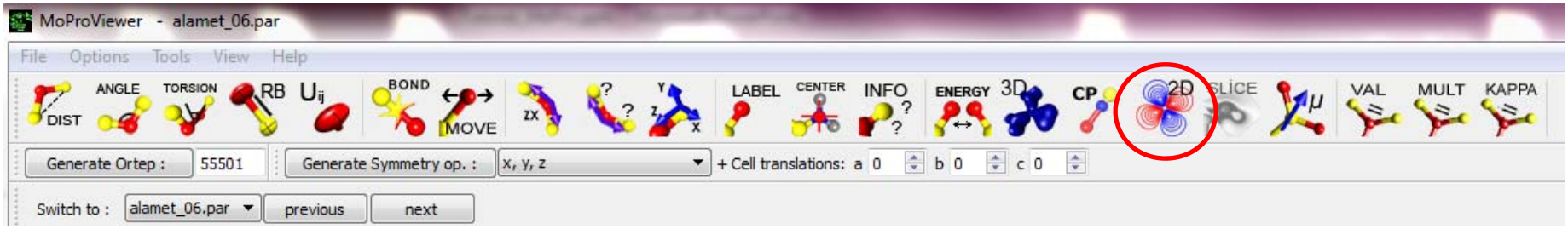


Check R-factor evolution

Check max Shift/sigma



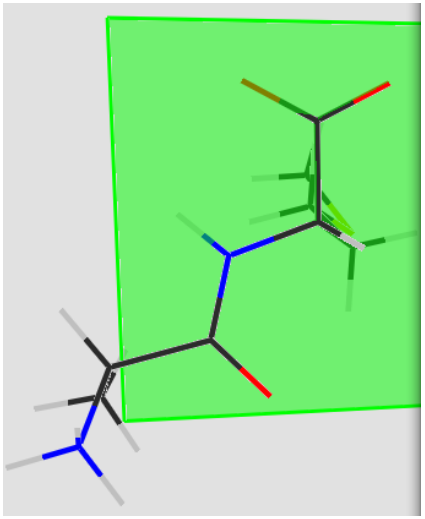
Step 17 Check Static Deformation Electron Density 2D maps

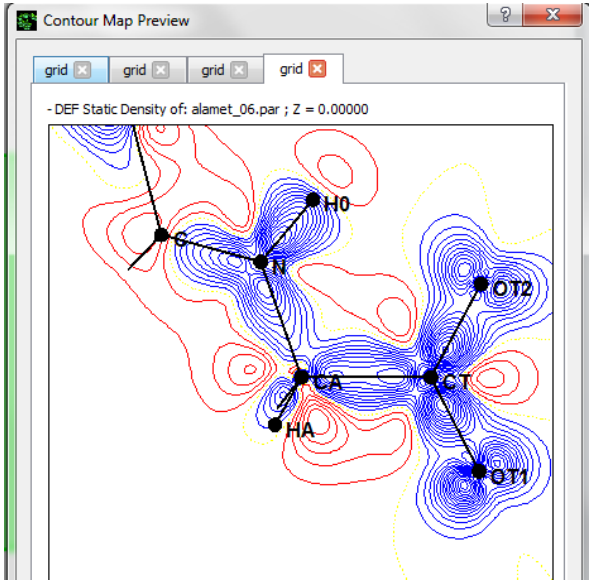


Choose

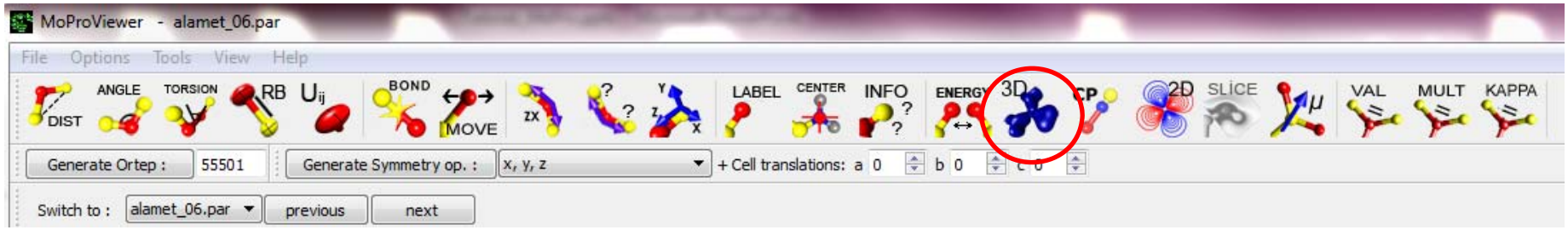
Triplets of connected atoms

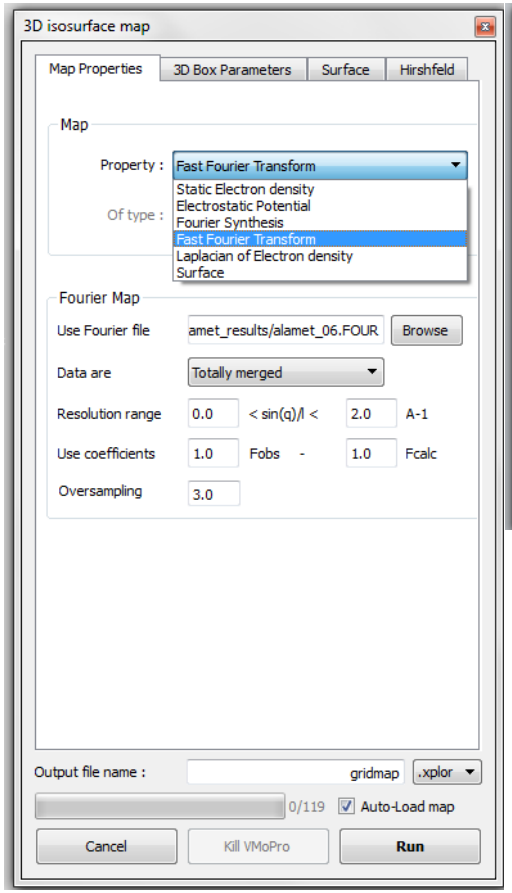
to define planes

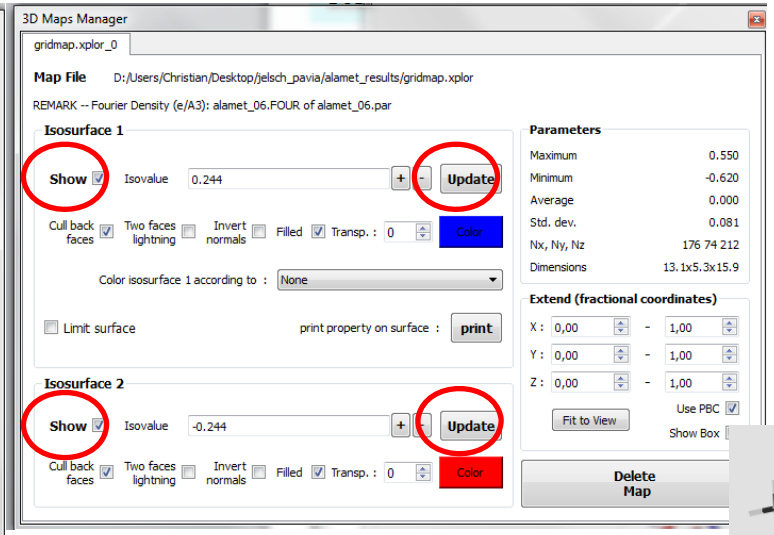




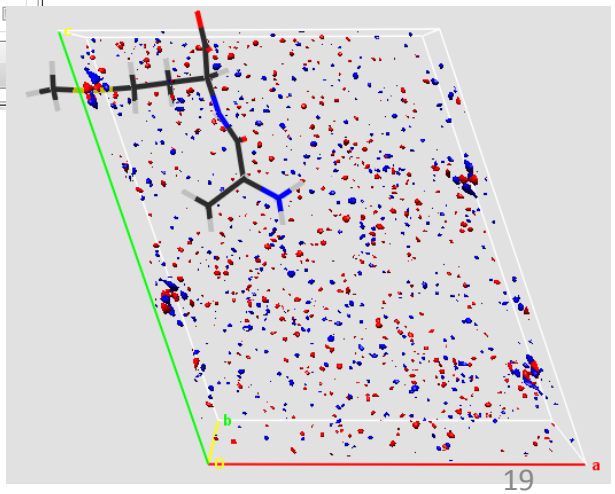
Step 18 Fast Fourier Transform 3D map



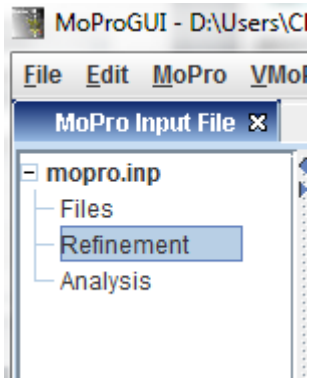


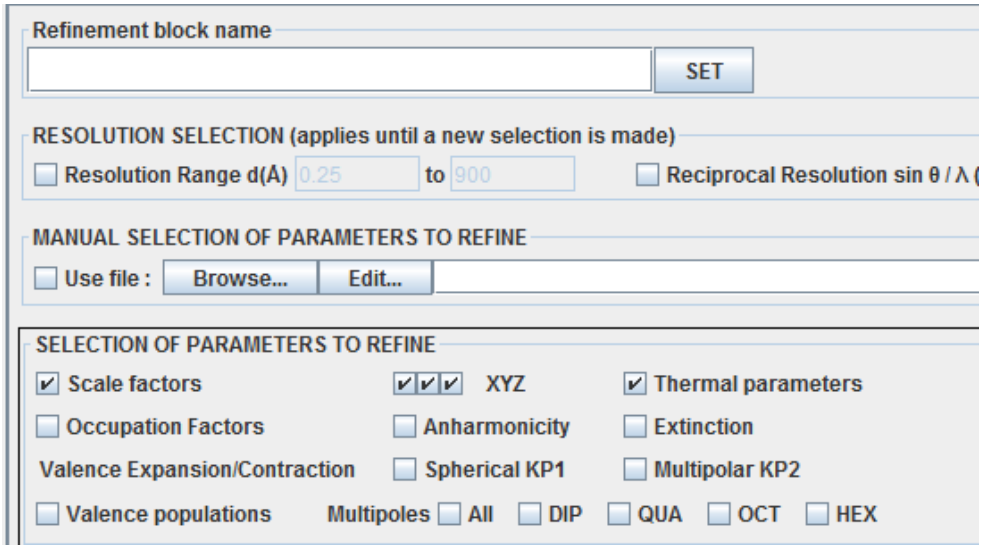


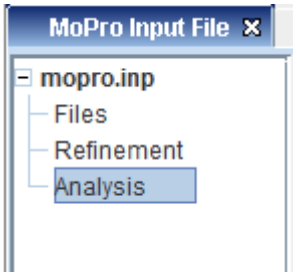
Residual Electron Density map in unit cell

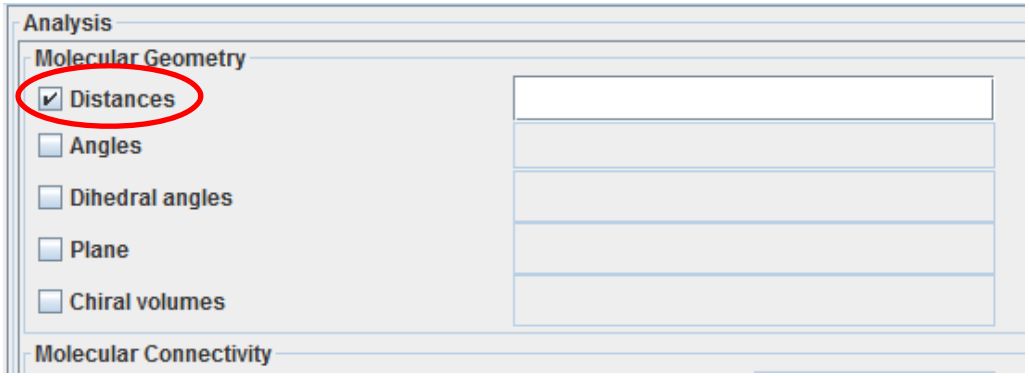


Step 19 Stereochemical analysis







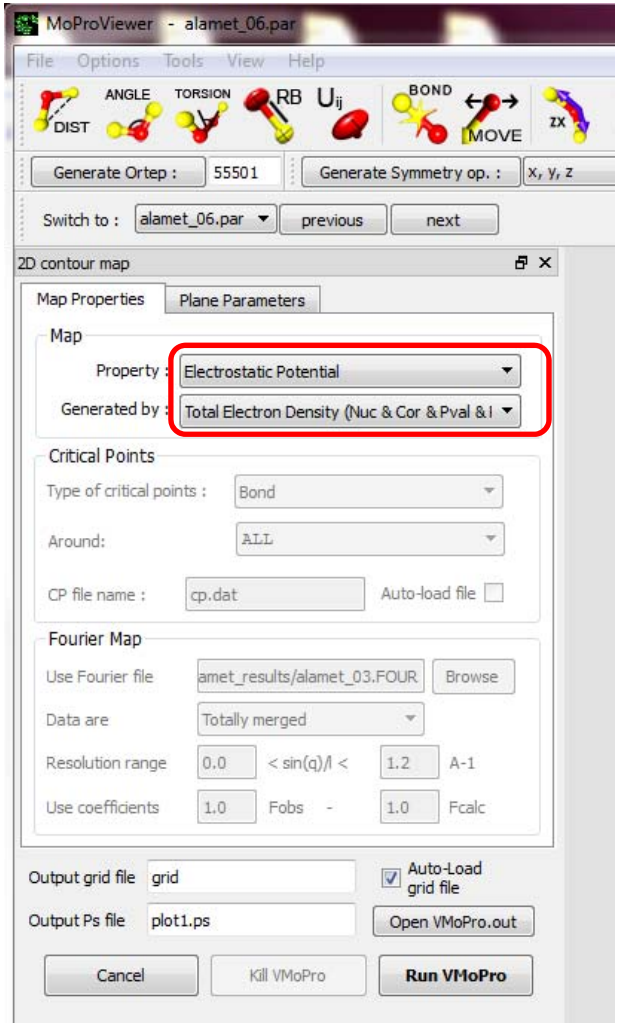


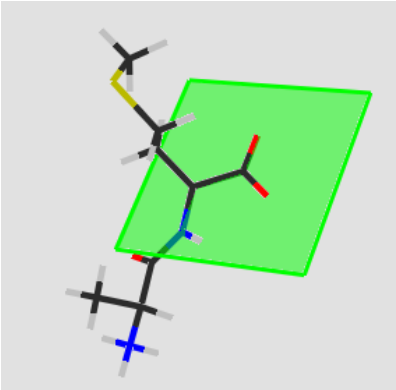
Refine at first structure to obtain sigmas of distances

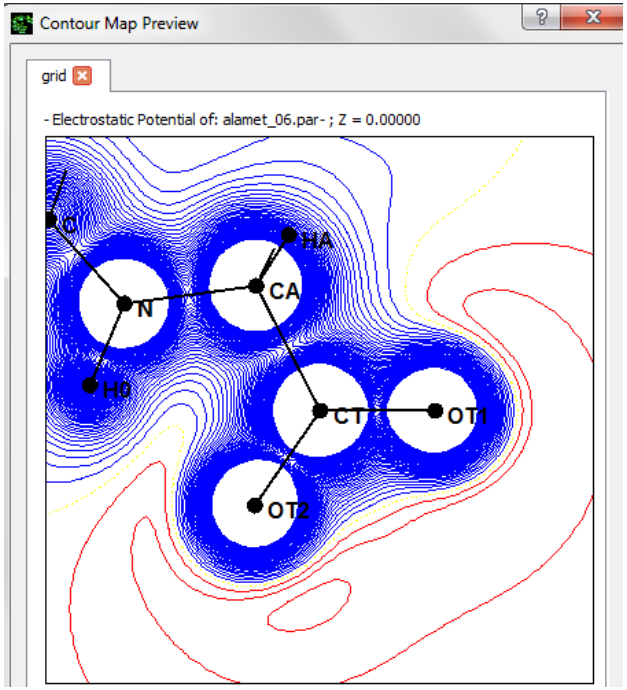
MoPro Output File

ATOM1				ATOM2			SYM2	DIST	sigDIST	refined xyz	xyz
NT	ala	1	--	CA	ala	1		1.481091	0.001594	+++	+++
NT	ala	1	--	H2	ala	1		1.030136	0.001247	+++	+++
NT	ala	1	--	H3	ala	1		1.034194	0.002353	+++	+++
NT	ala	1	--	H1	ala	1		1.036034	0.001297	+++	+++
CA	ala	1	--	C	ala	1		1.525269	0.000535	+++	+++

Step 20 2D map of Electrostatic Potential

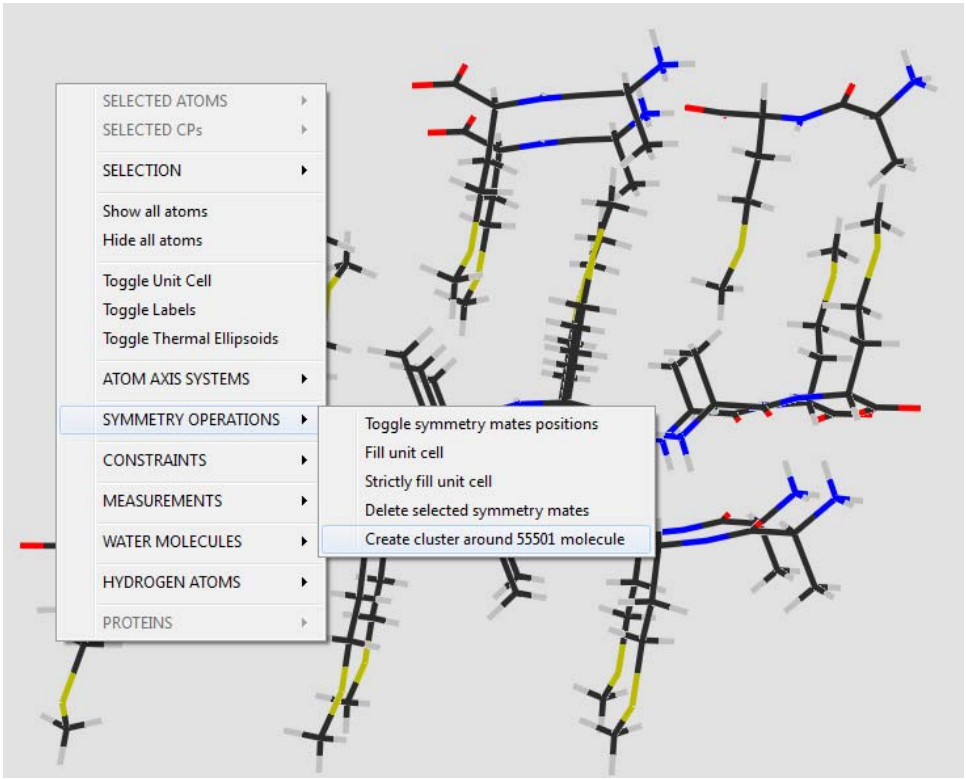


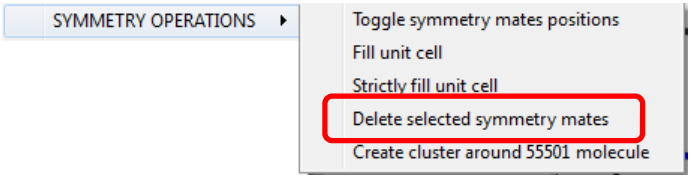


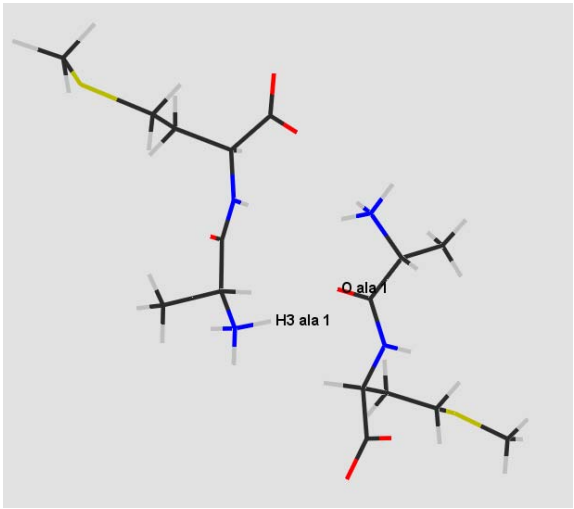


Step 21 Generate a dimer in MoProViewer

Click right on view



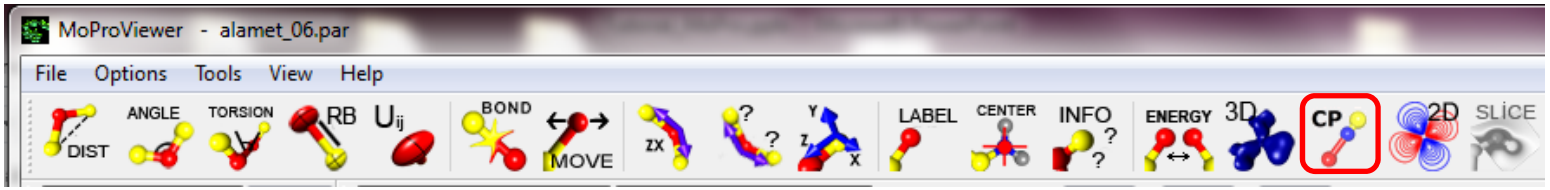


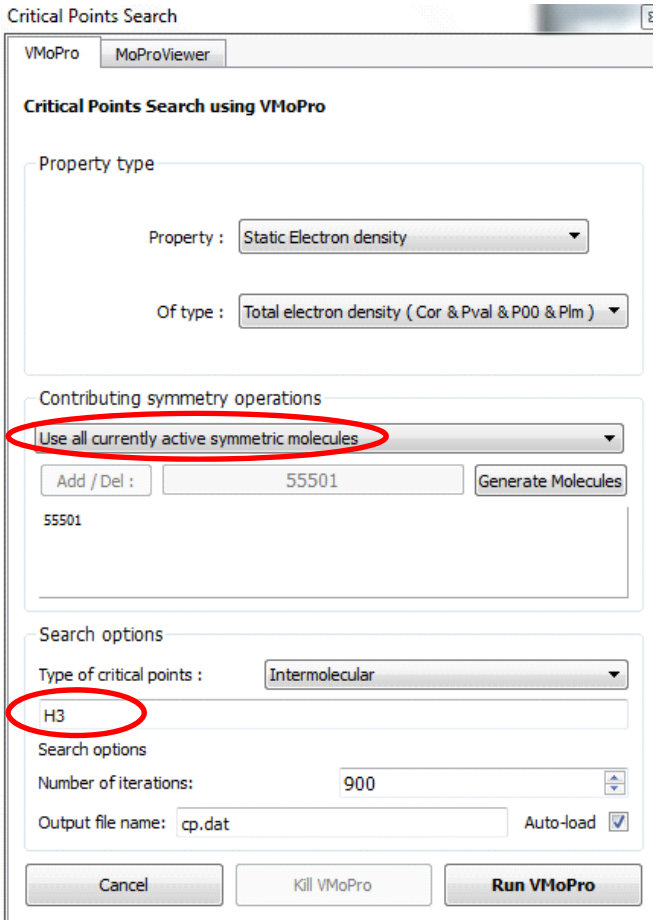


Keep a dimer like 55501 + 65602

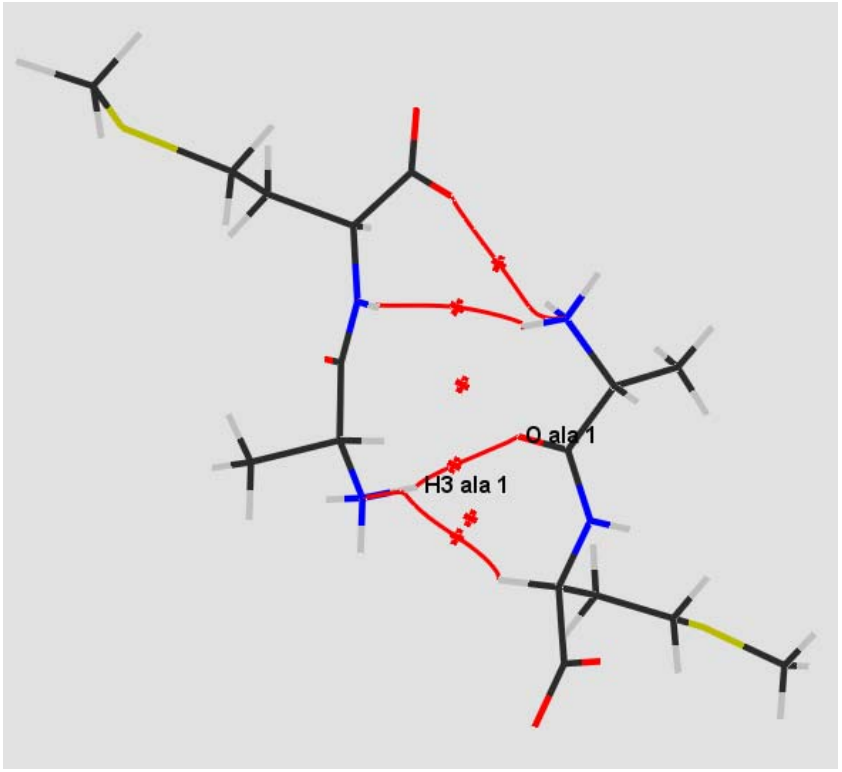
Ortep symmetry code
65602
Translation 1**a** + 0**b** + 1**c** & symmetry #02
6→1 5→0 4→-1

Step 22 Search Intermolecular critical points



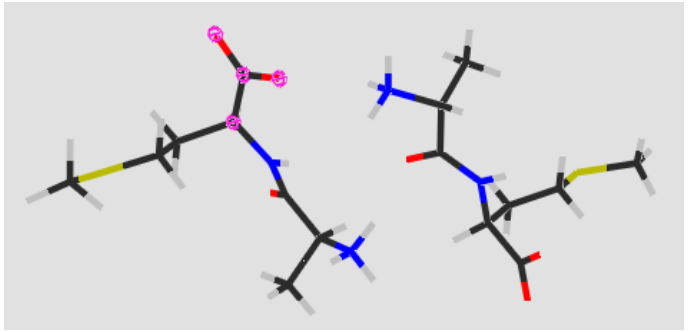


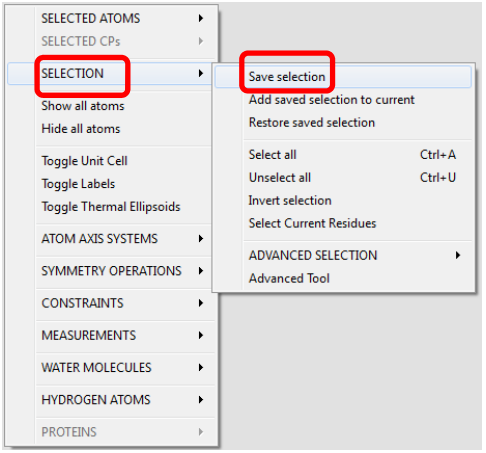
Search around atom H3 only (fast calculation)

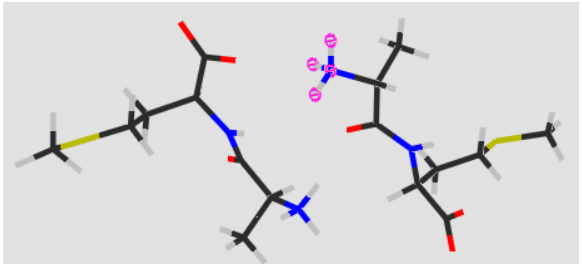


MoProViewer shows CPs & bond paths

Step 23 Compute electrostatic interaction energy of dimer



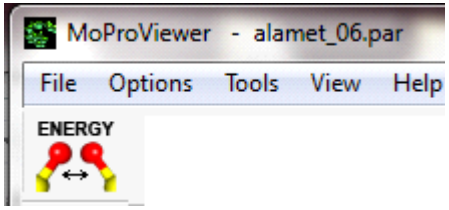




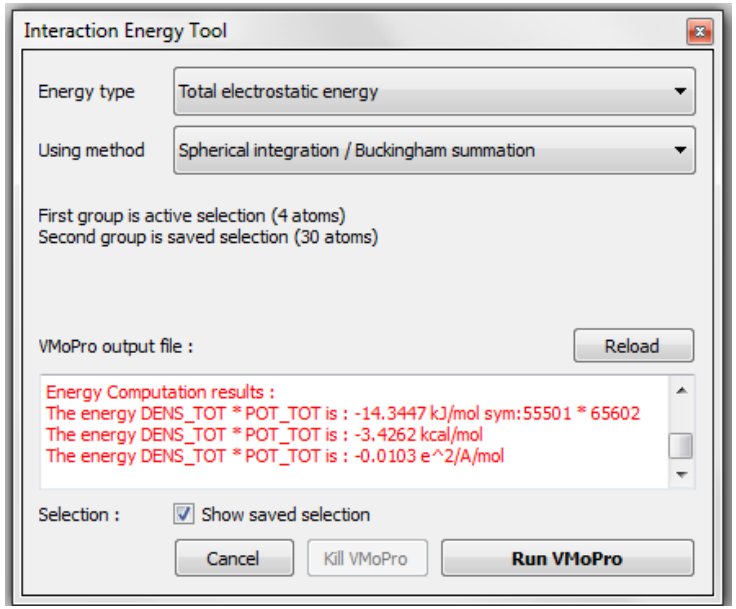
1) Select the carboxylate group

Right click, Selection / SAVE selection

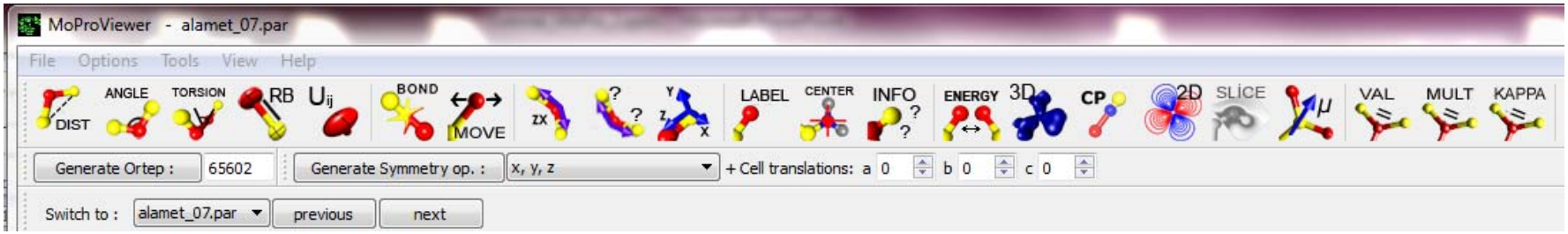
2) Select the NH3 group on the other molecule



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



Step 24 Discover the Tools of MoProViewer



Stereo-chemistry

Move atoms

Show local axes system for multipoles orientation

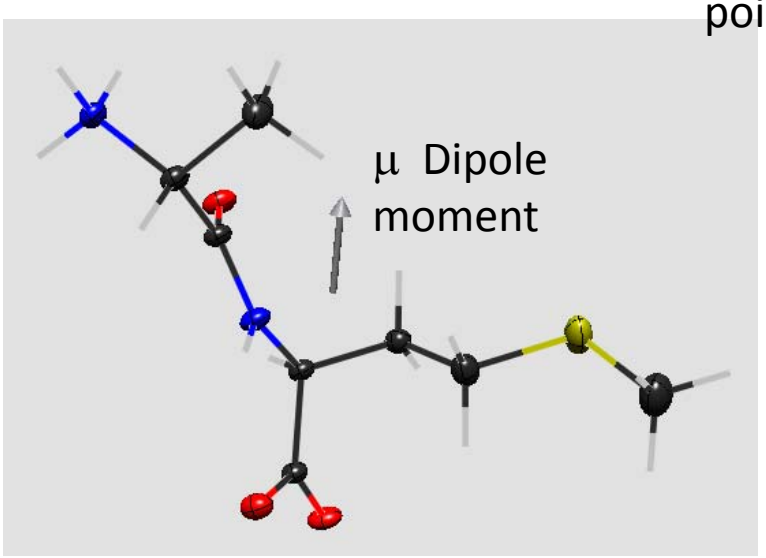
Compute 3D map

Compute 2D map

Critical points

Equivalence Constraints of atomic charge density

Uij Thermal ellipsoids



Step 25 Discover the MoPro Menus