Introduction to IQmol: Part I

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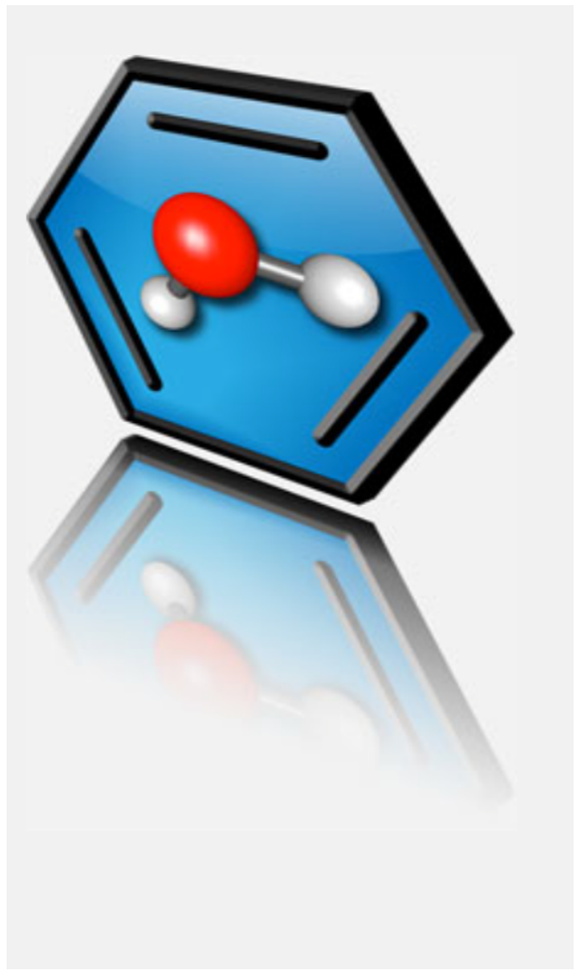
IQmol: Resources

- Written by Dr. Andrew Gilbert

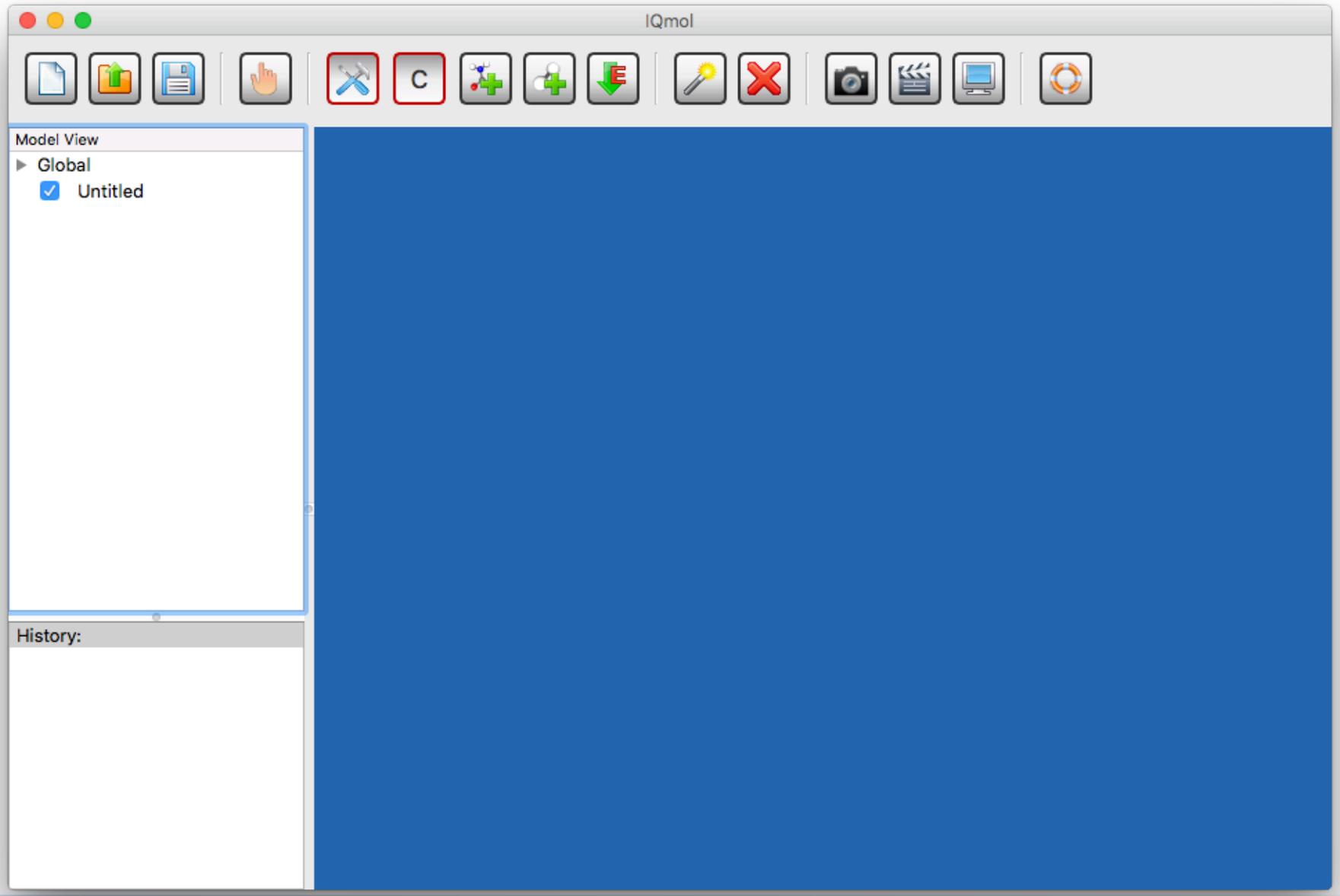
- Keep yourself up to date with IQmol website: http://iqmol.org

- **IQmol Youtube channel:** IQmol now has its own Youtube channel



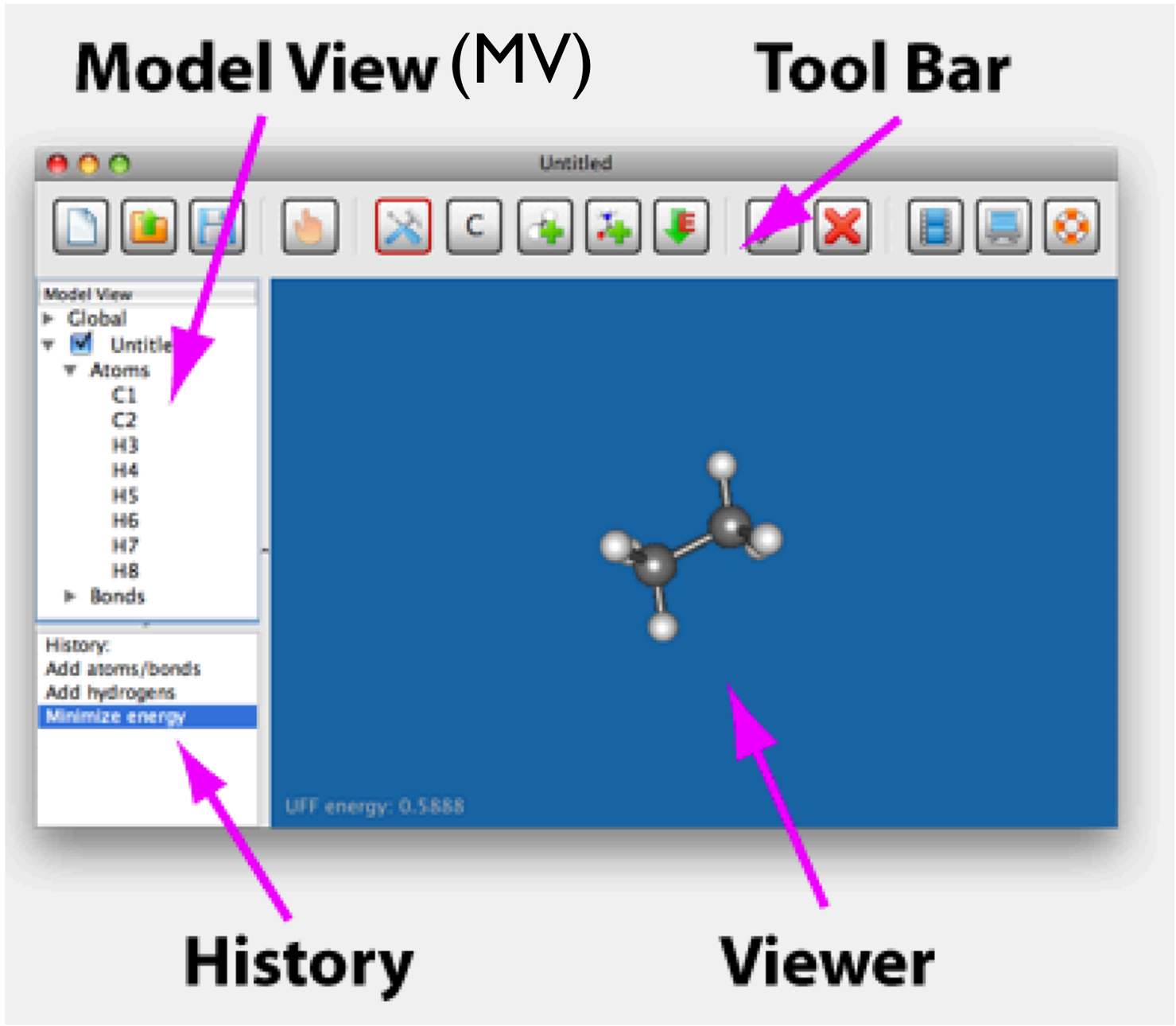
IQmol: Building molecules

- Open IQmol, the molecule building screen looks like this:



Iqmol 2.7.1 is used for this presentation

Iqmol: Quick overview



IQmol: Main build tools

Build Mode

Add Hydrogens

Minimize Energy (classical forcefield)

Build Elements

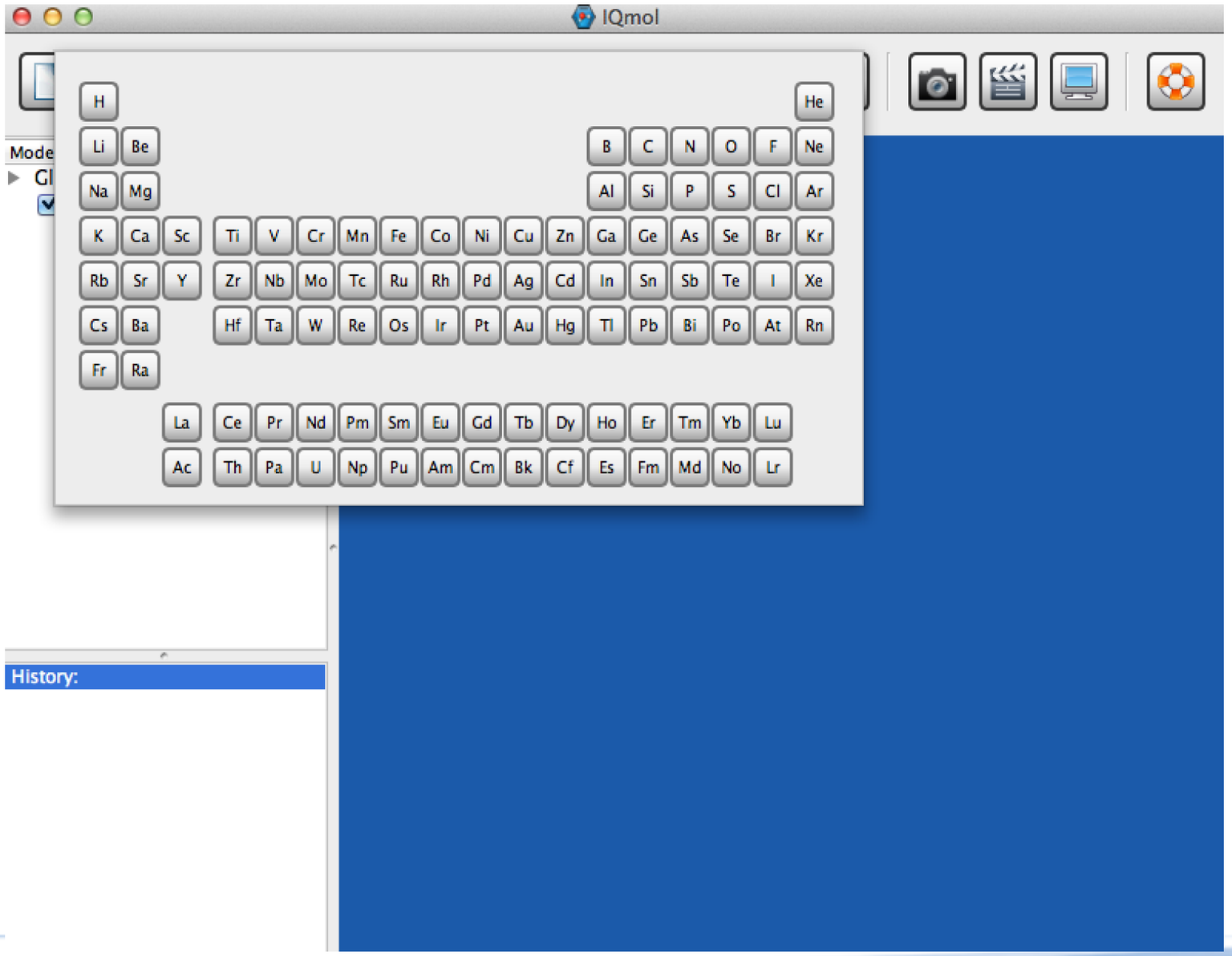
(periodic table)

Add Fragments

(pre-built molecules)

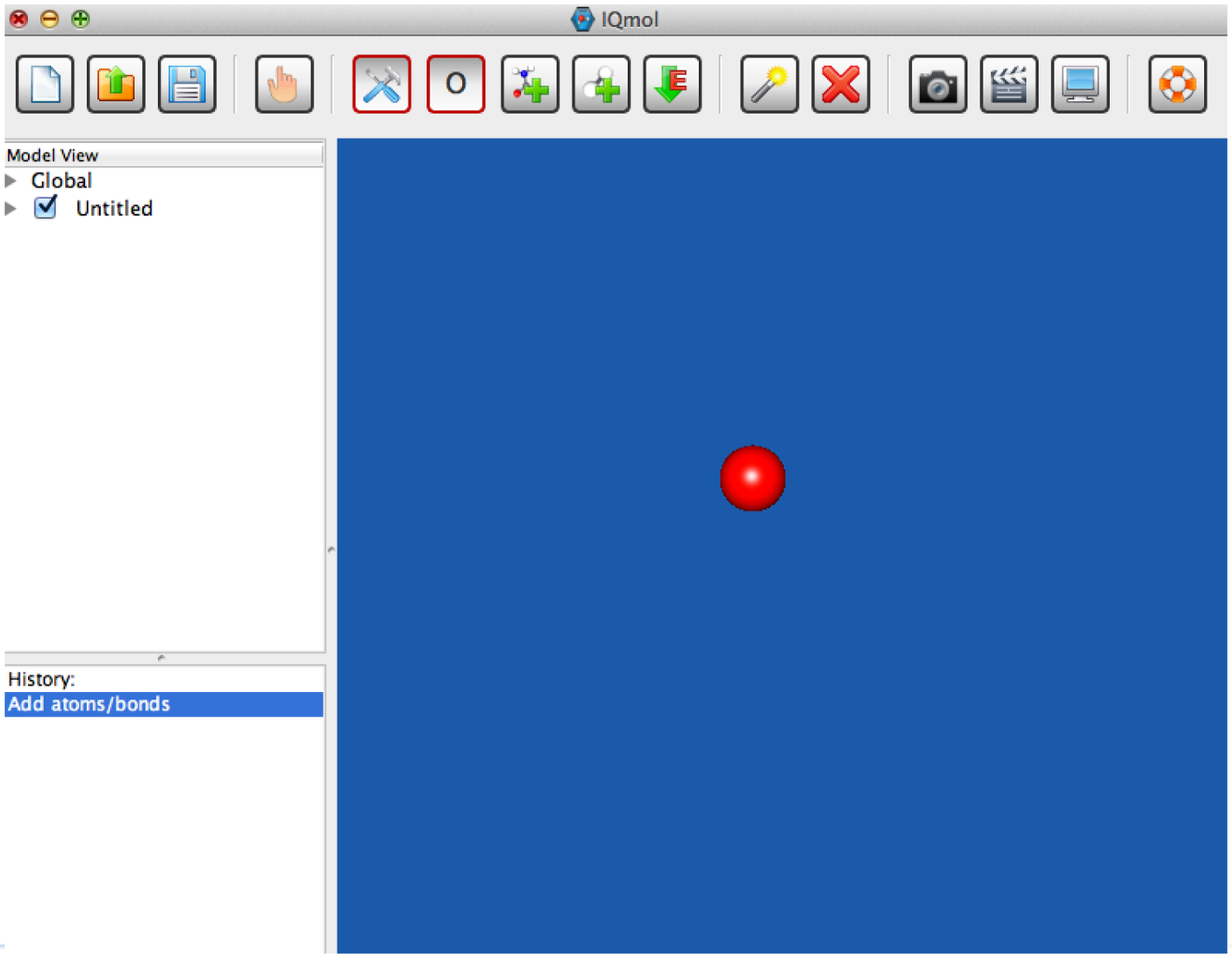
IQmol: Building molecules

- Click the “Build Element” : periodic table pops up:



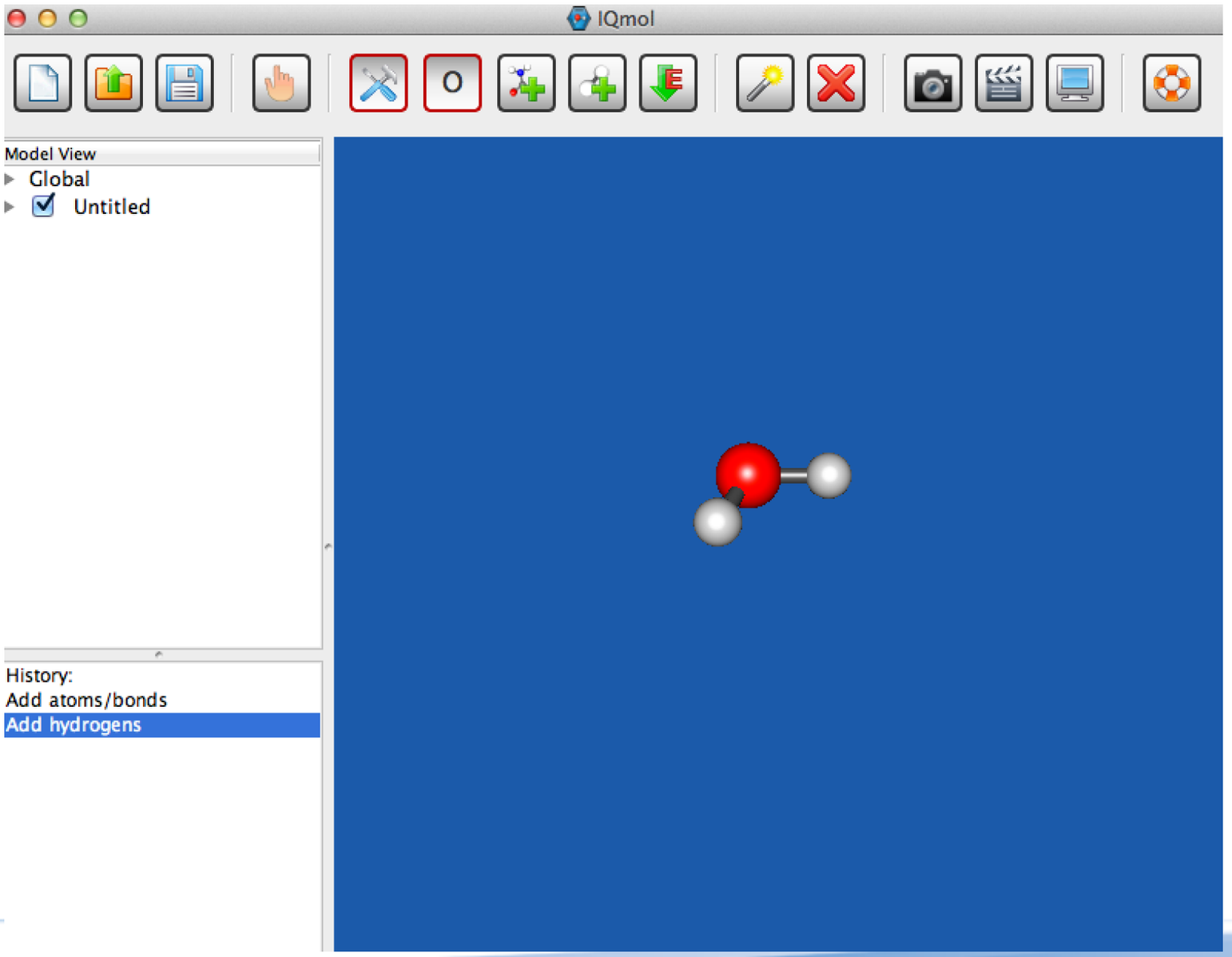
IQmol: Selecting atom

- Select an atom, for example Oxygen: O
- Click in the blue screen (Viewer) area to place the Oxygen atom



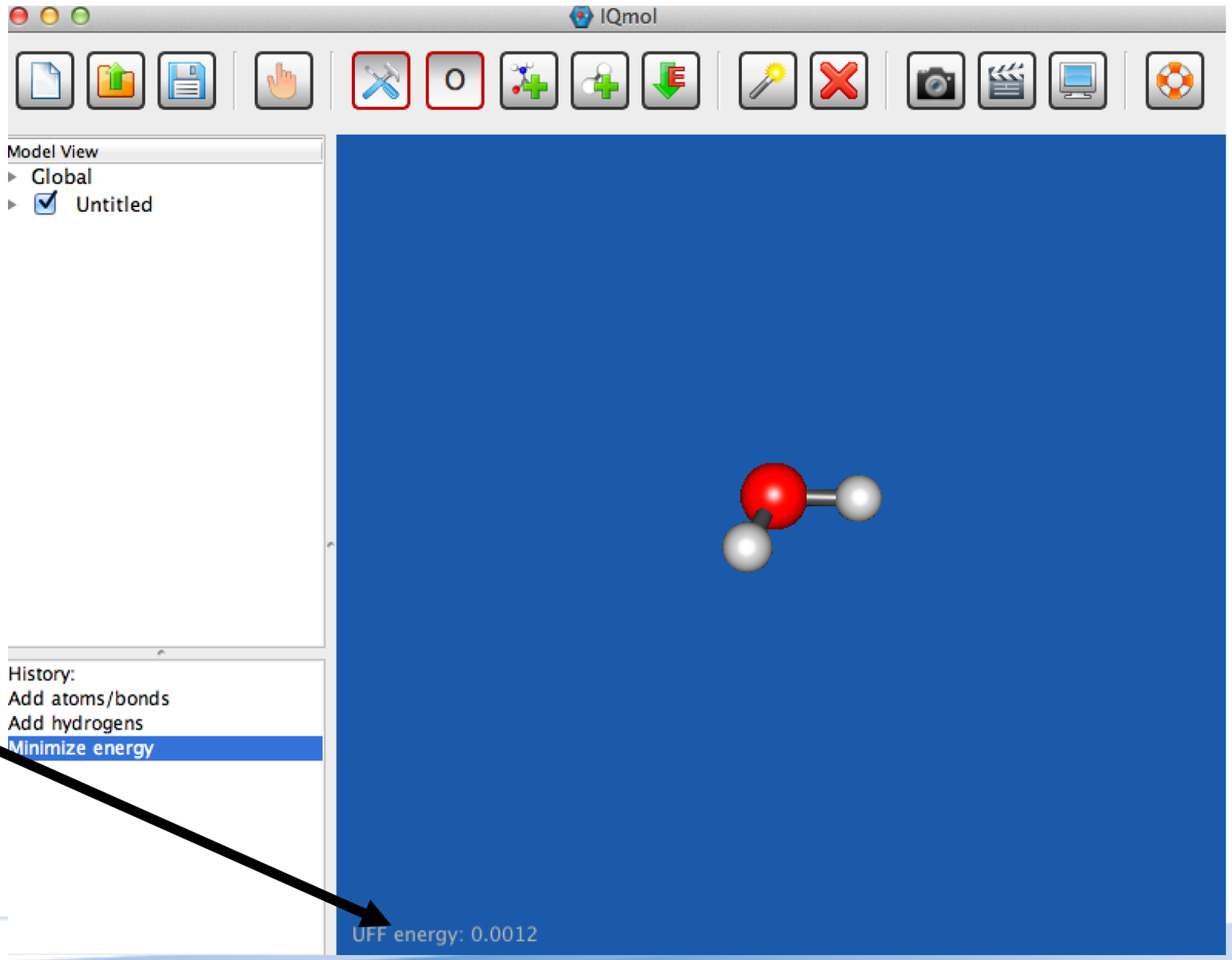
IQmol: Add Hydrogen

- Click the “Add Hydrogens” button: 



IQmol: Classical minimizer

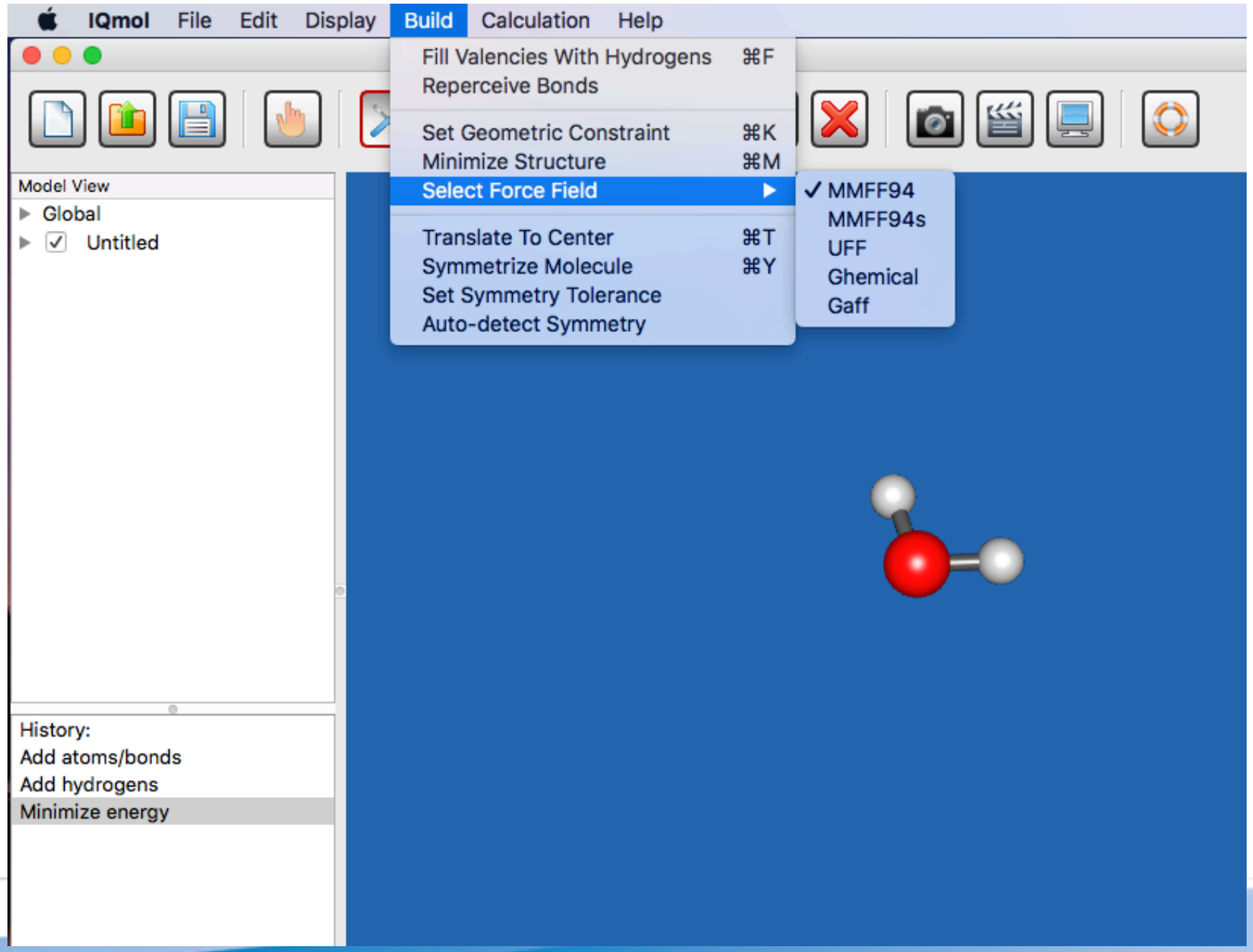
- Click the “Minimize Energy” button to get a more realistic structure



Energy of the current structure

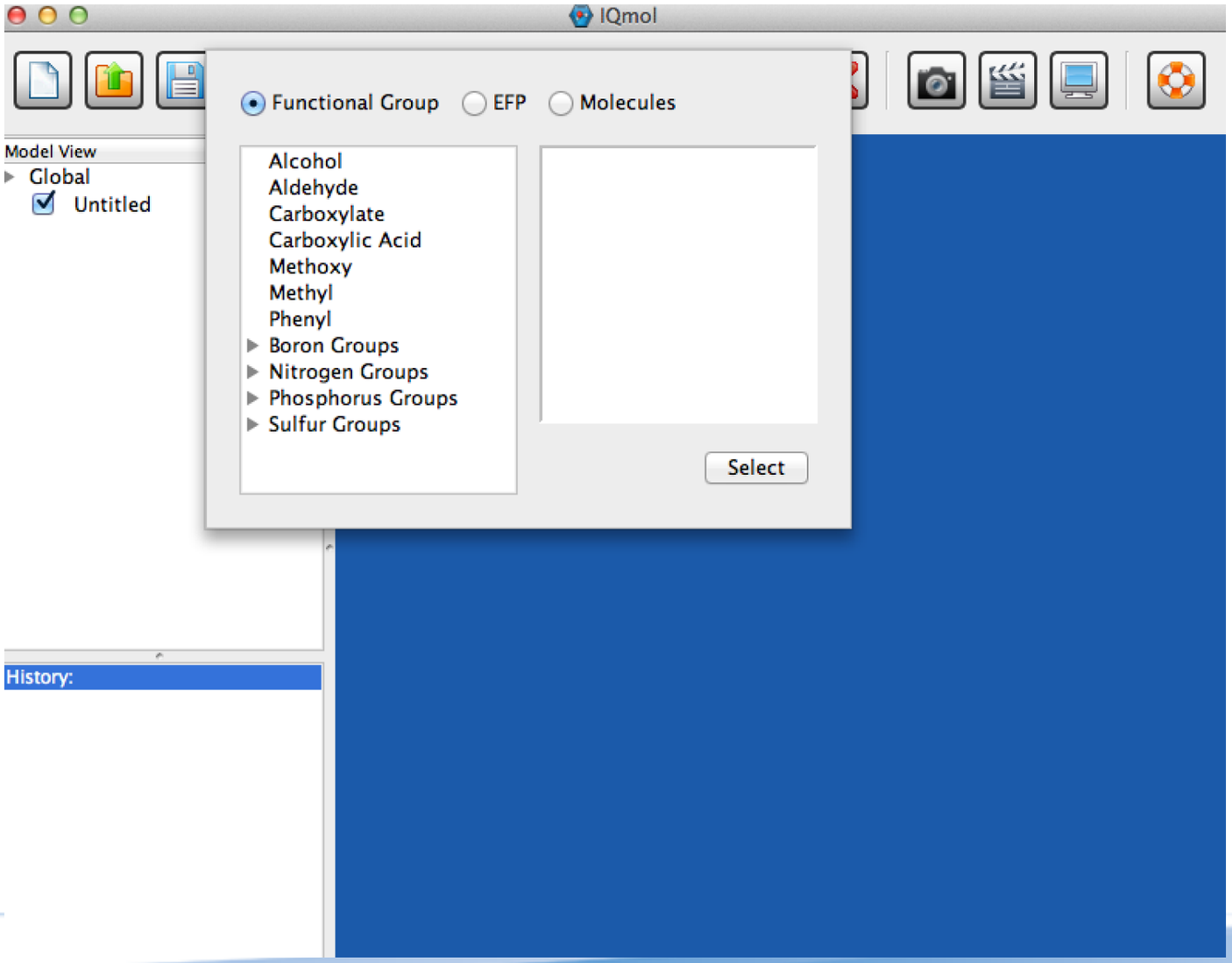
IQmol: Classical minimizer

- Build —> Select Force Field: allows you to choose different force field



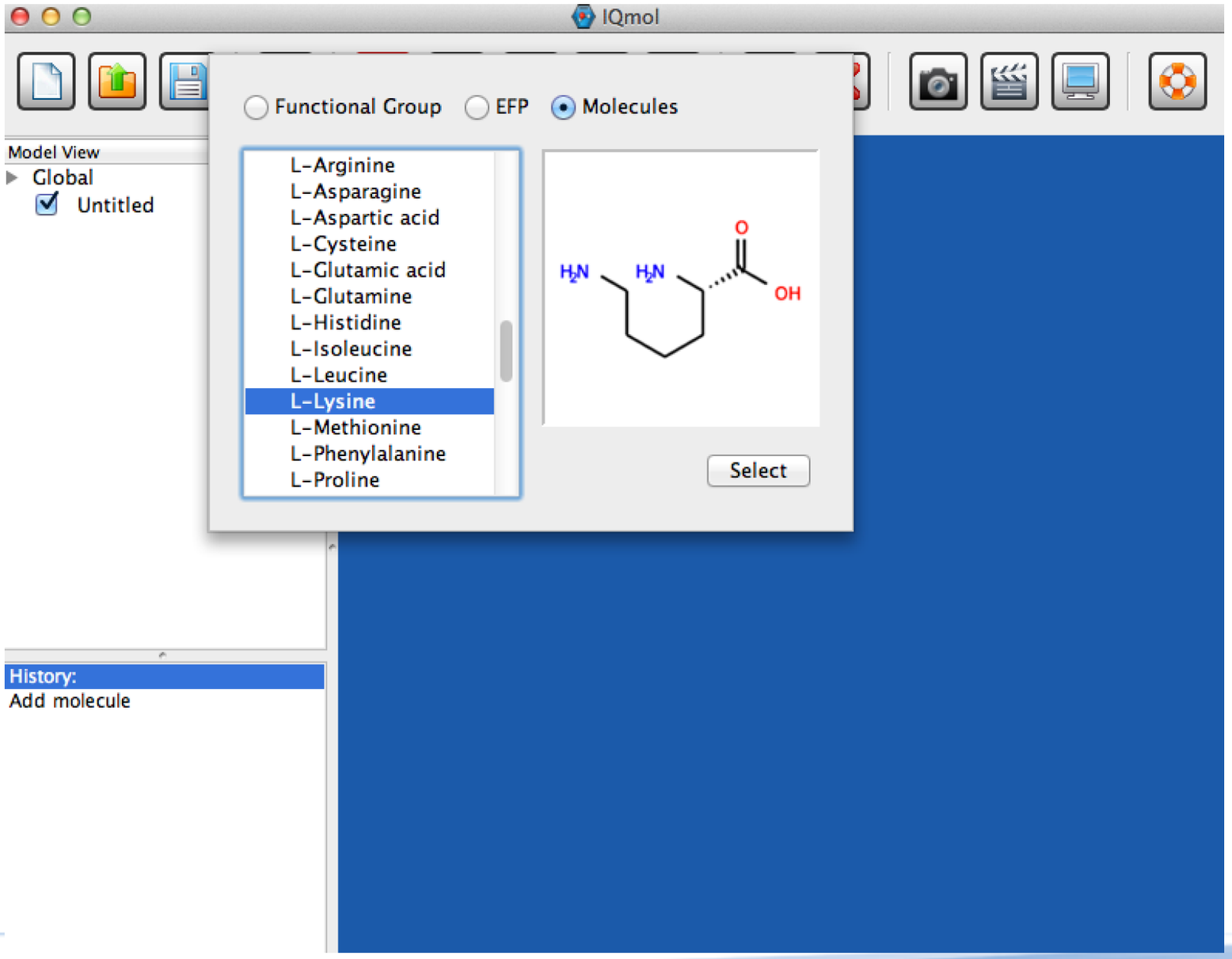
IQmol: Pre-build molecules

- Pre-build molecule library ("Add Fragments" button ) contains various molecules that can be used to build more complex molecules



IQmol: Pre-build molecules

- Click on the “Add Fragment” button , then choose amino_acids/L-lysine.



IQmol: Manipulation Mode

- Click on the “Manipulate” mode 

Activating this mode changes the cursor to . This is the default mode for the viewer and allows the molecule to be rotated and zoomed.

The manipulate mode implements the following mouse functions:

- **Left click and drag:** Rotate the view of the molecule. Cursor changes to
- **Middle click and drag:** Zoom in and out. Cursor changes to
- **Right click and drag:** Translate the view of the molecule. Cursor changes to

Rotation of all atoms: Left click + drag	Rotation of selected atoms: CTRL + left click +drag
Translation of all atoms: R click + drag	Translation of selected atoms: CTRL + L click + drag

Replace CTRL with command key for Mac

IQmol: Select Mode

- Click on the “Select” mode 

Activating this mode changes the cursor to ⊹. This mode can also be activated using the *shift key* when in manipulate mode.

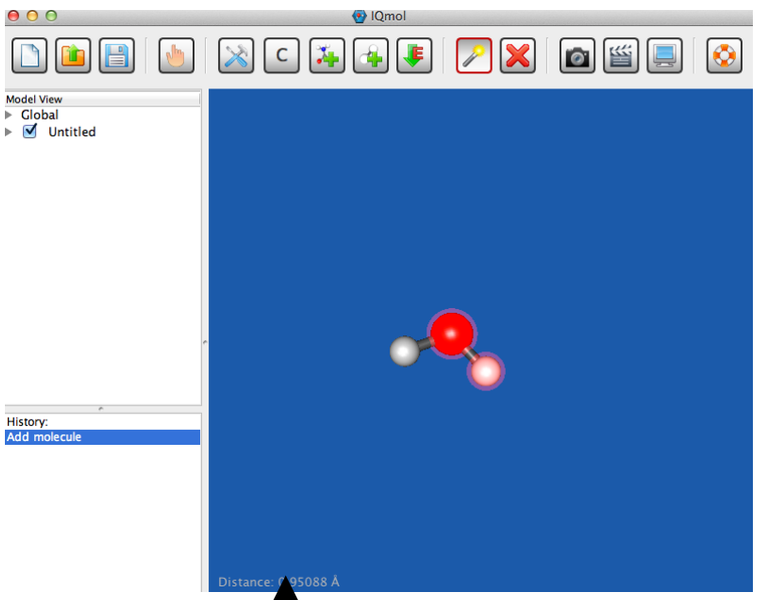
The select mode implements the following mouse functions:

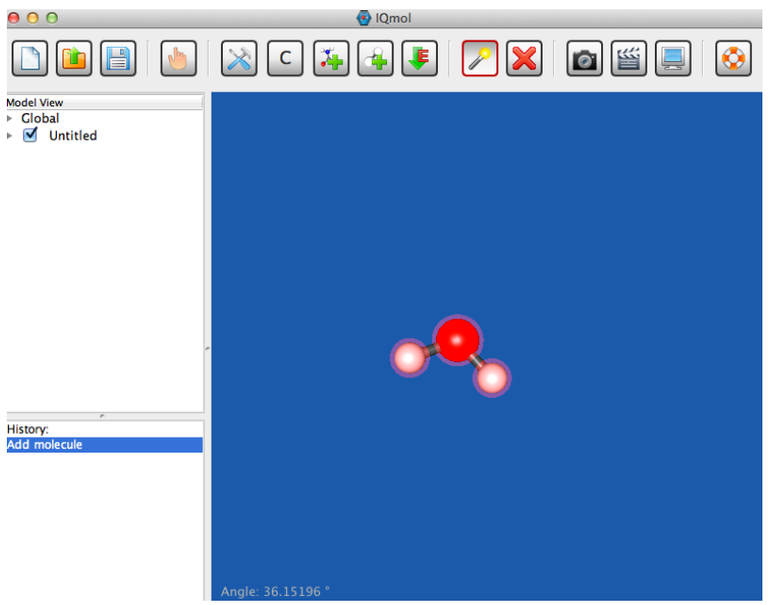
- **Left click:** Adds atom or bond to selection.
- **Click and drag:** Creates a selection rectangle, all atoms and bonds within the selection rectangle are added to the selection.
- **Right click:** Removes atom or bond from selection.

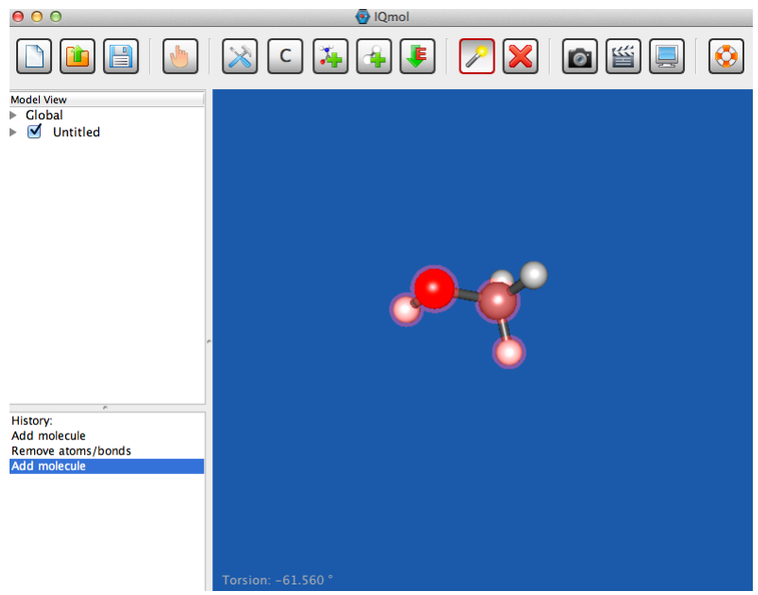
- Press “CTRL” and the left/right mouse (two fingers on Mac Trackpad) button to move the group of selected atoms [Replace CTRL with command key for Mac. For Mac Tracpad do the corresponding finger gesture]

IQmol: Measuring bond length, angles, and dihedrals

- Click the select button 
- Select 2, 3 or 4 atoms as necessary
- the measured bond length or angle or dihedral is displayed in the bottom corner:







The bond length is displayed here

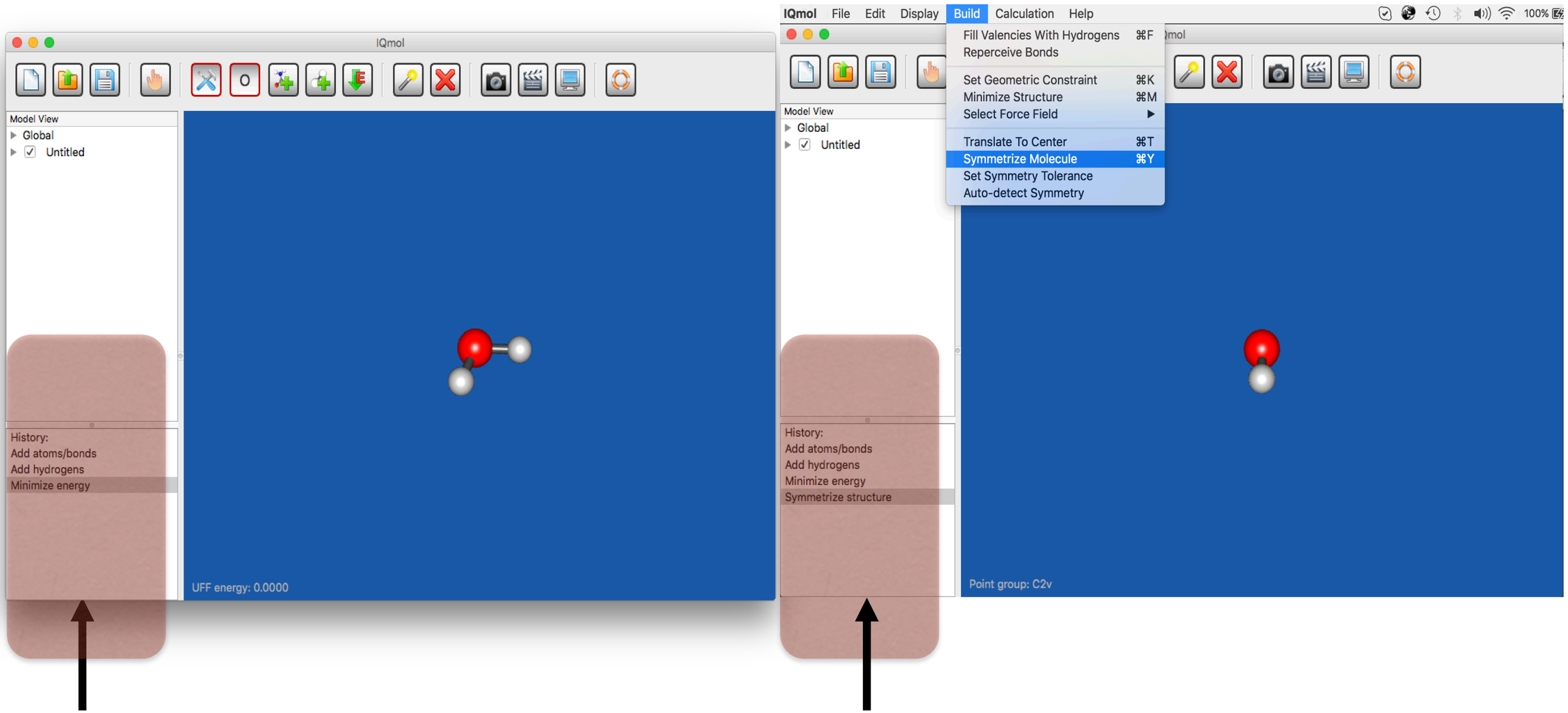
Performing Q-Chem calculations
Example 1: H_2O

Prerequisite: Consult IQmol-Server-Setup tutorial

H2O

- Build molecule, clean-up (force-field opt-n), check symmetry (symmetrize molecule)
- Optimize B3LYP/6-31G*
- Play with changing the view of the molecule, move it around, zoom
- Use ‘Select’ feature to measure bonds and angles
- Look at MOs: HOMO, HOMO-1; LUMO
- Run FREQ job, look at vibrations (click versus double-click)

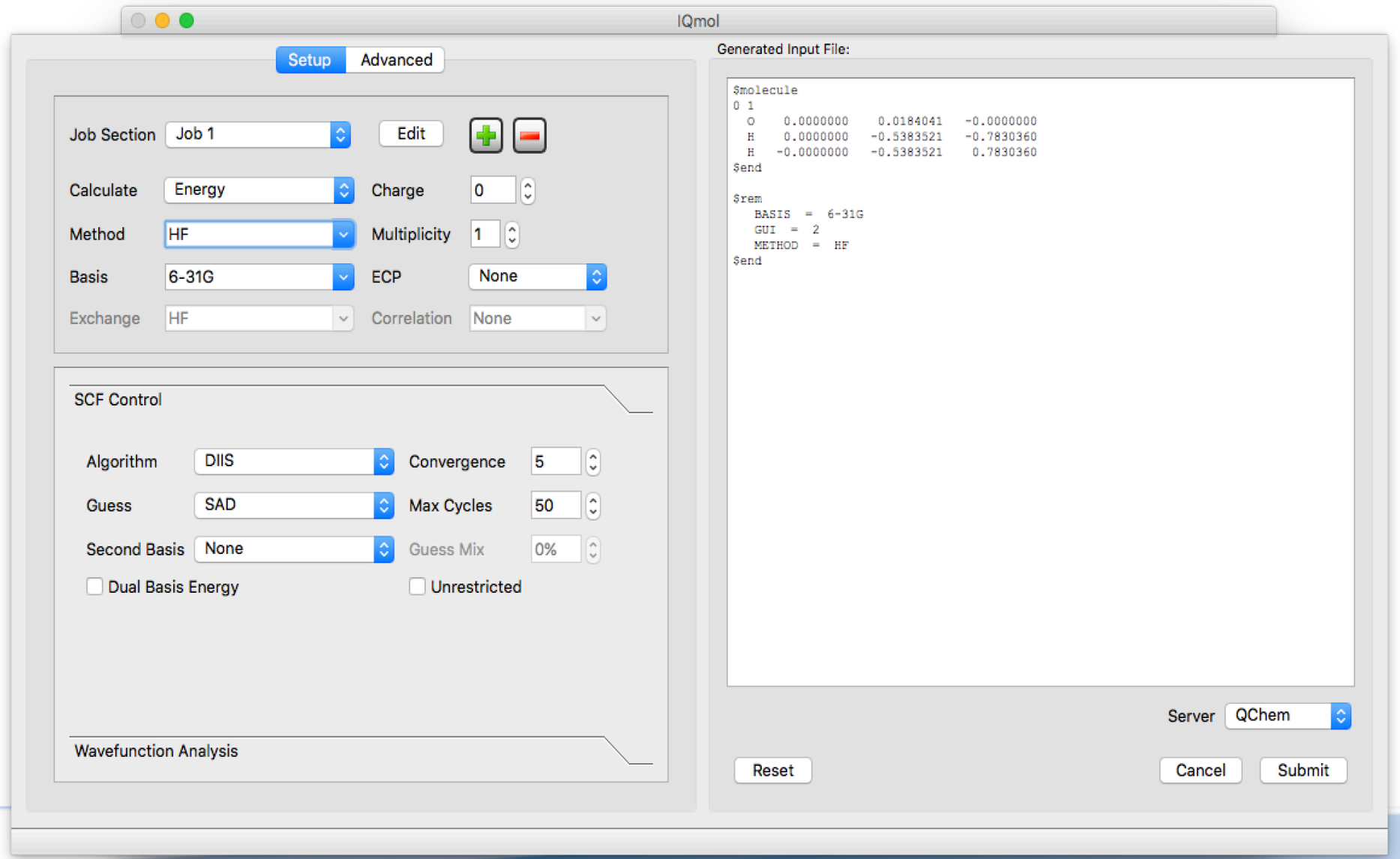
Building up/Check symmetry



Performing Q-Chem Calculations

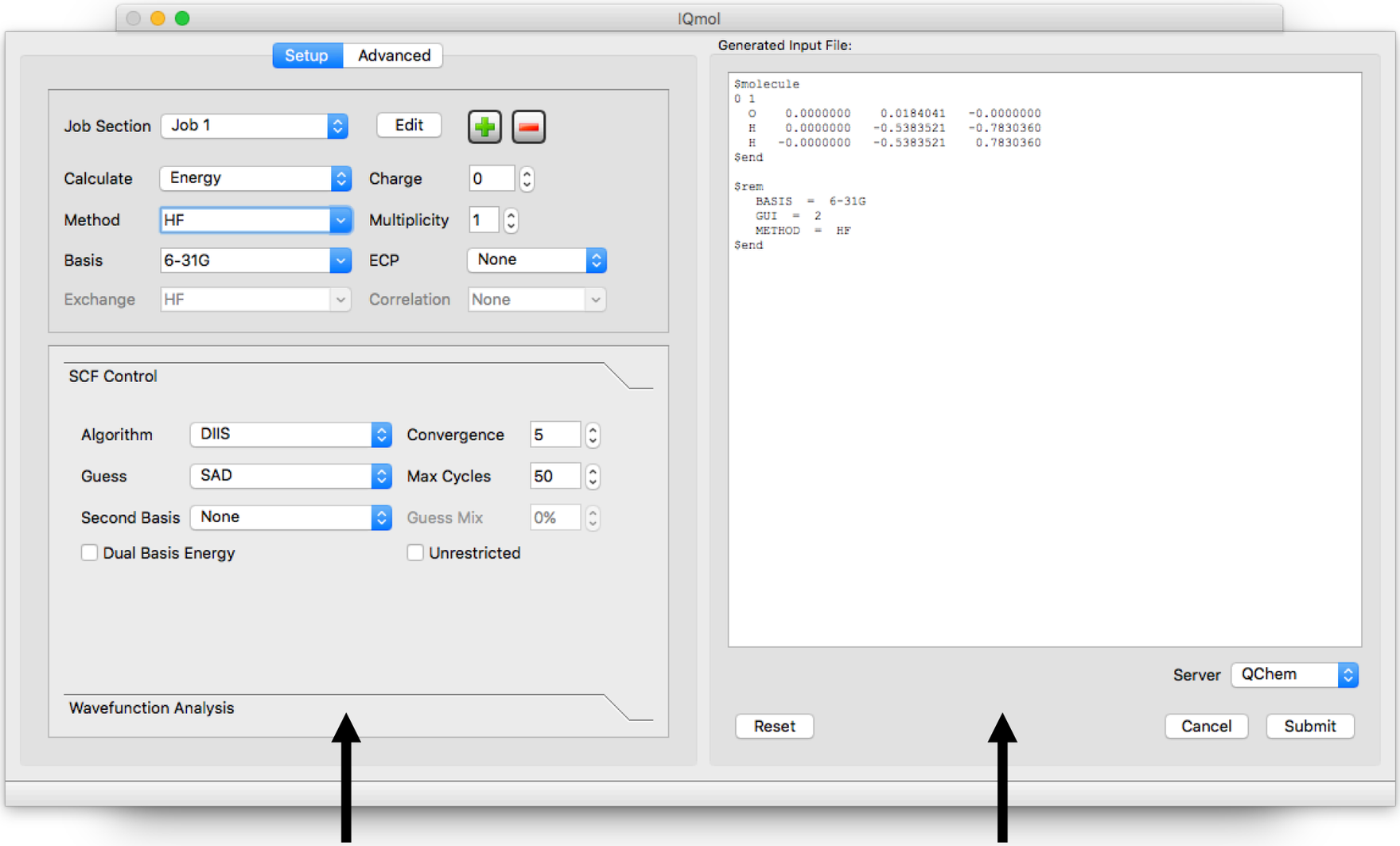
From menu bar: File Edit Display Build Calculation Help

- **Calculation** → **Q-chem Setup;** open Q-chem User Interface (QUI) input editor



QUI

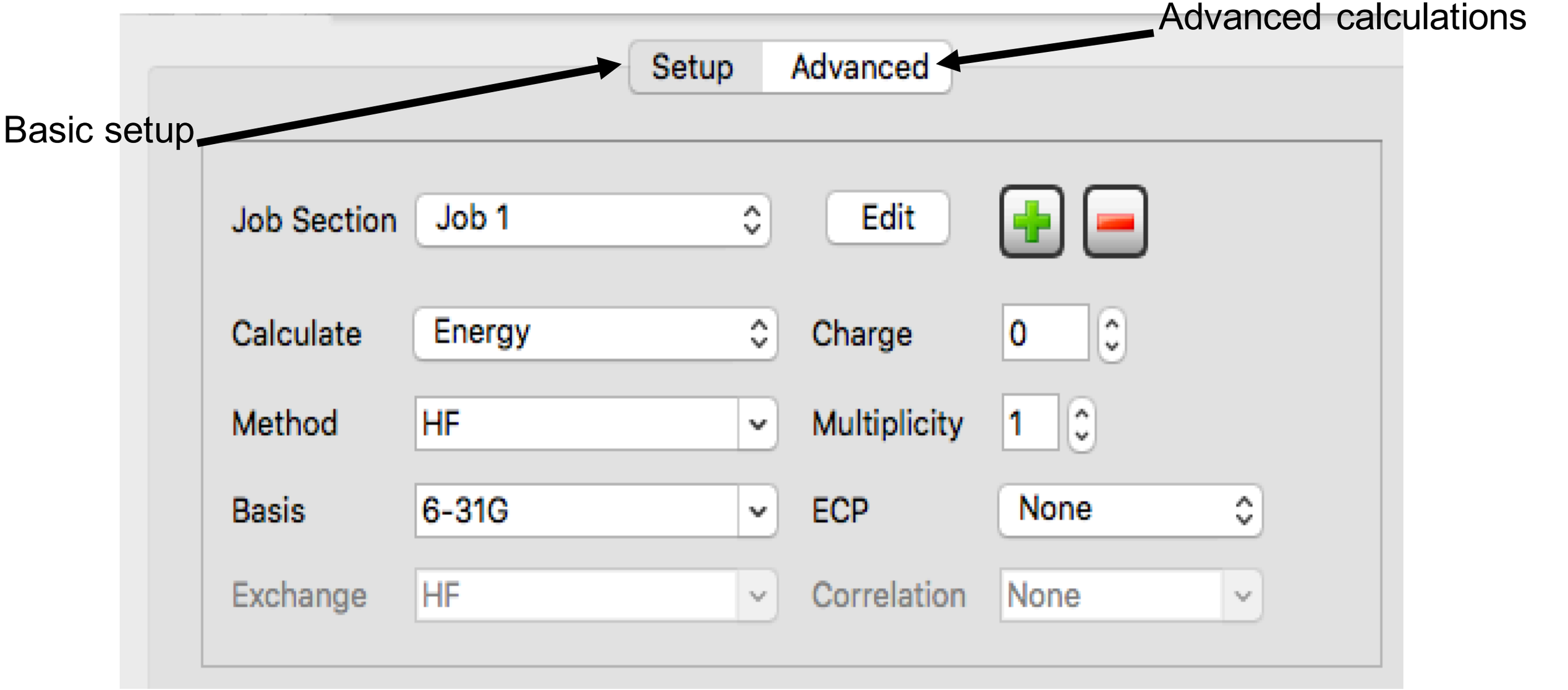
- QUI has 2 windows



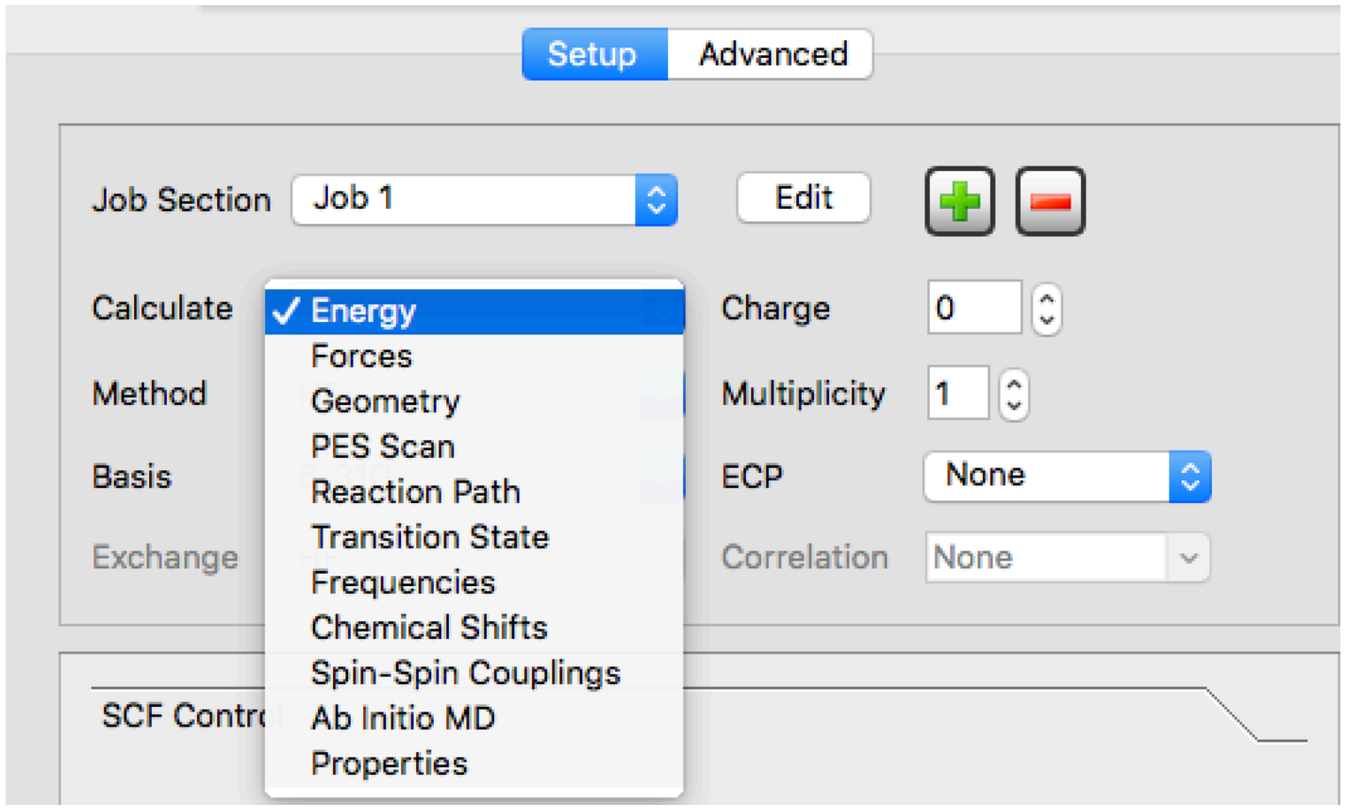
Details of the calculation

Preview of the input file

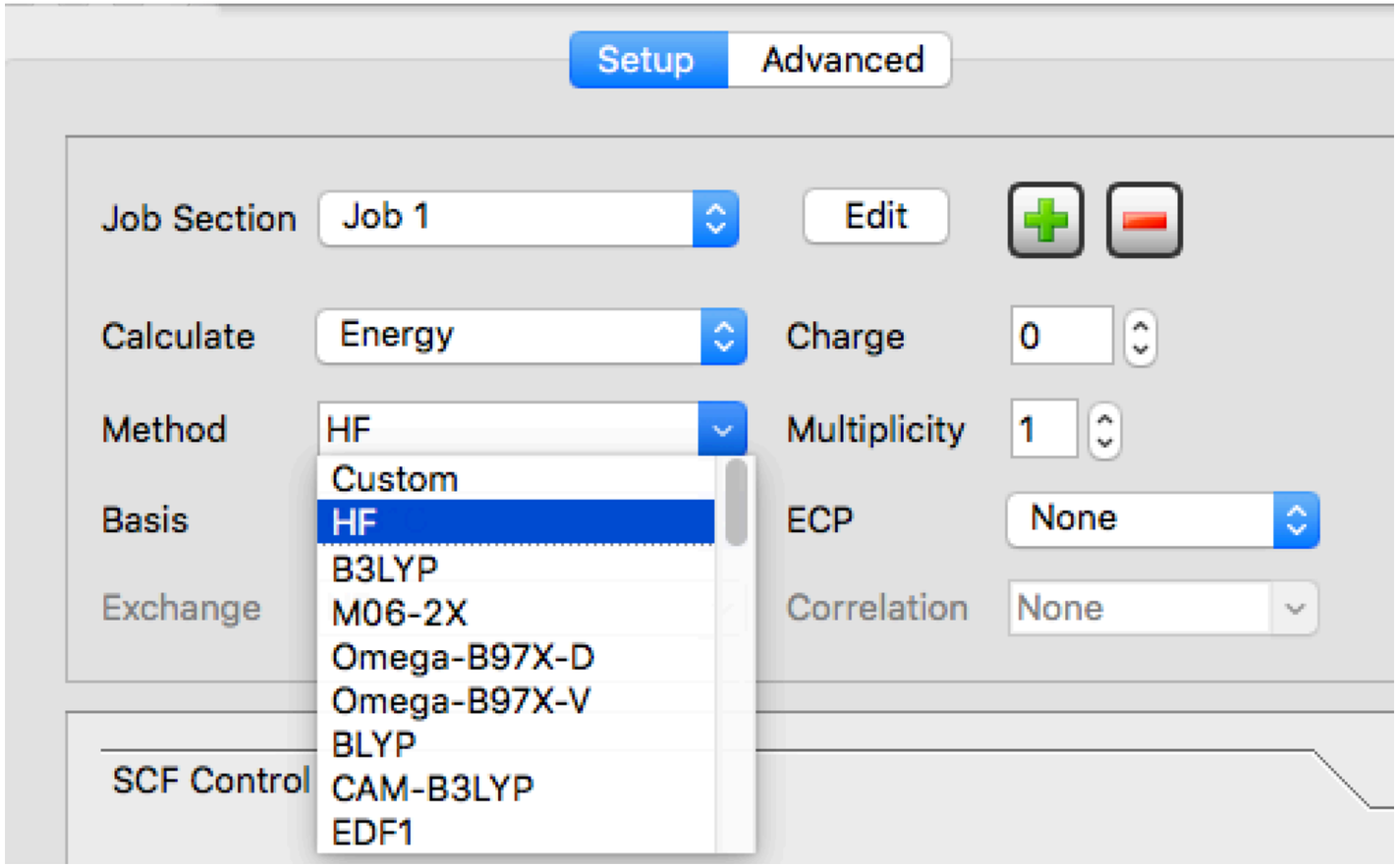
- There are 2 windows in “Computational details” section



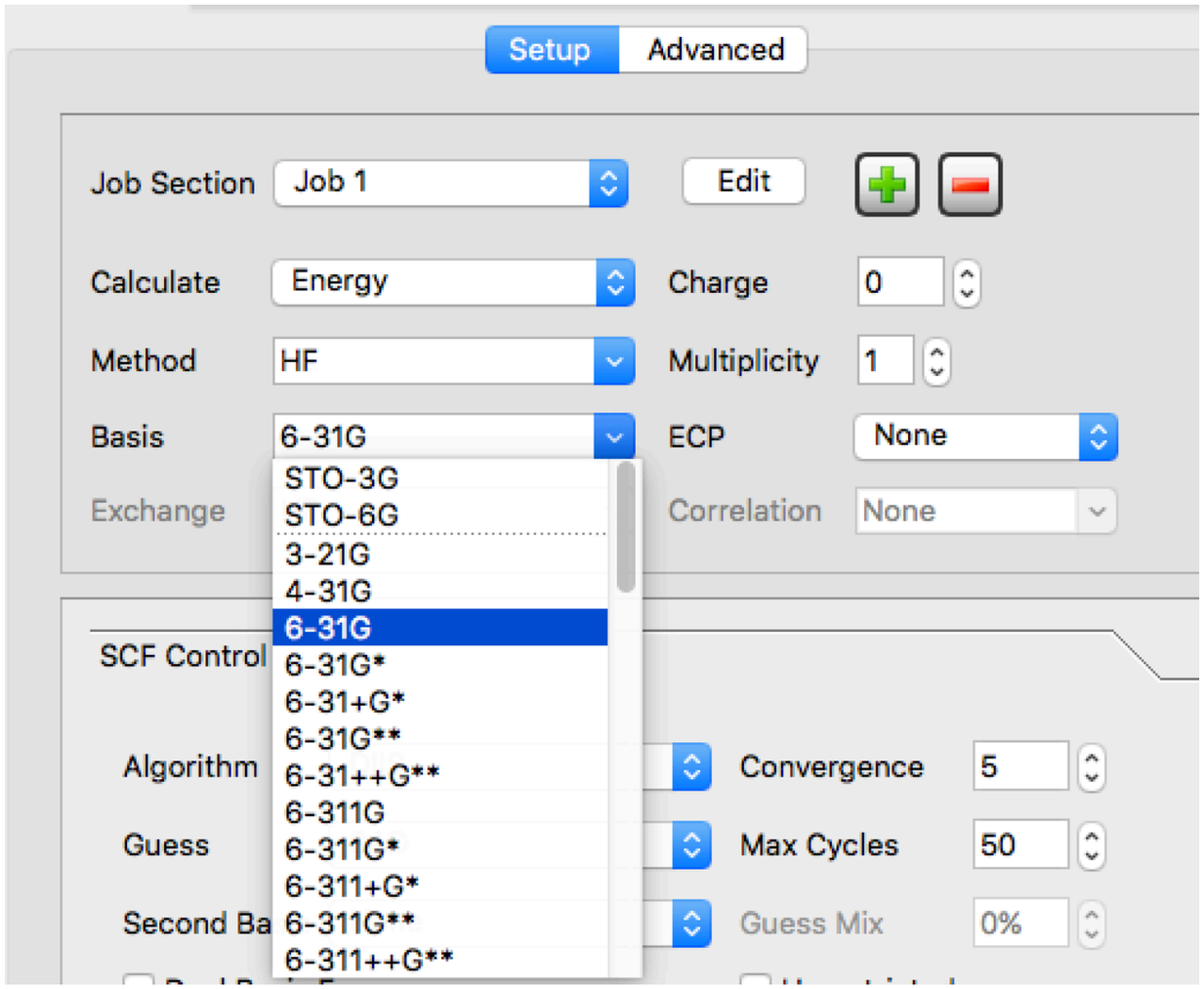
Setting up the job type, method, basis set



Setting up the job type, method, basis set

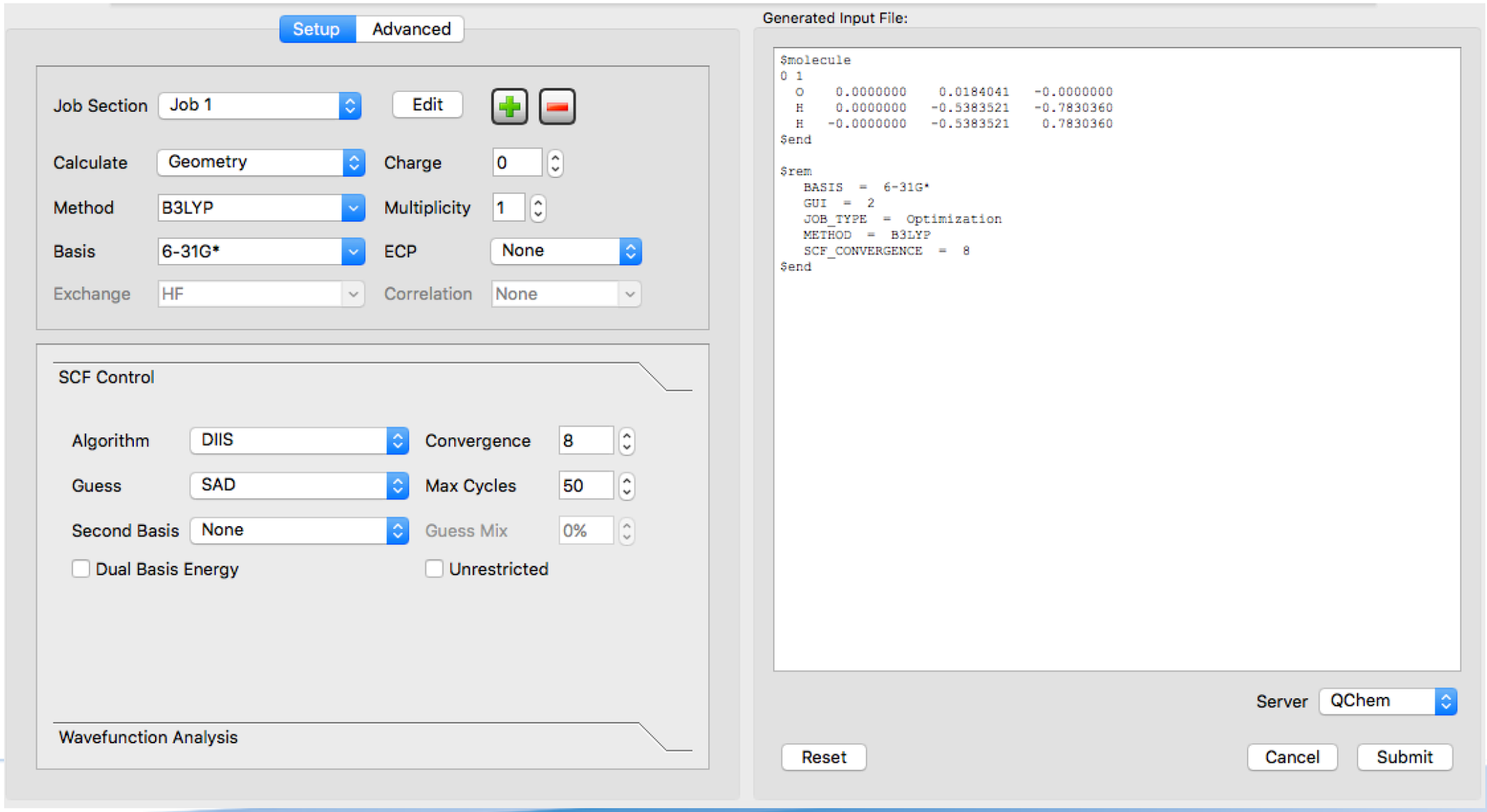


Setting up the job type, method, basis set



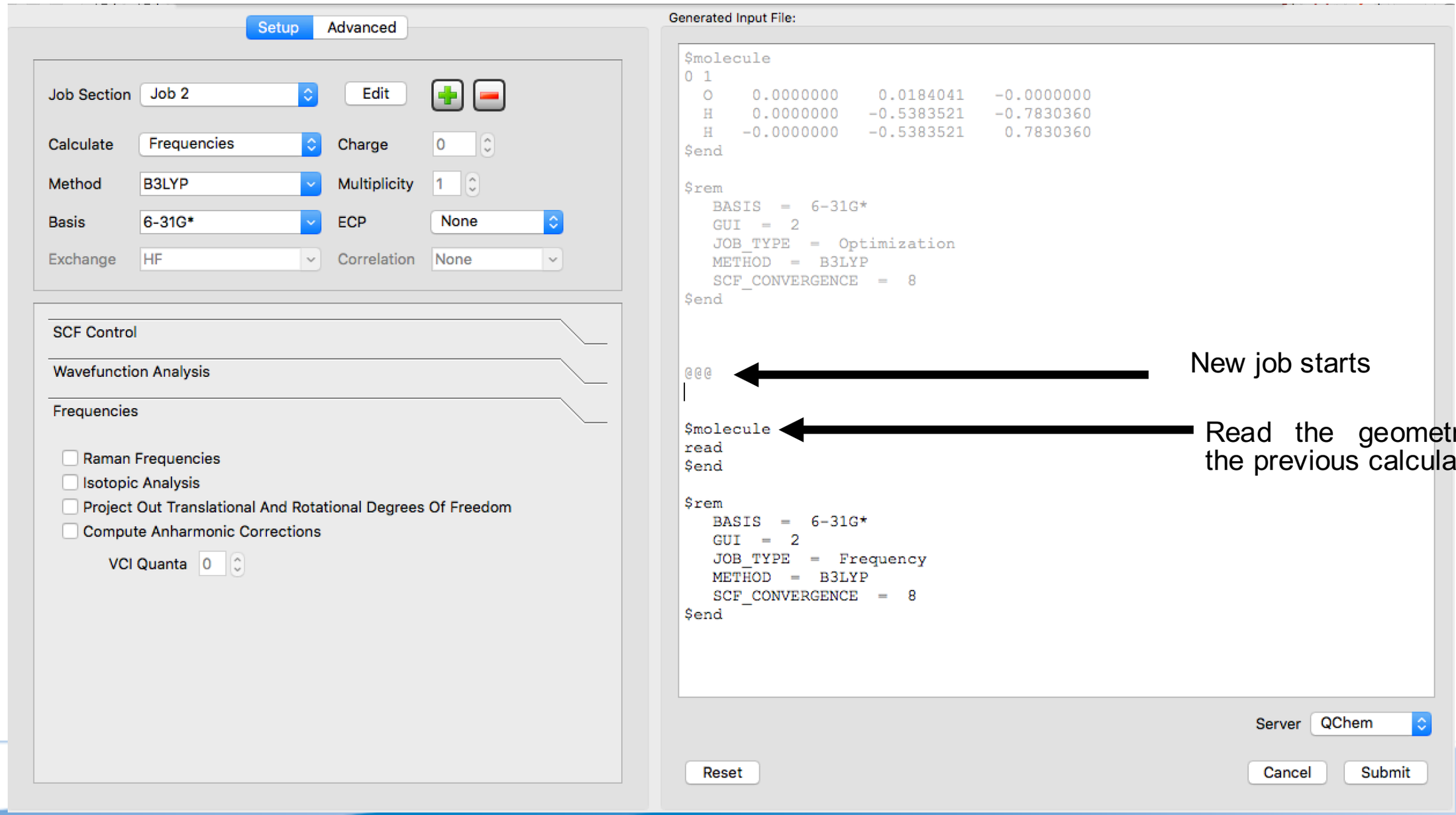
H_2O: Optimization and Frequency

- Take H_2O molecule and perform “Optimization” and “Frequency” analysis
- First optimization:



H_2O: Optimization and Frequency

- Use add button to submit multiple jobs within one input file: such as optimization and frequency to be performed subsequently



Input editing

- One can manually modify the input preview
- $rem section

Generated Input File:

```
$molecule
0 1
  O     0.0000000     0.0184041    -0.0000000
  H     0.0000000    -0.5383521    -0.7830360
  H    -0.0000000    -0.5383521     0.7830360
$end

$rem
   BASIS  =  6-31G*
   GUI  =  2
   JOB_TYPE  =  Optimization
   METHOD  =  B3LYP
   SCF_CONVERGENCE  =  8
$end
```

Server QChem

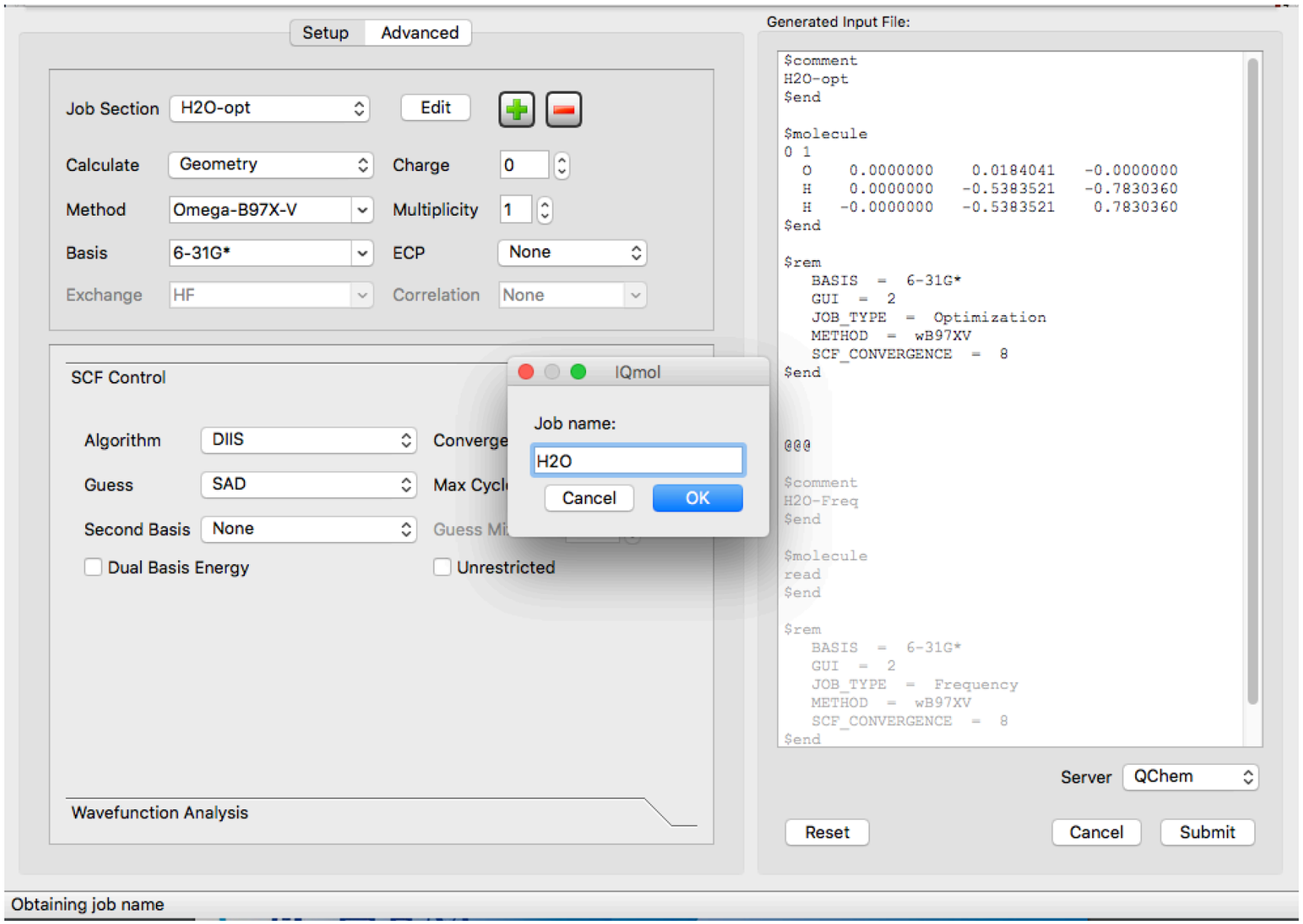
Reset Cancel Submit

Saving input file

- Save the input on a disk: **File** → **save as**
- Use **.inp** for name of the input file

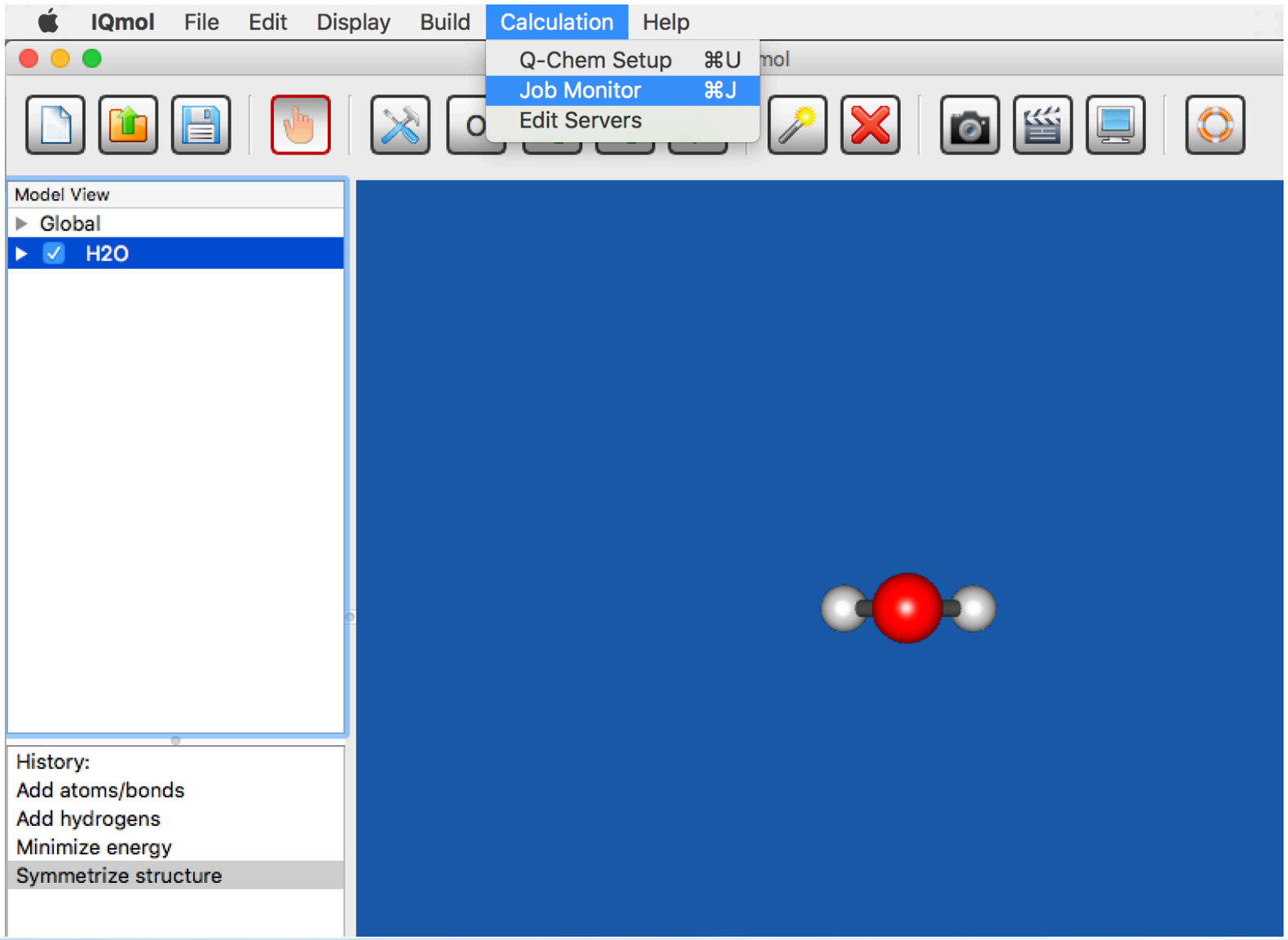
Submitting job to Iqmol server iqmol.q-chem.com

Give a name and remember it.



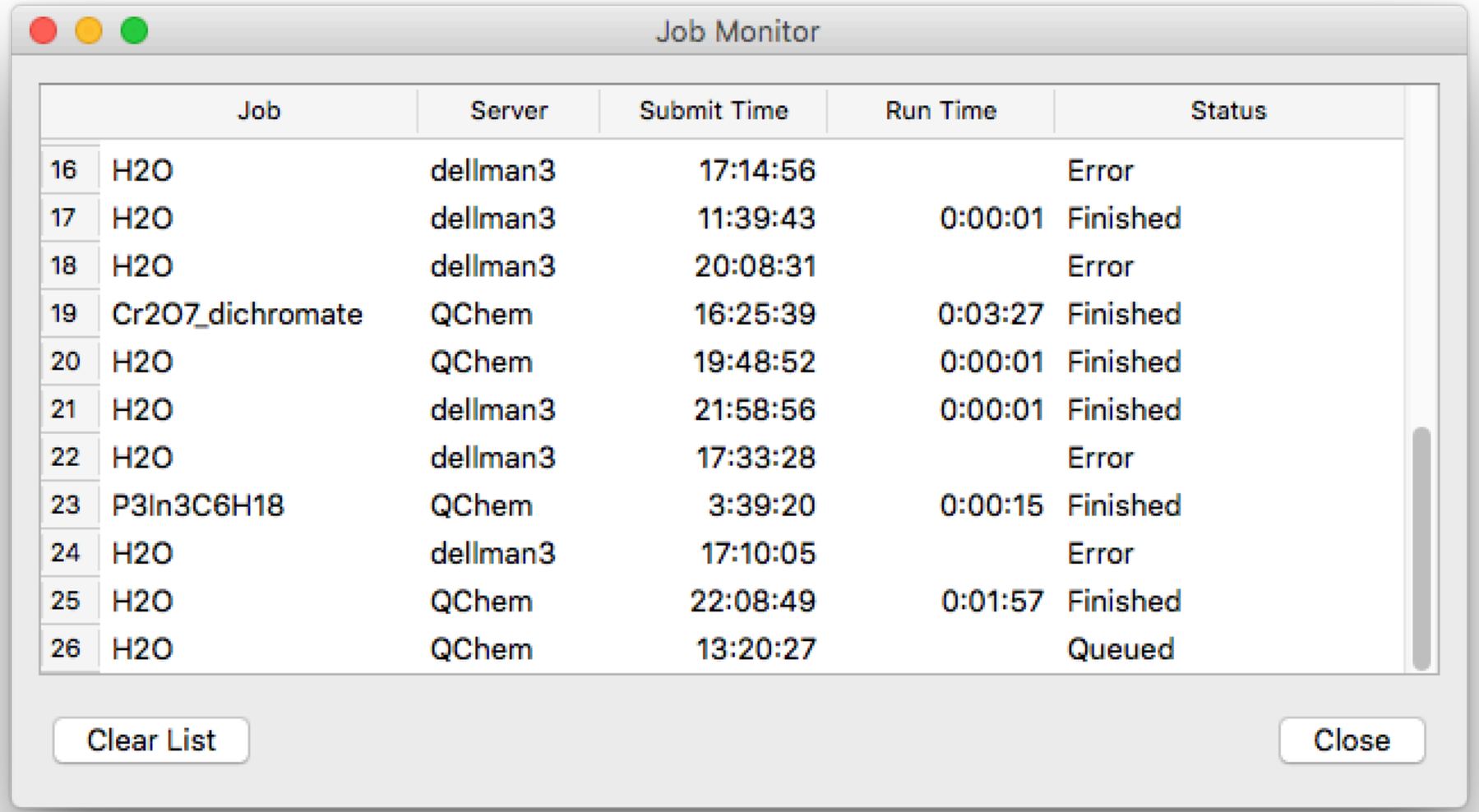
Job Status

- Check the job status by selecting: “**Calculation —>Job Monitor**”



Monitoring submitted job

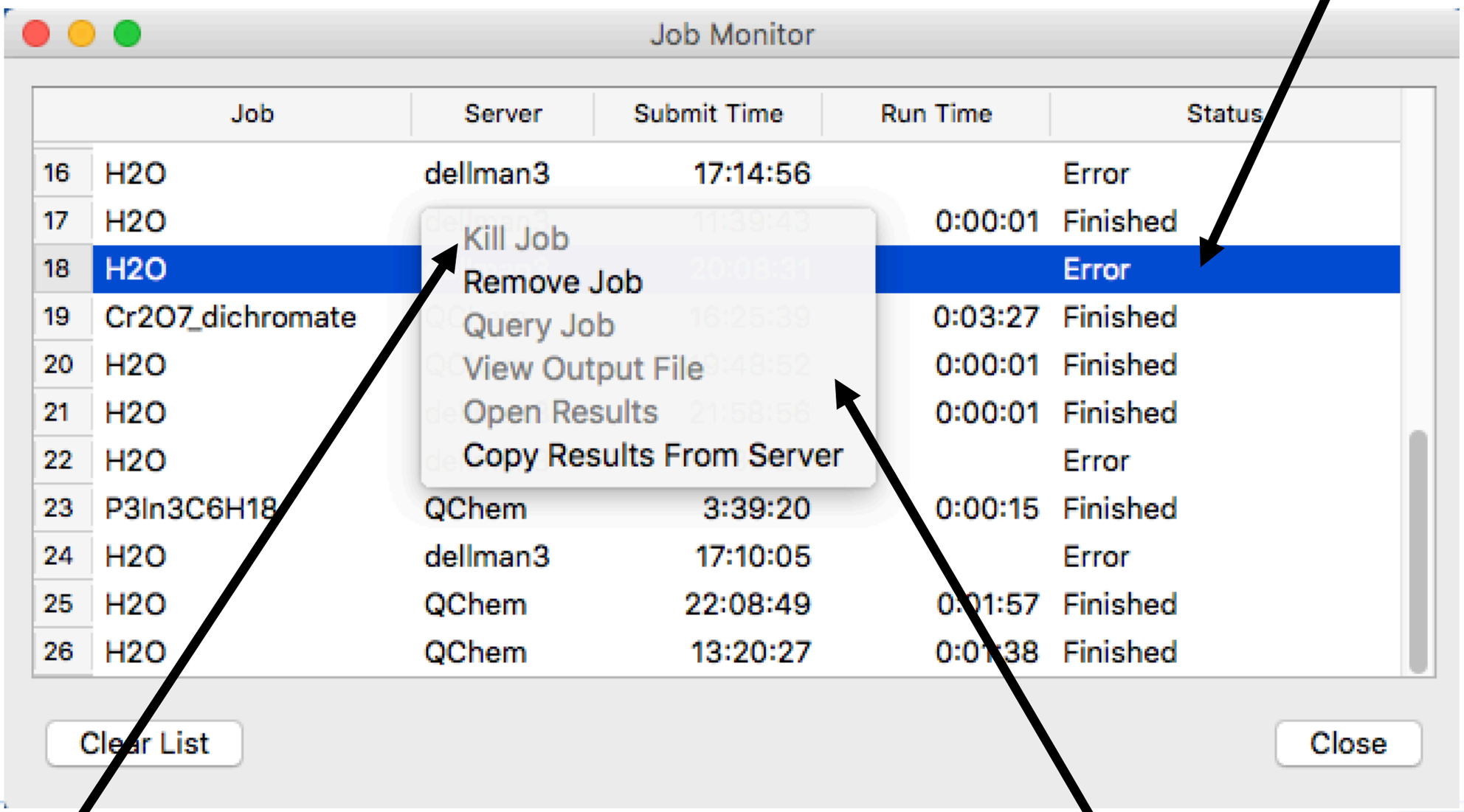
- Check the job status by selecting: "**Calculation —>Job Monitor**"



Monitoring submitted job

use left mouse button to select the job

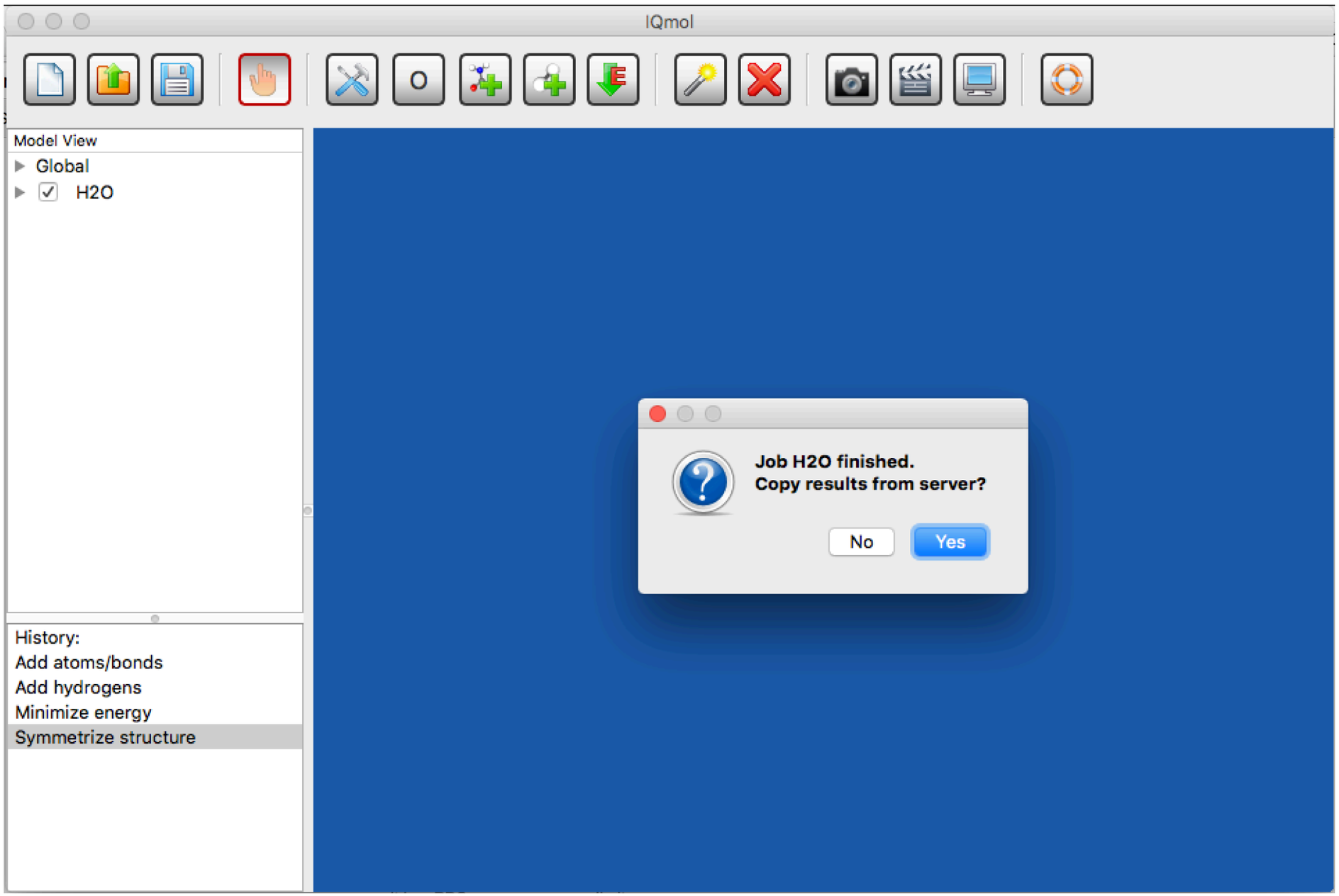
- Job status:



kill the job by selecting this option

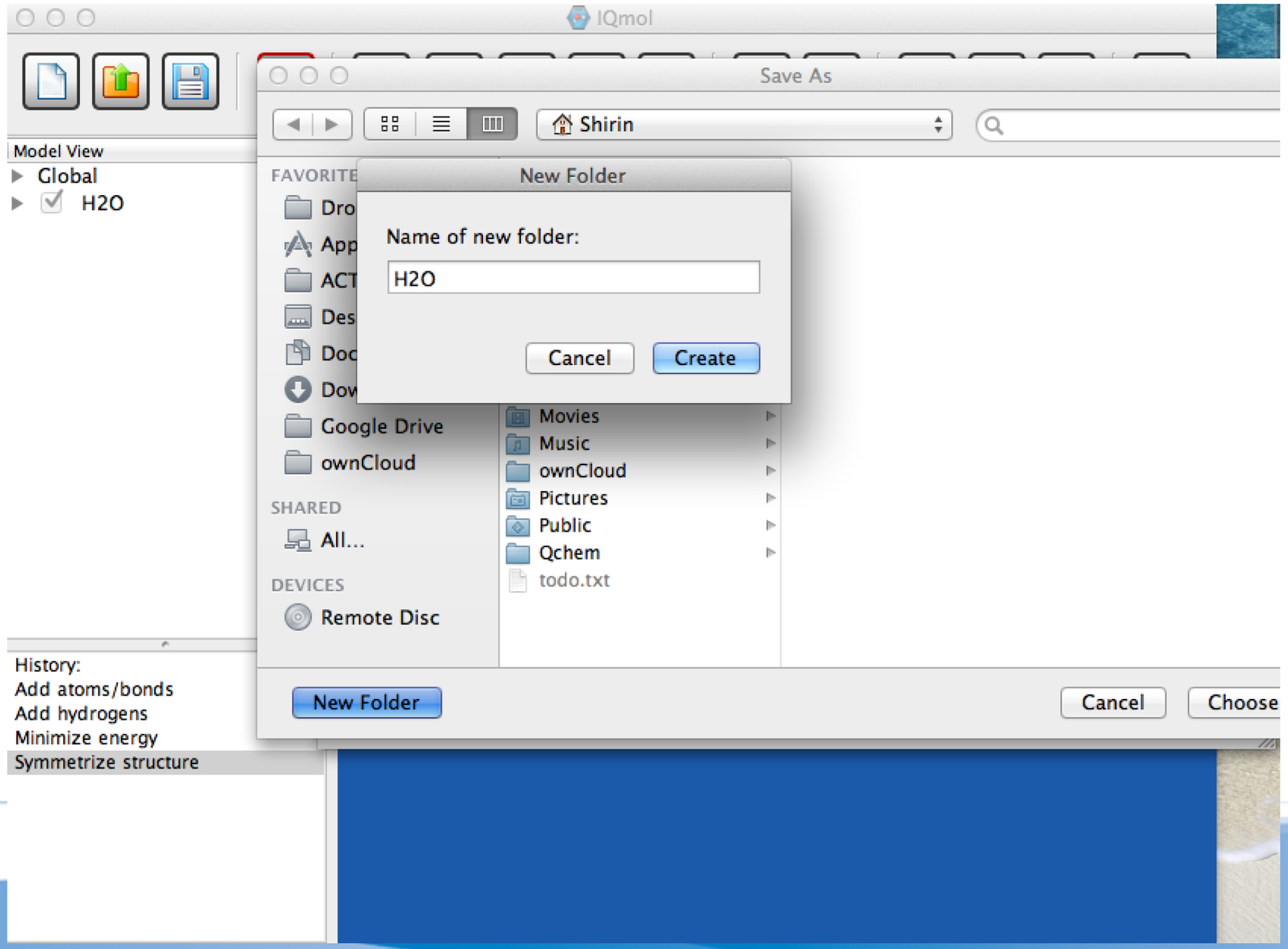
use right mouse button to see this menu

Job is finished



Copy files to your laptop

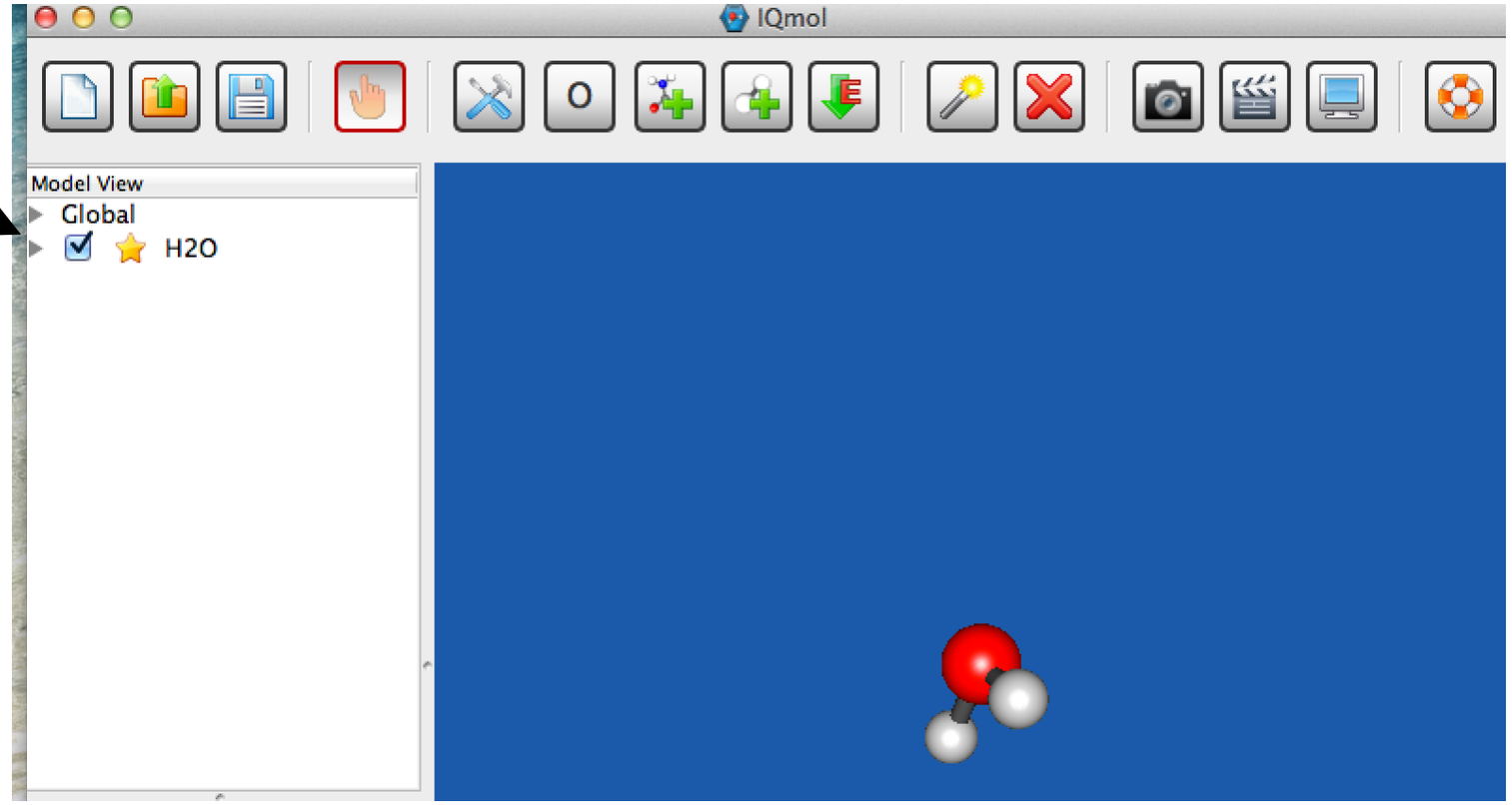
Create new folder to store output files:



After you copied files to your laptop

Golden star shows that it is copied properly.

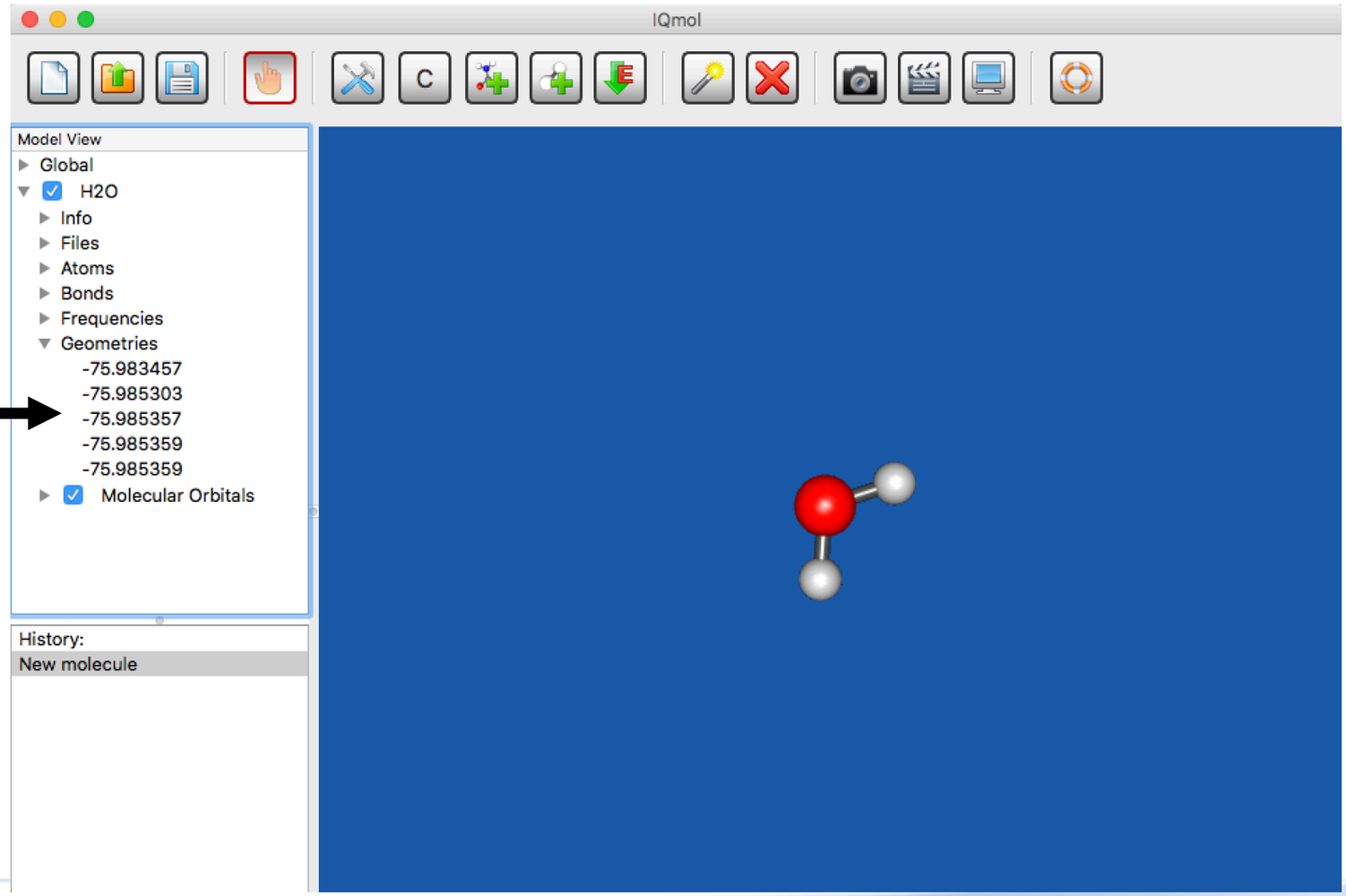
Click the checkbox !



Analyzing Output: Optimization

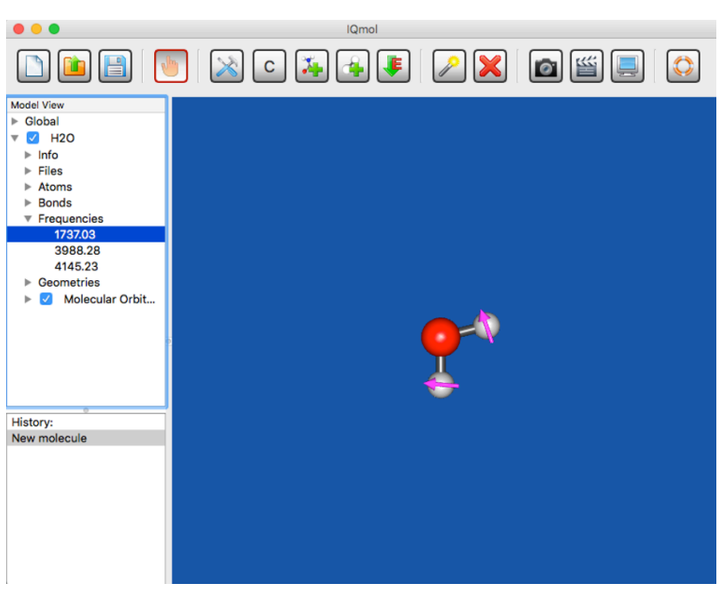
- After the calculations has been completed, open the .out (output) with IQmol. The example here is H_2O after optimization and frequency analysis.
- Click the small arrow next to the checkbox to see various calculated properties

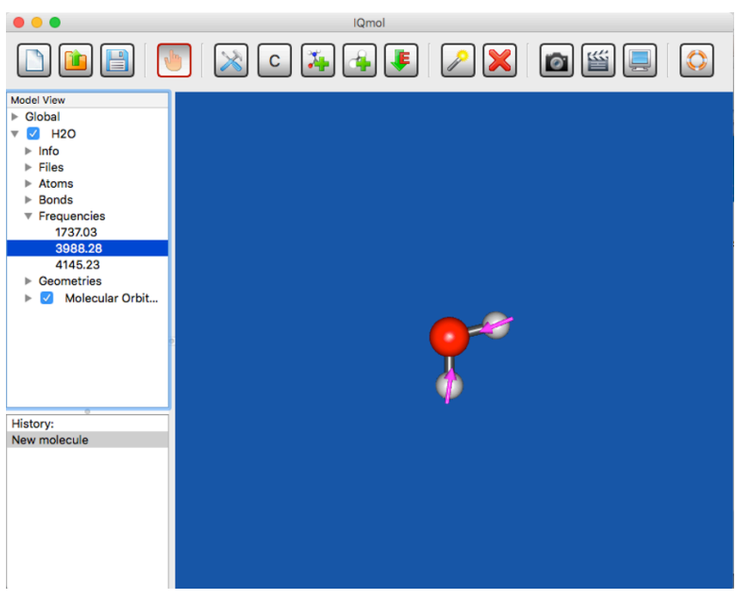
Clicking the arrow next to **Geometries** gives the calculated energy at every step of optimization

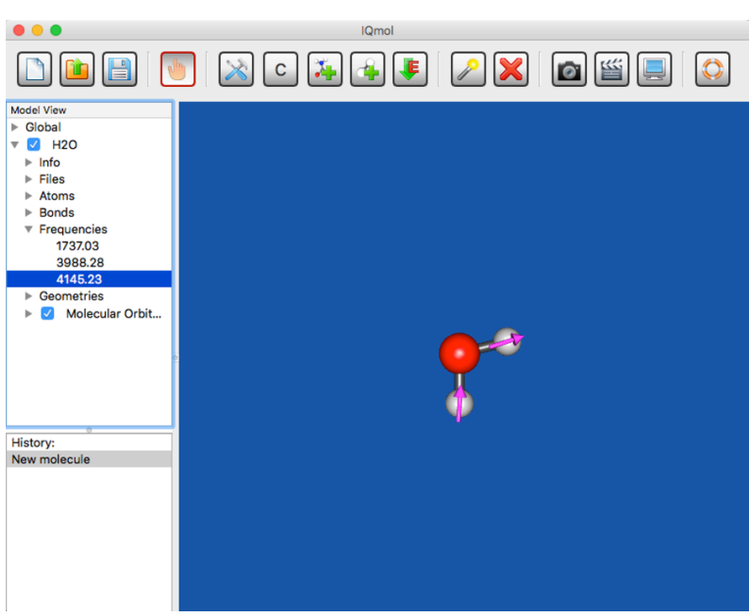


Analyzing Output: Frequencies

- Clicking the arrow next to **Frequencies** gives the calculated frequencies and displaced vectors for each frequency (for H_2O: 3N-6=3 vibrational frequencies)
- Double click at each value to animate the vibration

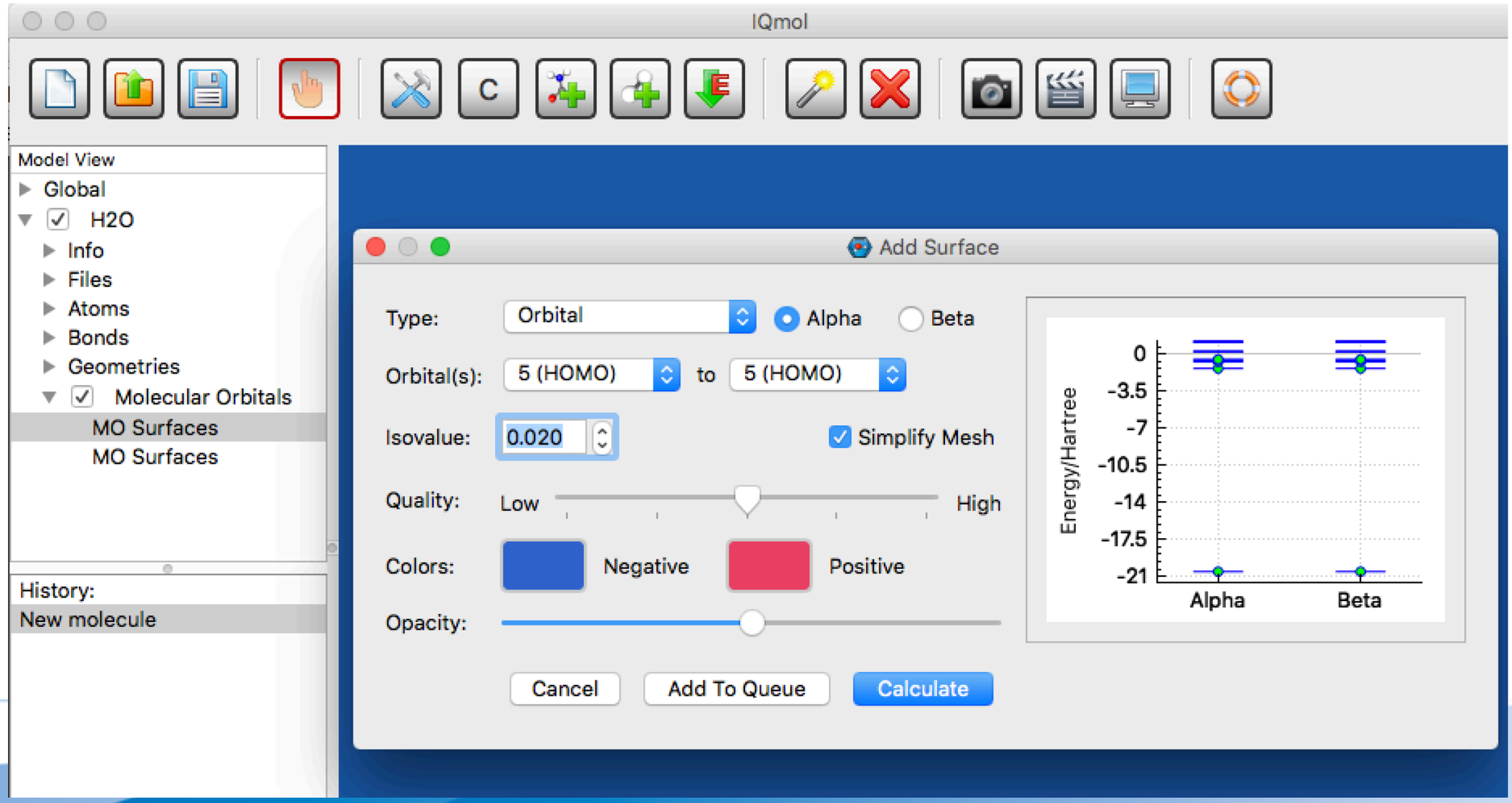






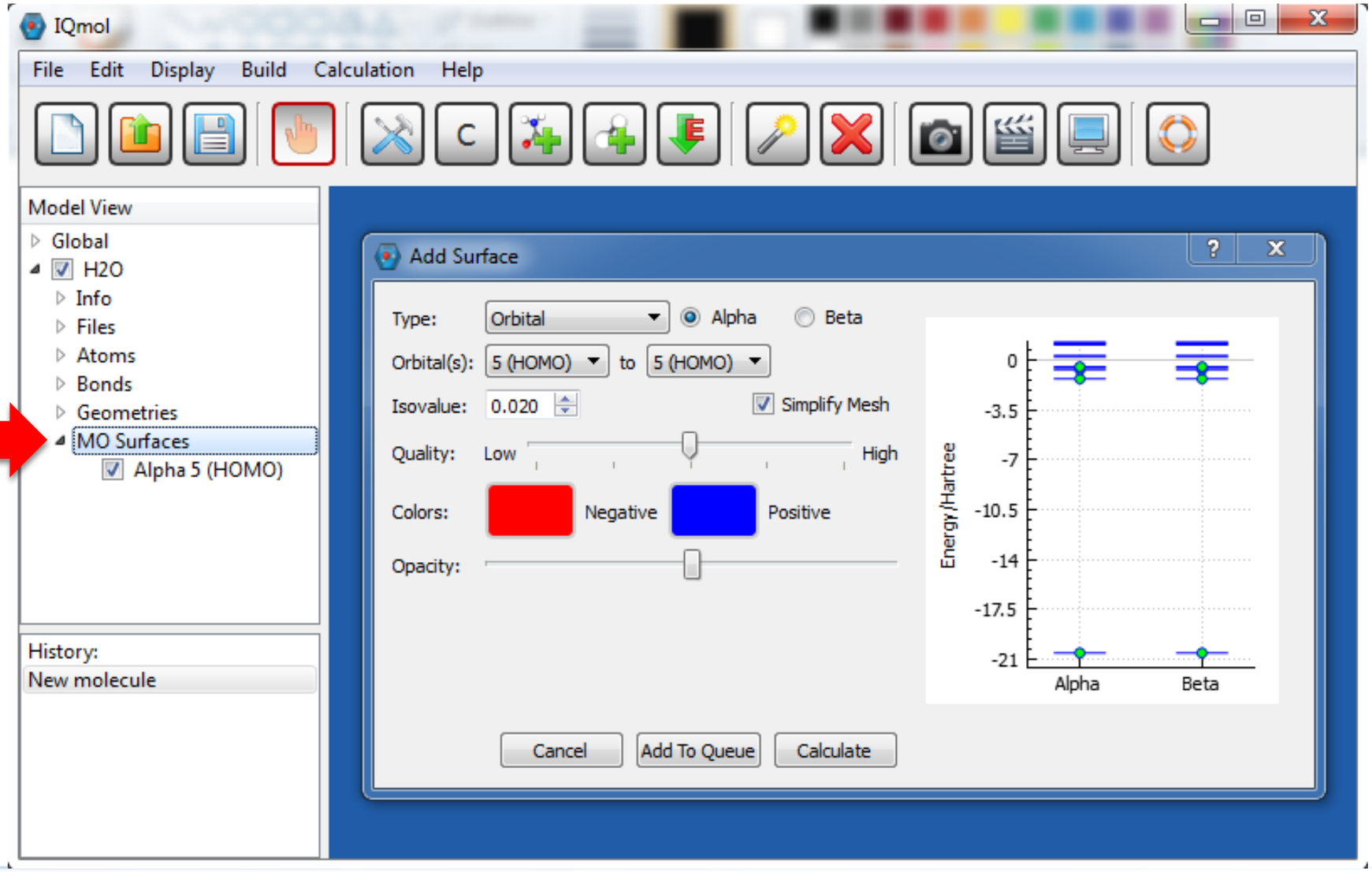
Analyzing Output: Orbitals, Density, Spin Density ,…

- **Must add GUI = 2 in the $ rem section** (IQmol does it by default)
- Open **.Fchk** file to see orbitals, density, spin density and so on.
- Double click on **MO Surfaces** under **Molecular Orbitals** (mac) and a window pops up



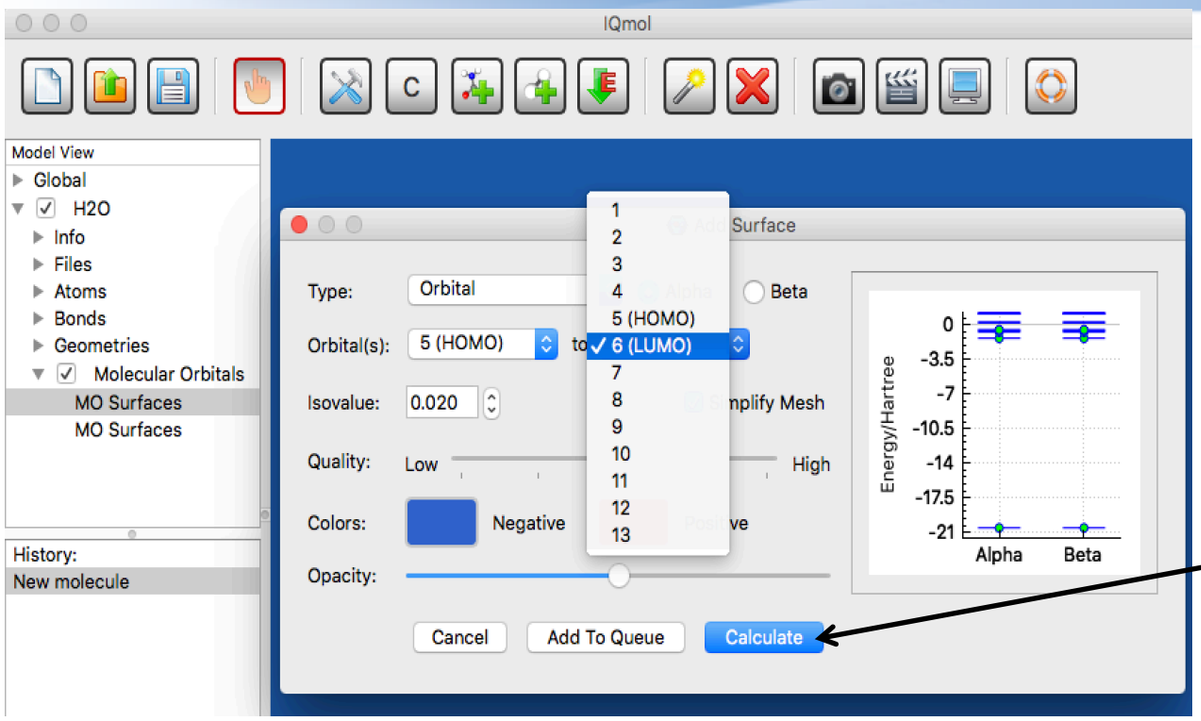
Analyzing Output: Orbitals, Density, Spin Density ,…

- For MS Windows views are little different
- Just double click on **MO Surfaces** and "Add Surface" window pops up

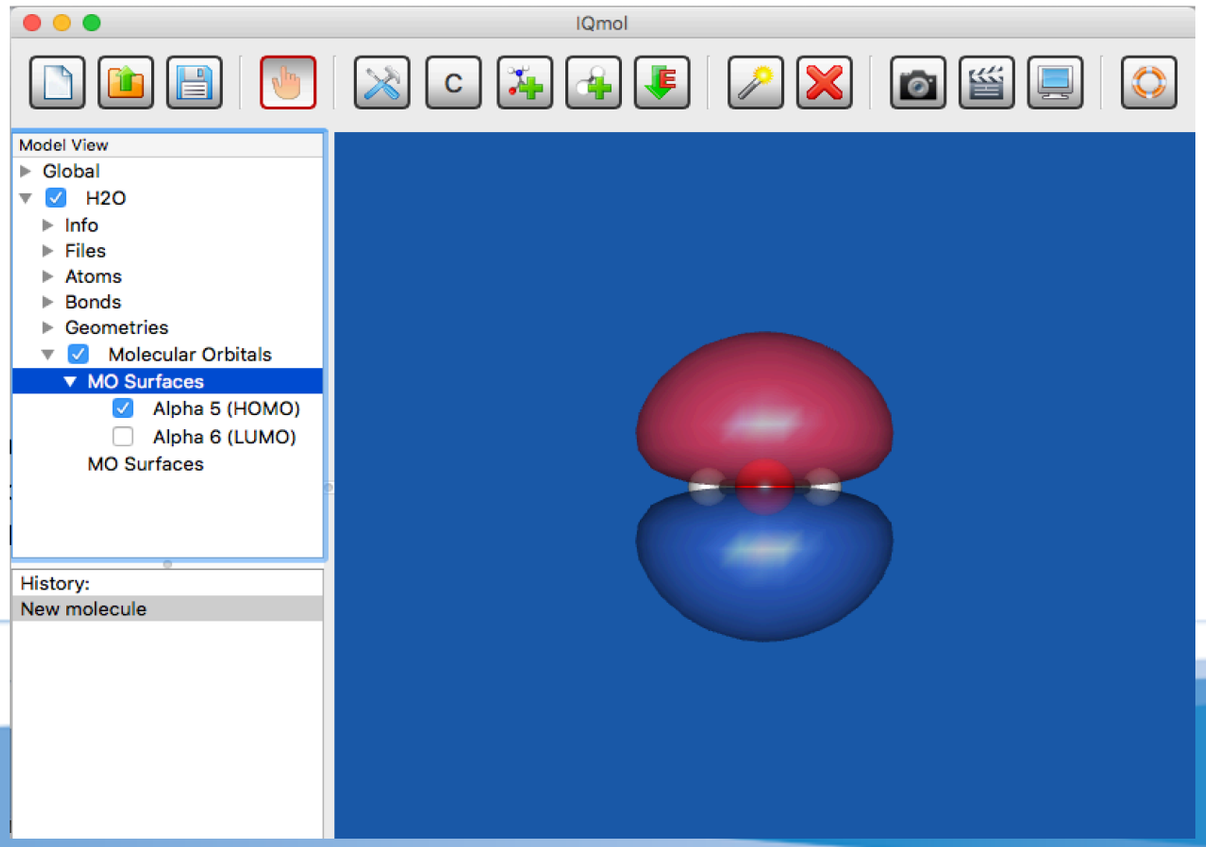


Screen shot from Windows 7

Analyzing Output: Orbitals, Density, Spin Density ,…



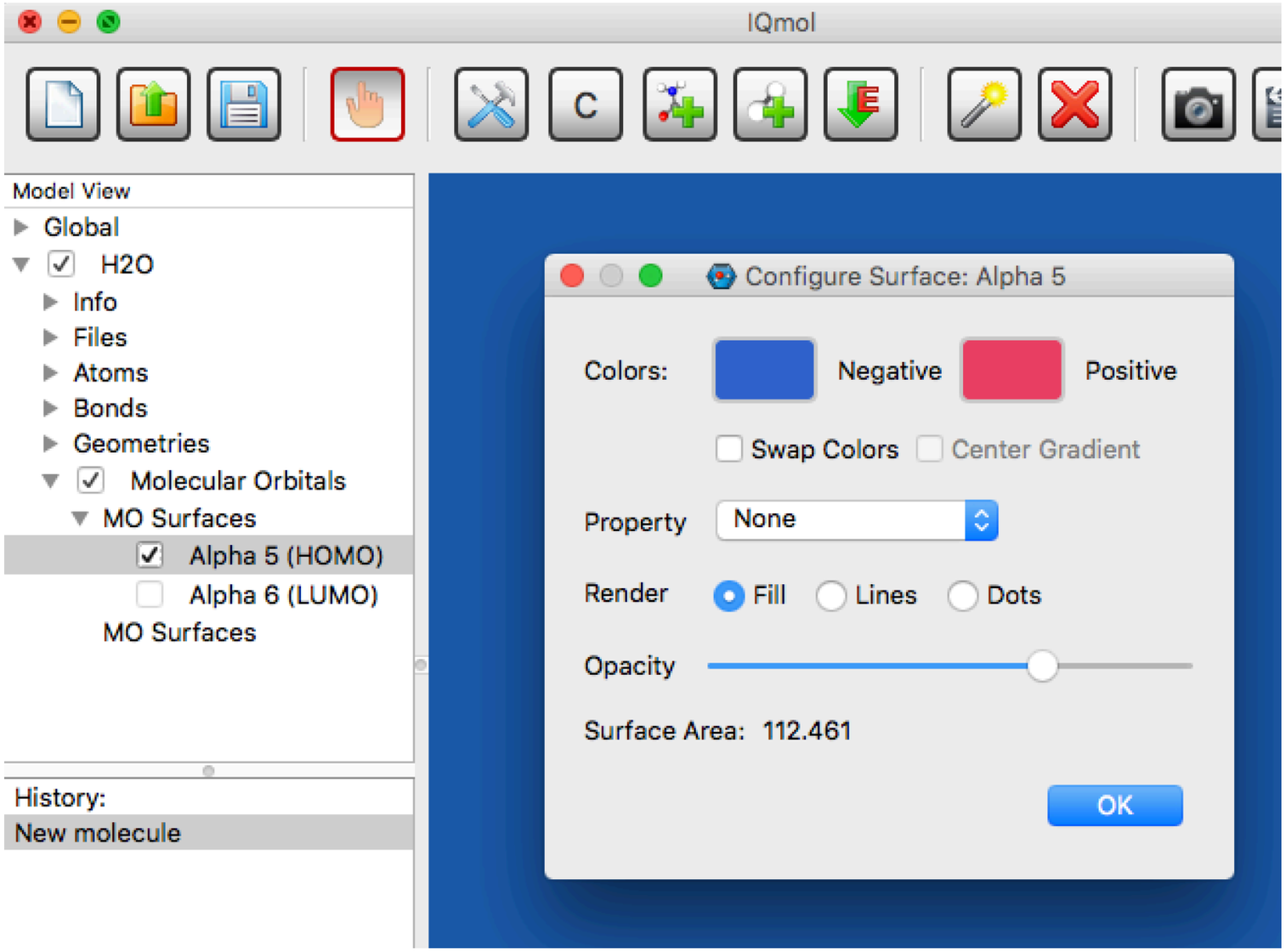
- Select orbital
- Select the relevant orbital (default: HOMO)
- Select the quality you want
- Click **calculate**



- Click the arrow next to **MO Surfaces** to see the orbitals one by one by clicking the checkbox of the corresponding orbital (do not forget to uncheck the old one)
- Use “Manipulate Mode" to better see the orbital
- To save the screen: **File —> Save Picture**

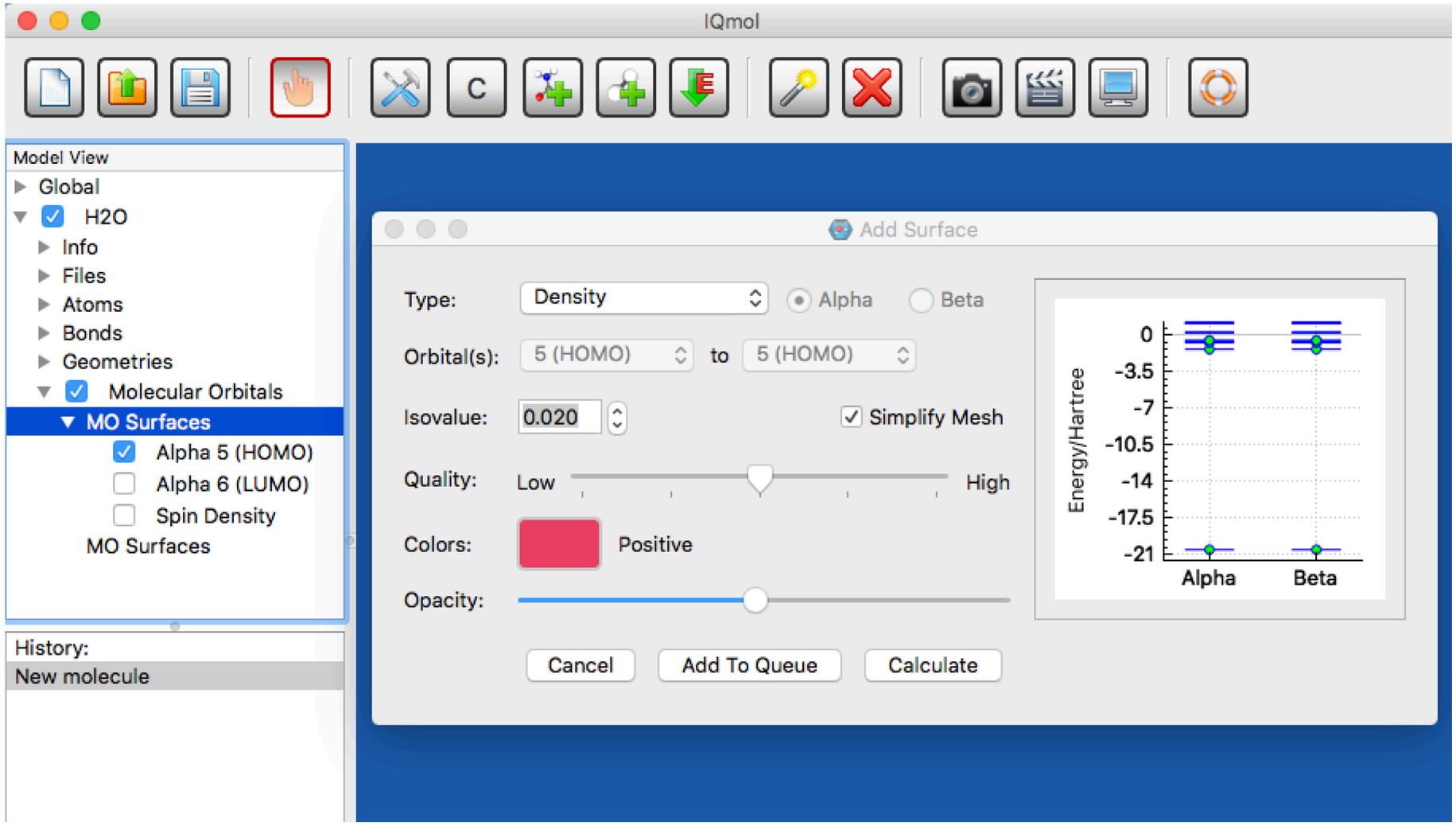
Analyzing Output: Orbitals, Density, Spin Density ,…

- To change the quality of the surface double click on the orbital being displayed in MV.



Analyzing Output: Orbitals, Density, Spin Density ,…

- Double click on **MO Surface** again from MV panel
- “Add Surface” window will pop up again
- Select different properties to be calculated; spin density, density, and so on….



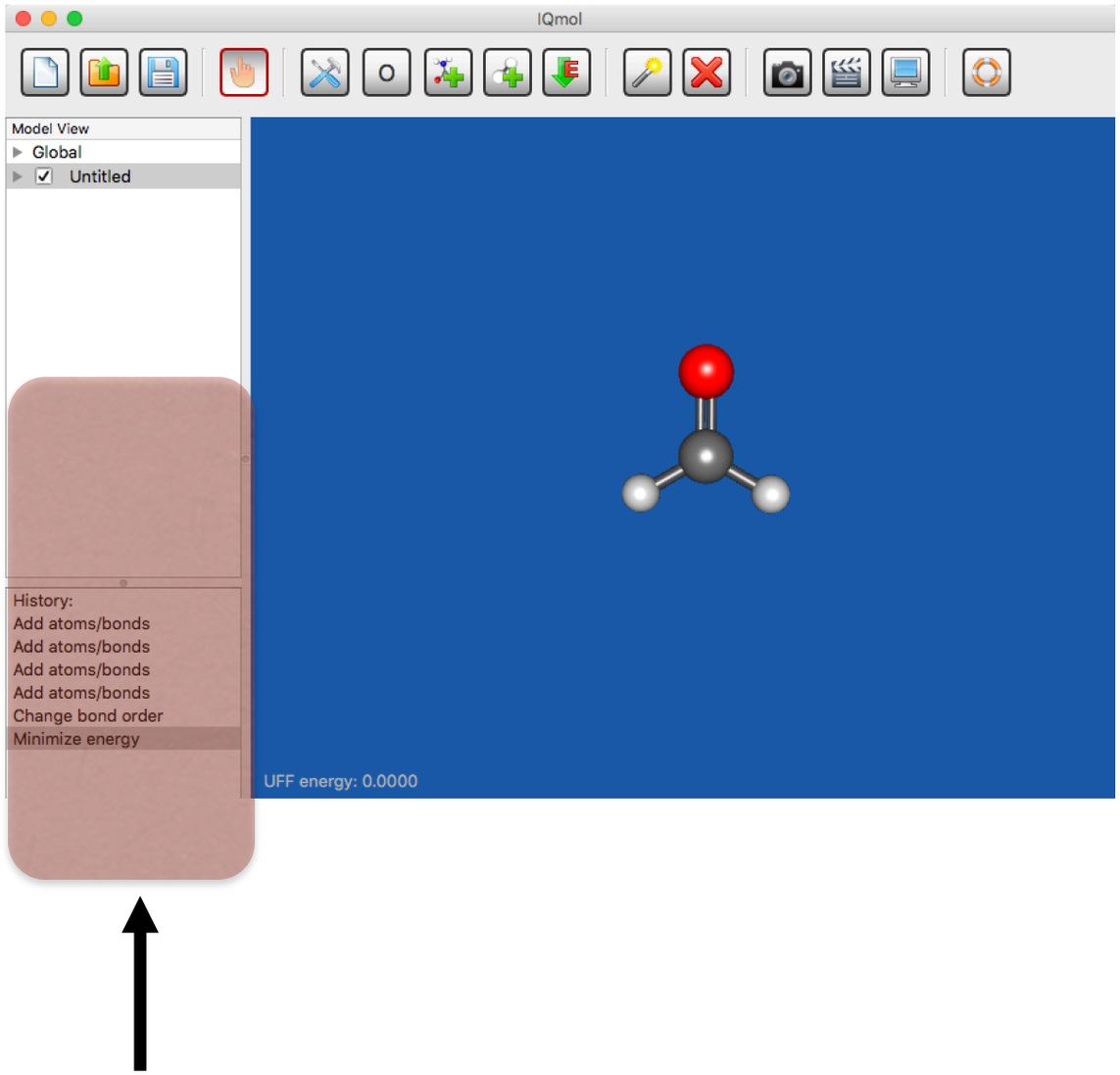
Performing Q-Chem calculations

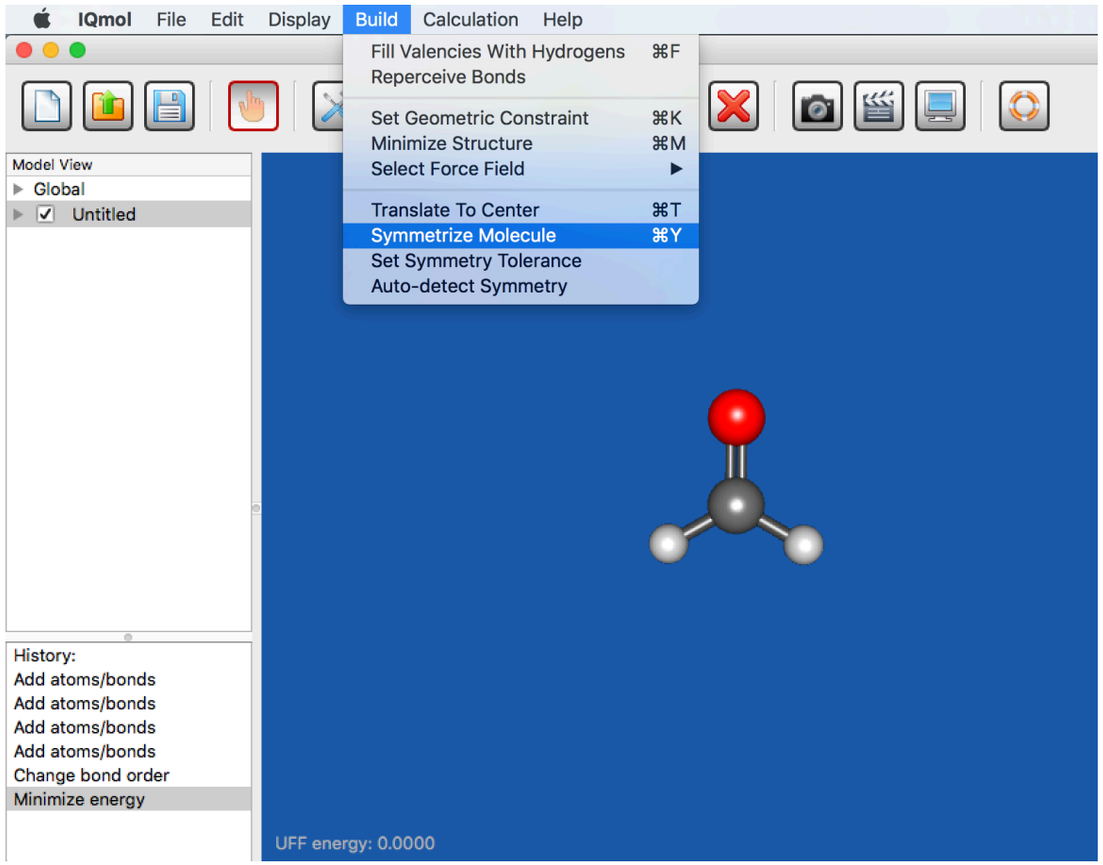
Example 2: CH_2O (Formaldehyde)

Formaldehyde

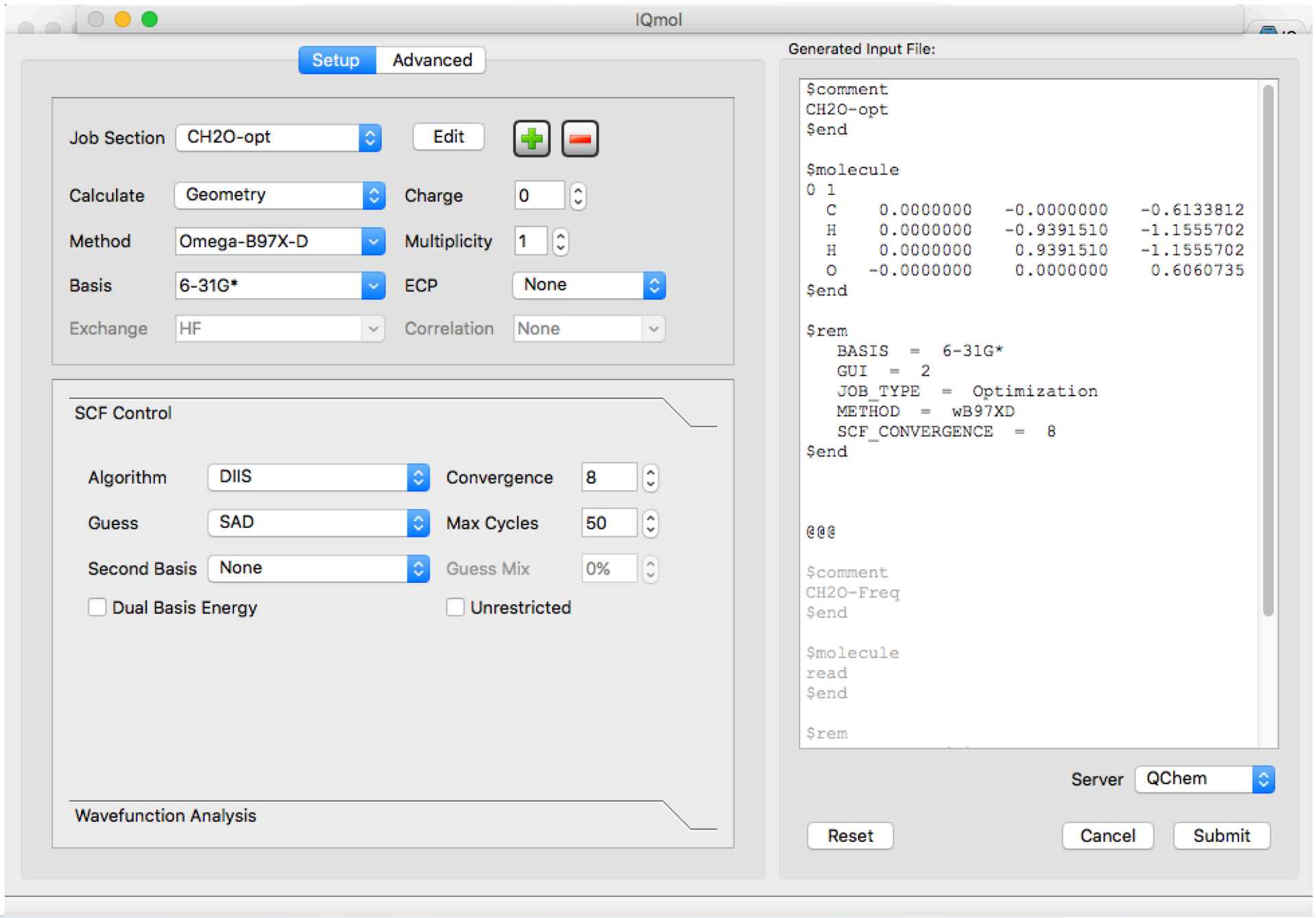
- Build molecule, clean-up (force-field opt-n), check symmetry (symmetrize molecule)
- Optimize wB97X-D/6-31+G*
- Play with changing the view of the molecule, move it around, zoom
- Use ‘Select’ feature to measure bonds and angles
- Look at MOs: HOMO, HOMO-1, LUMO
- Run FREQ job, look at vibrations (click versus double-click)
- Advanced: Run NBO analysis, look at NBO charges and bond orders

Building up/Check symmetry

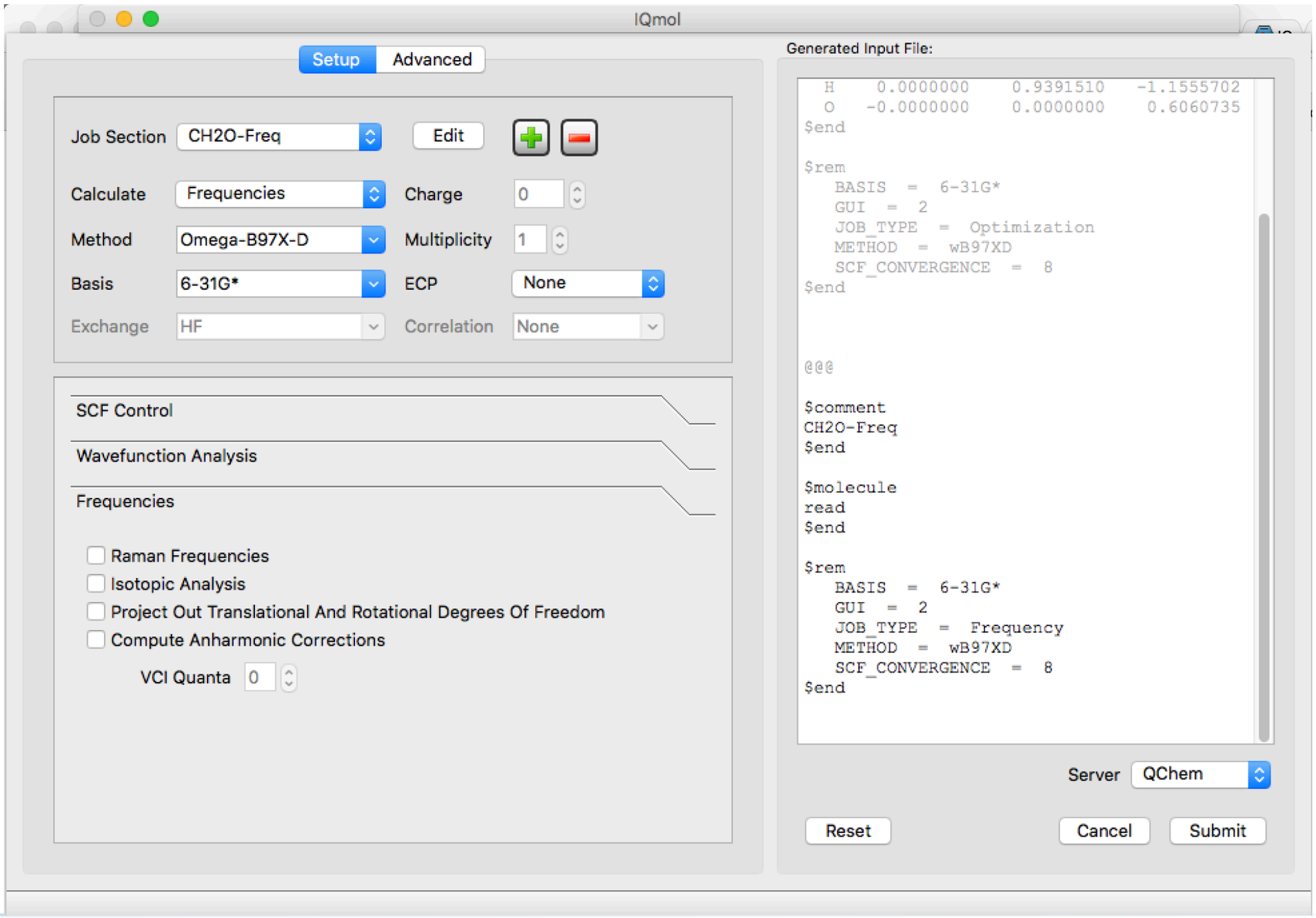




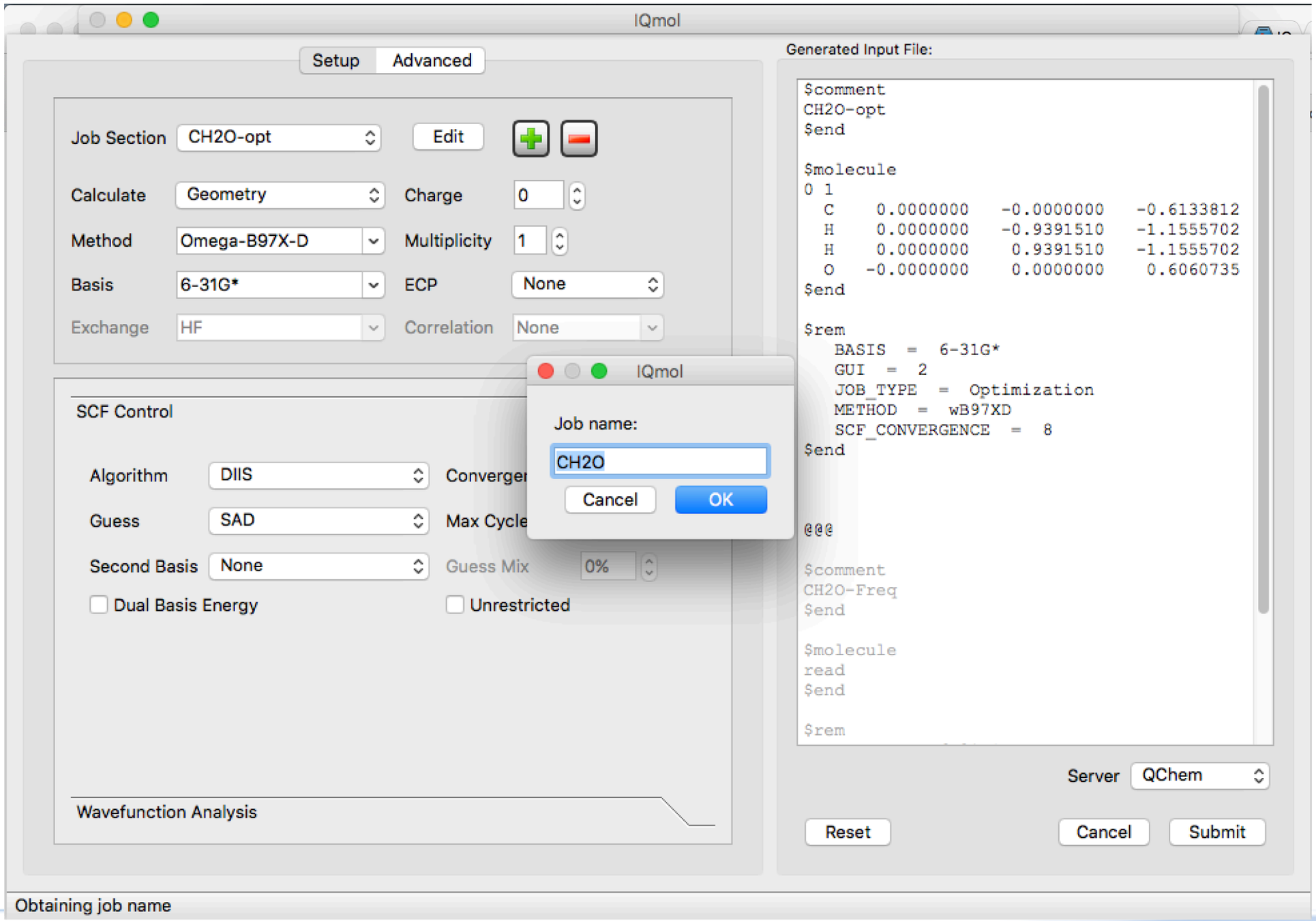
CH_2O Optimization



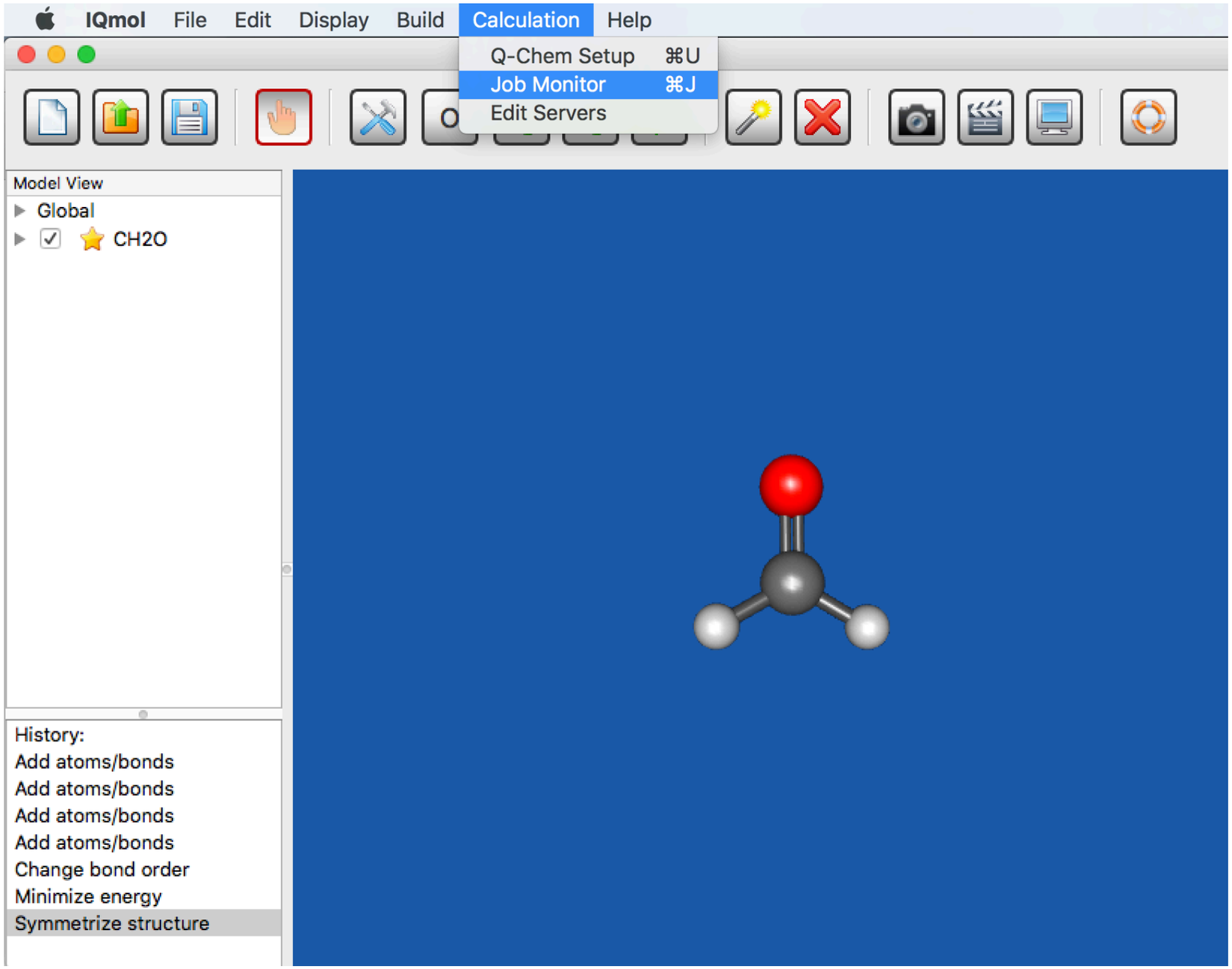
CH_2O Frequency



Submitting job to QChem



Monitoring submitted job



Monitoring submitted job

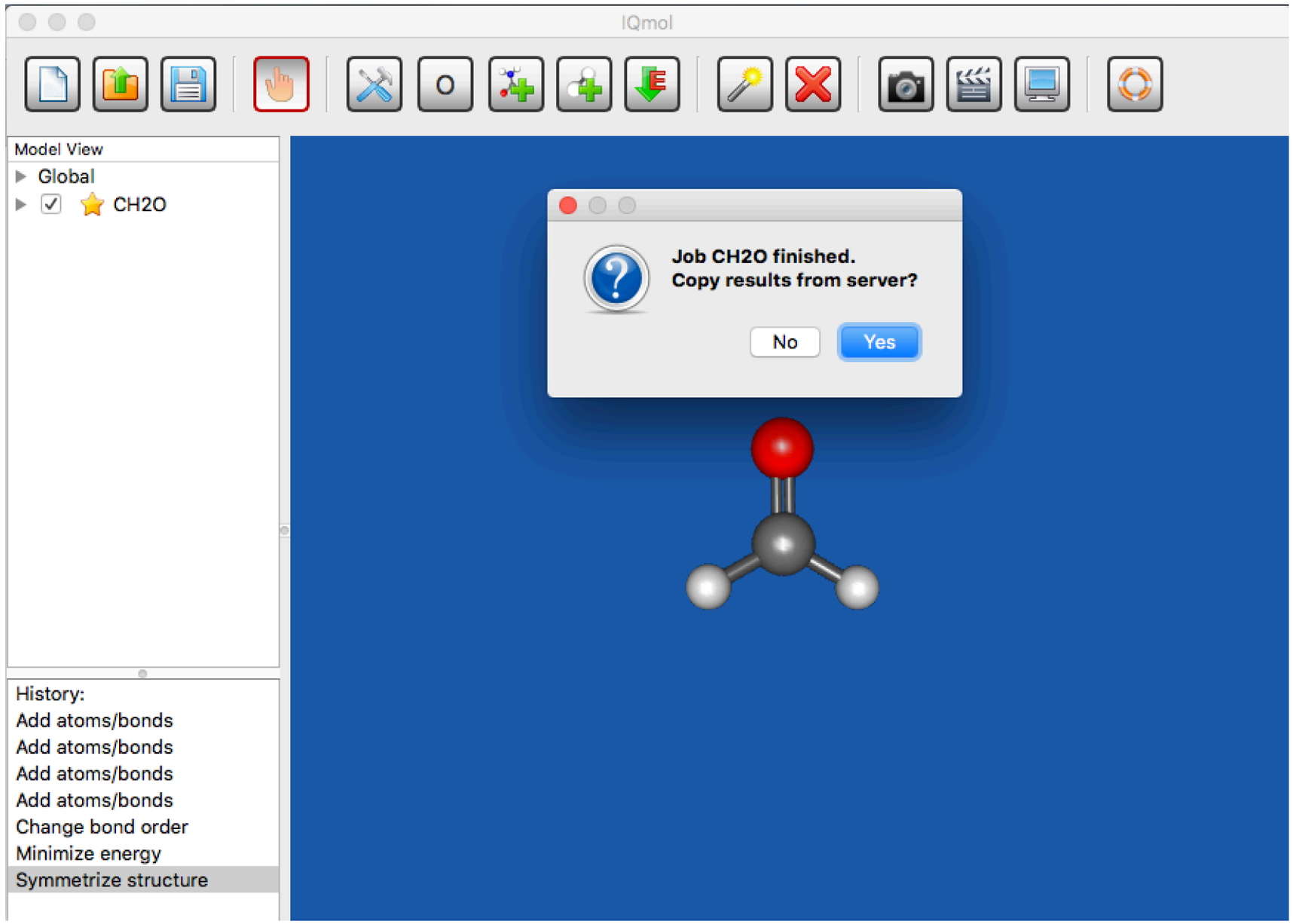
Job Monitor

	Job	Server	Submit Time	Run Time	Status
31	Cr2O7_dichromate	QChem	16:25:39	0:03:27	Finished
32	H2O	QChem	22:08:49	0:01:57	Finished
33	CH2O	QChem	11:20:08	0:00:20	Finished
34	CH2O	QChem	11:23:59		Finished
35	CH2O	QChem	11:25:04		Finished
36	CH2O	QChem	11:26:25		Finished
37	CH2O	QChem	11:26:56		Finished
38	CH2O	QChem	11:28:03		Queued

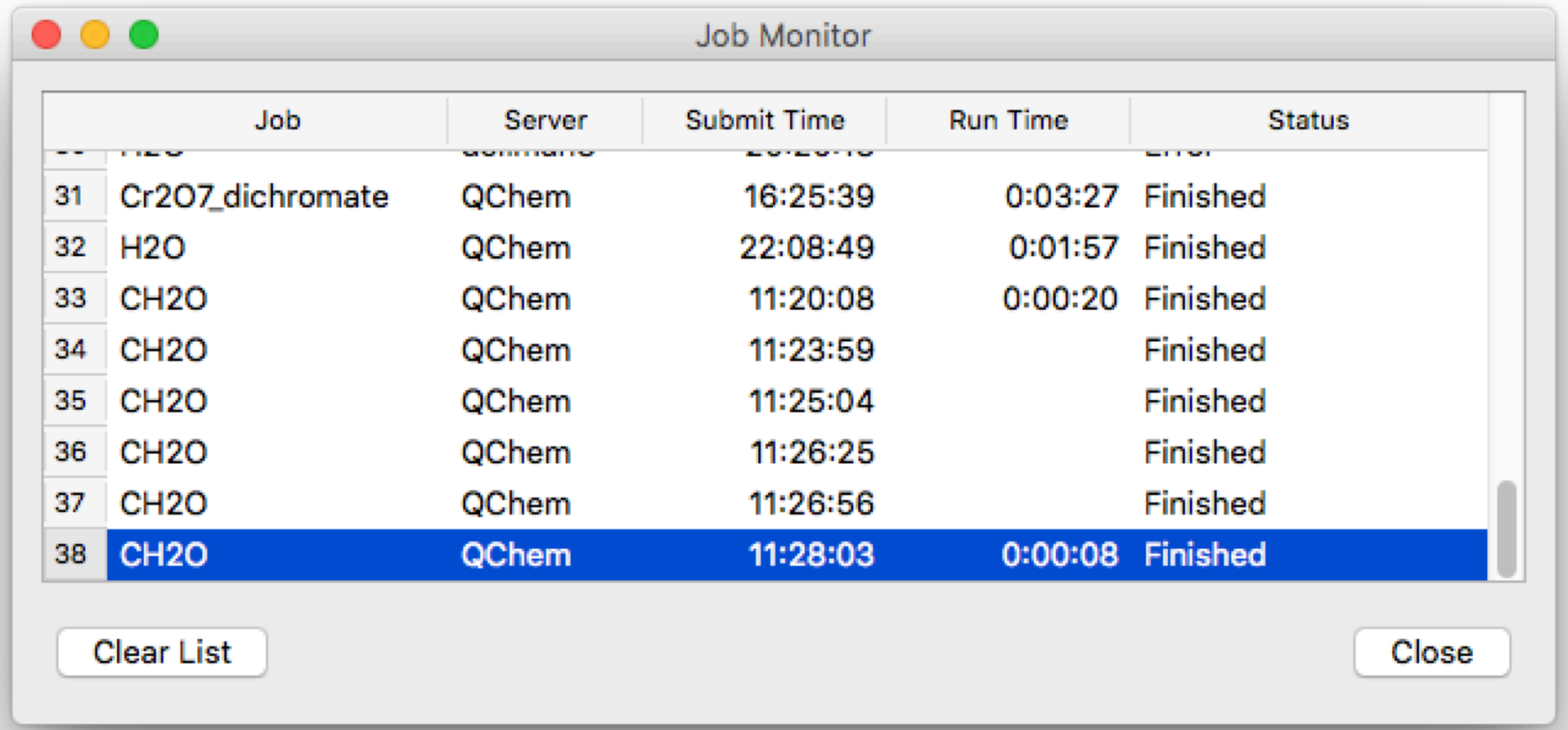
Clear List

Close

Job is finished

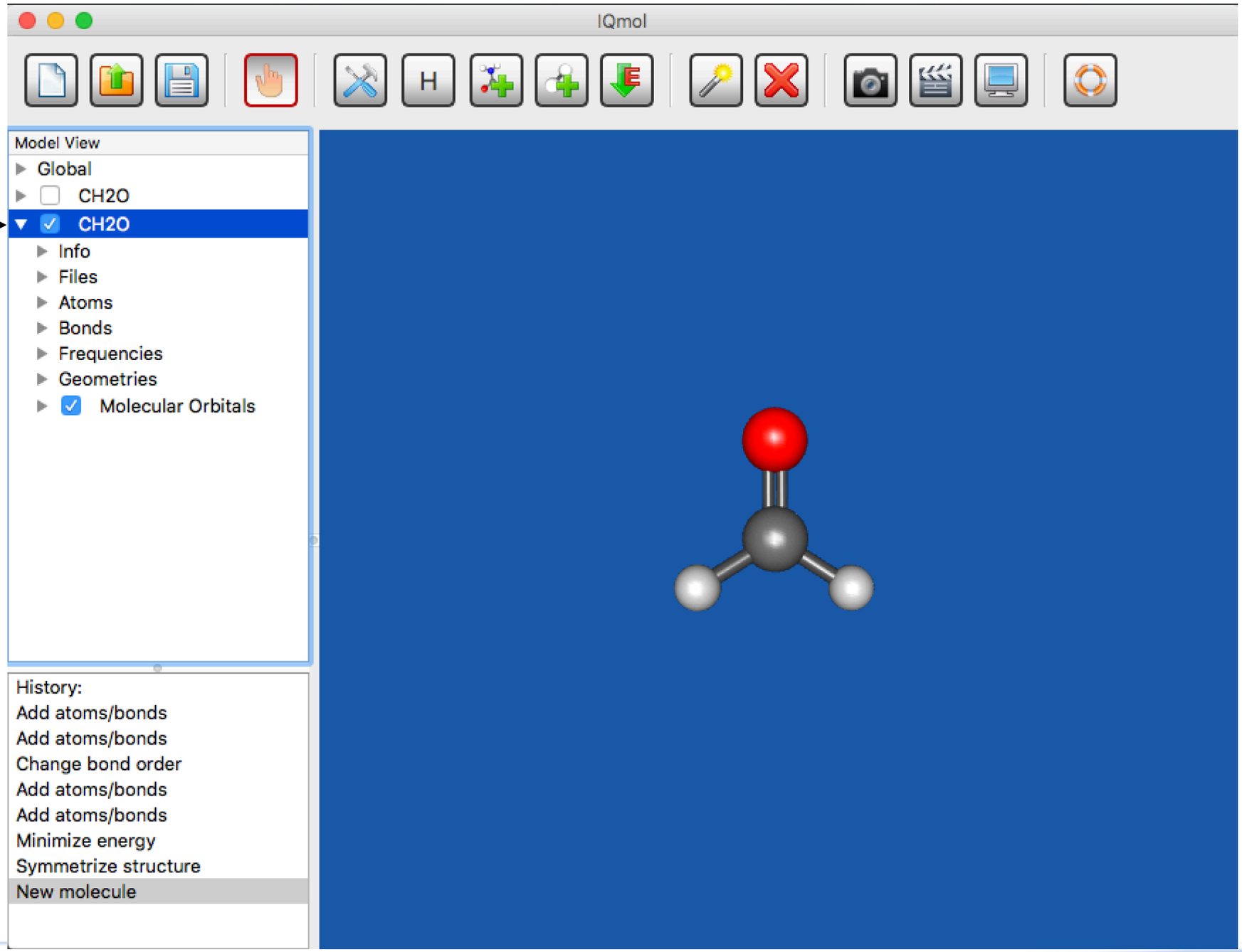


Copy files to your laptop

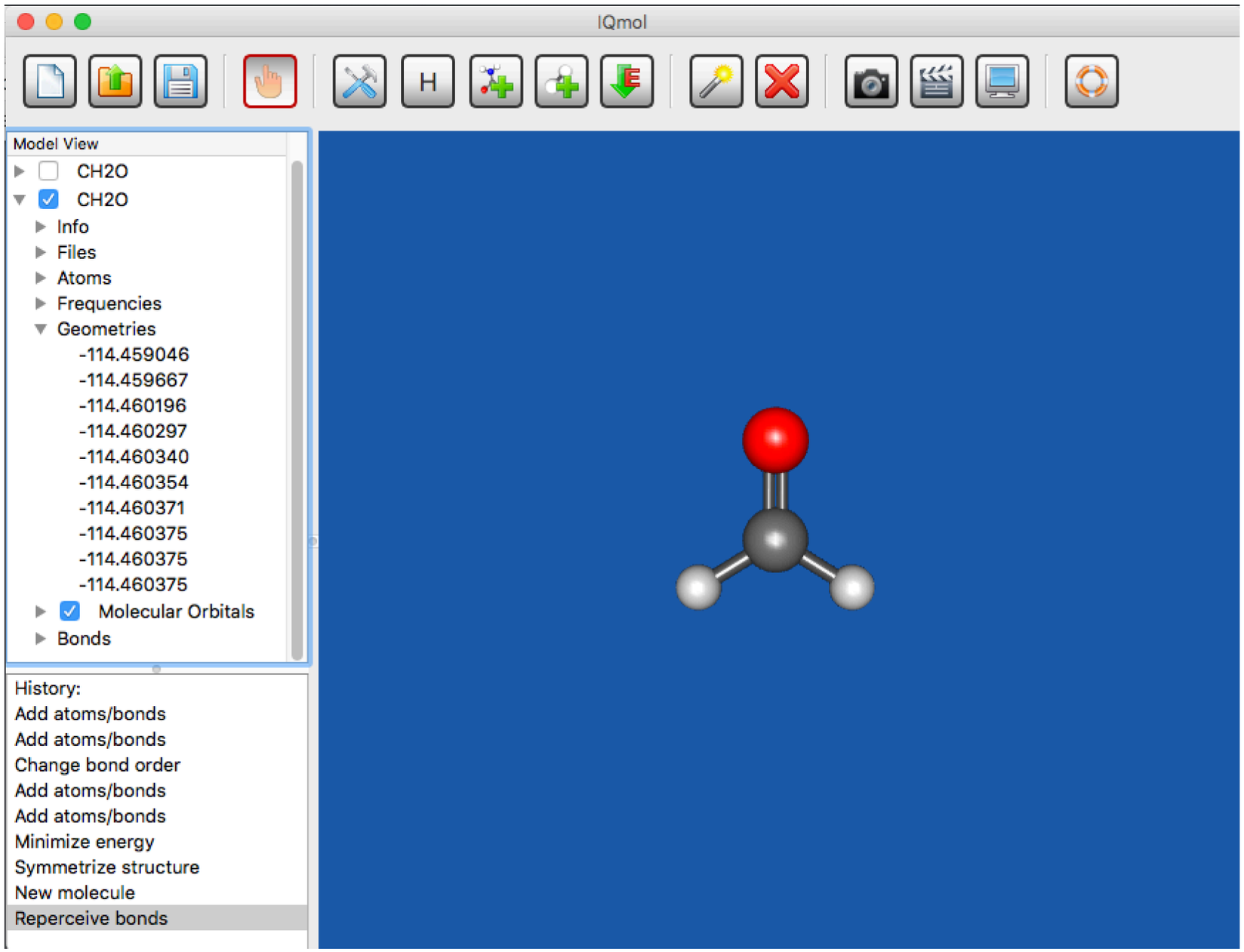


Analyze the output

click checkbox

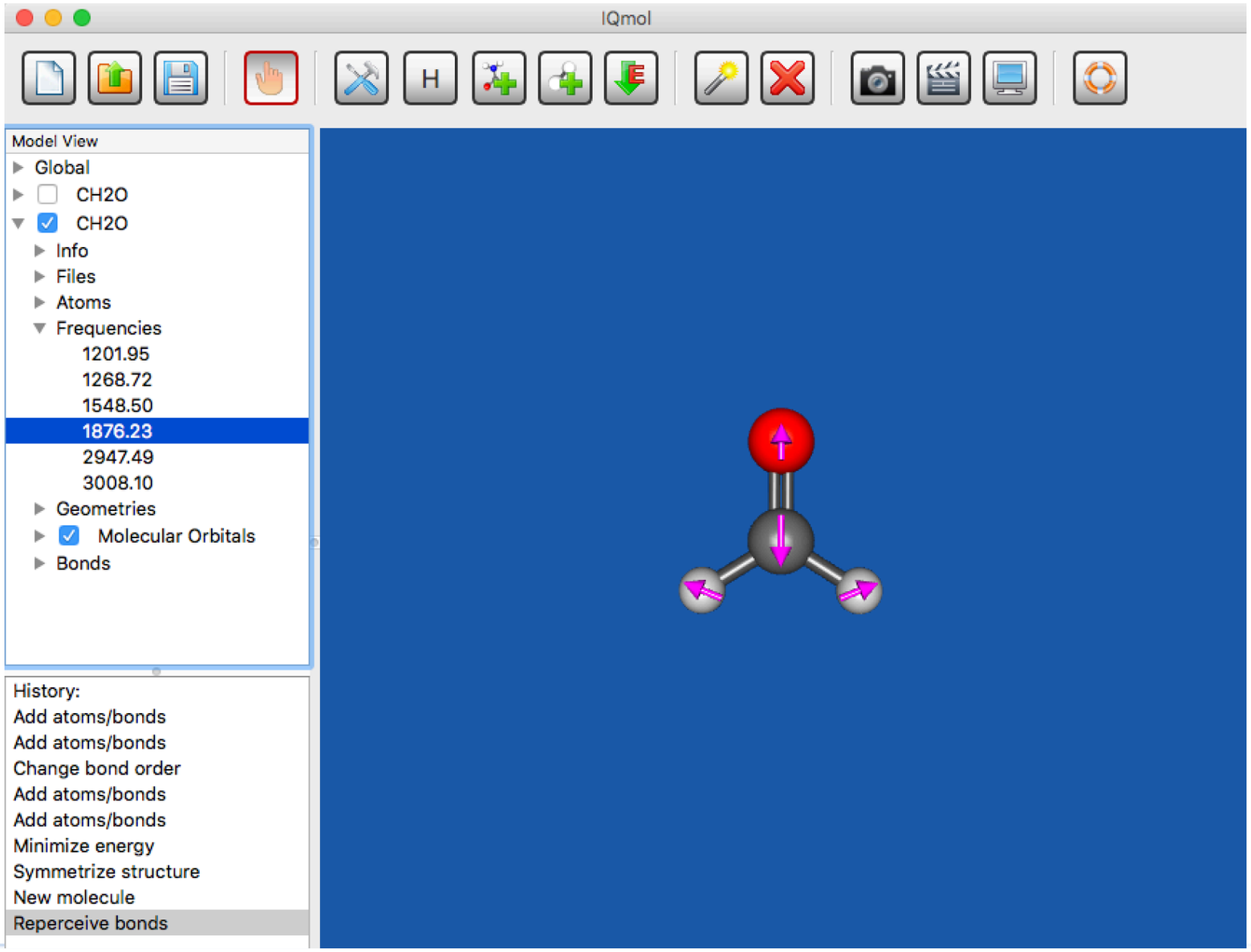


Optimization cycles



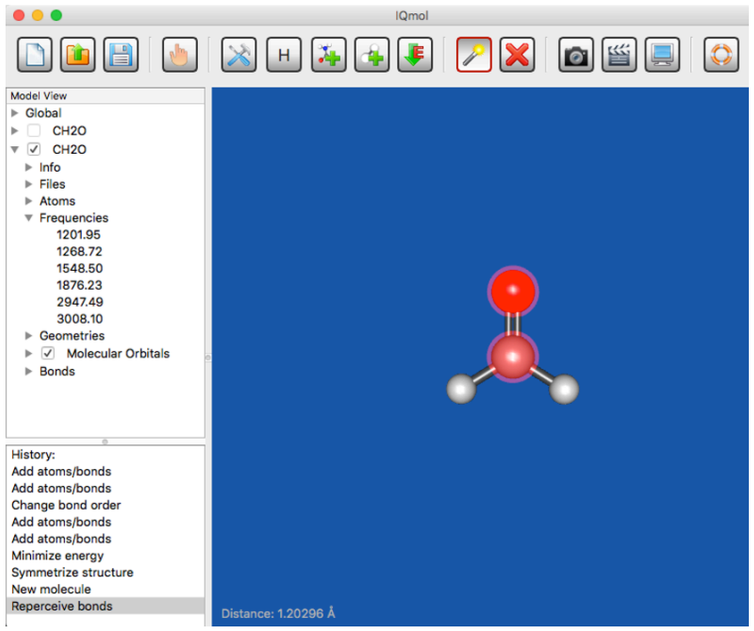
Frequencies

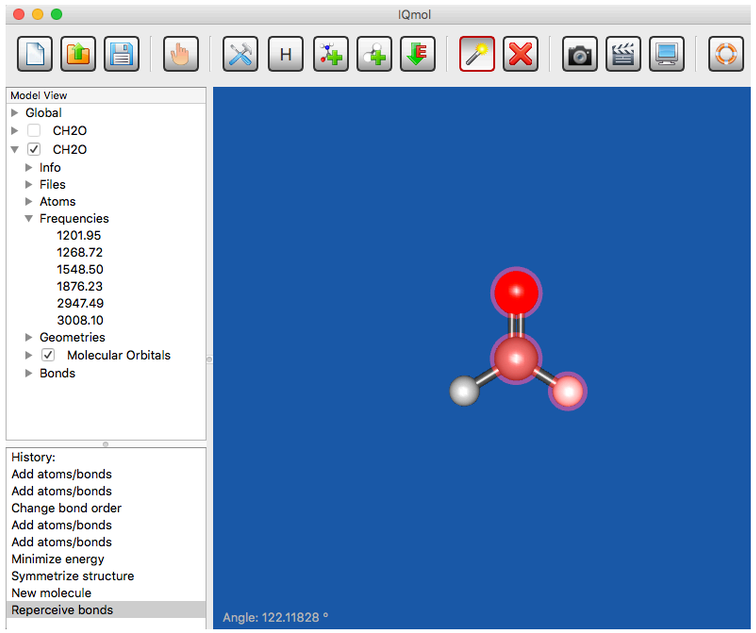
3N-6= 6 vibrational frequency

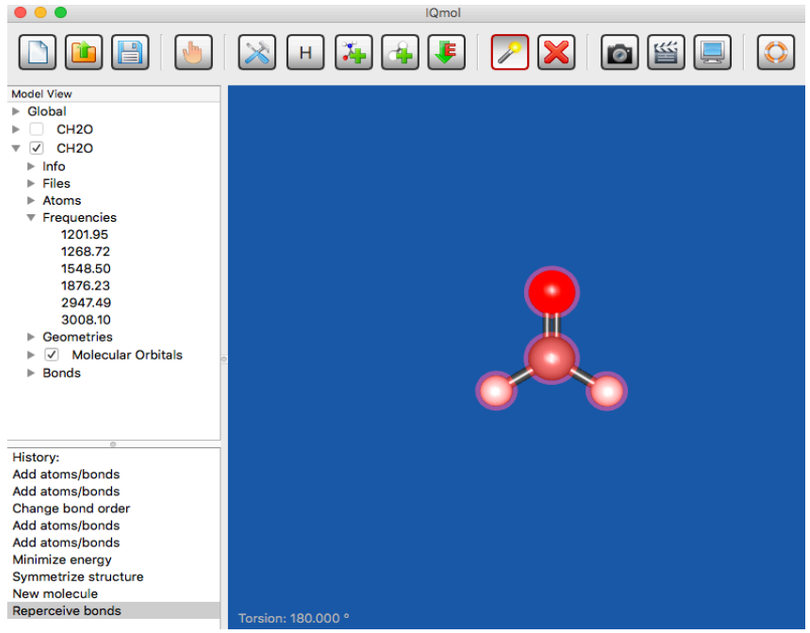


Measuring parameters

- Use “Select” mode to choose a bond, angle, torsion, …

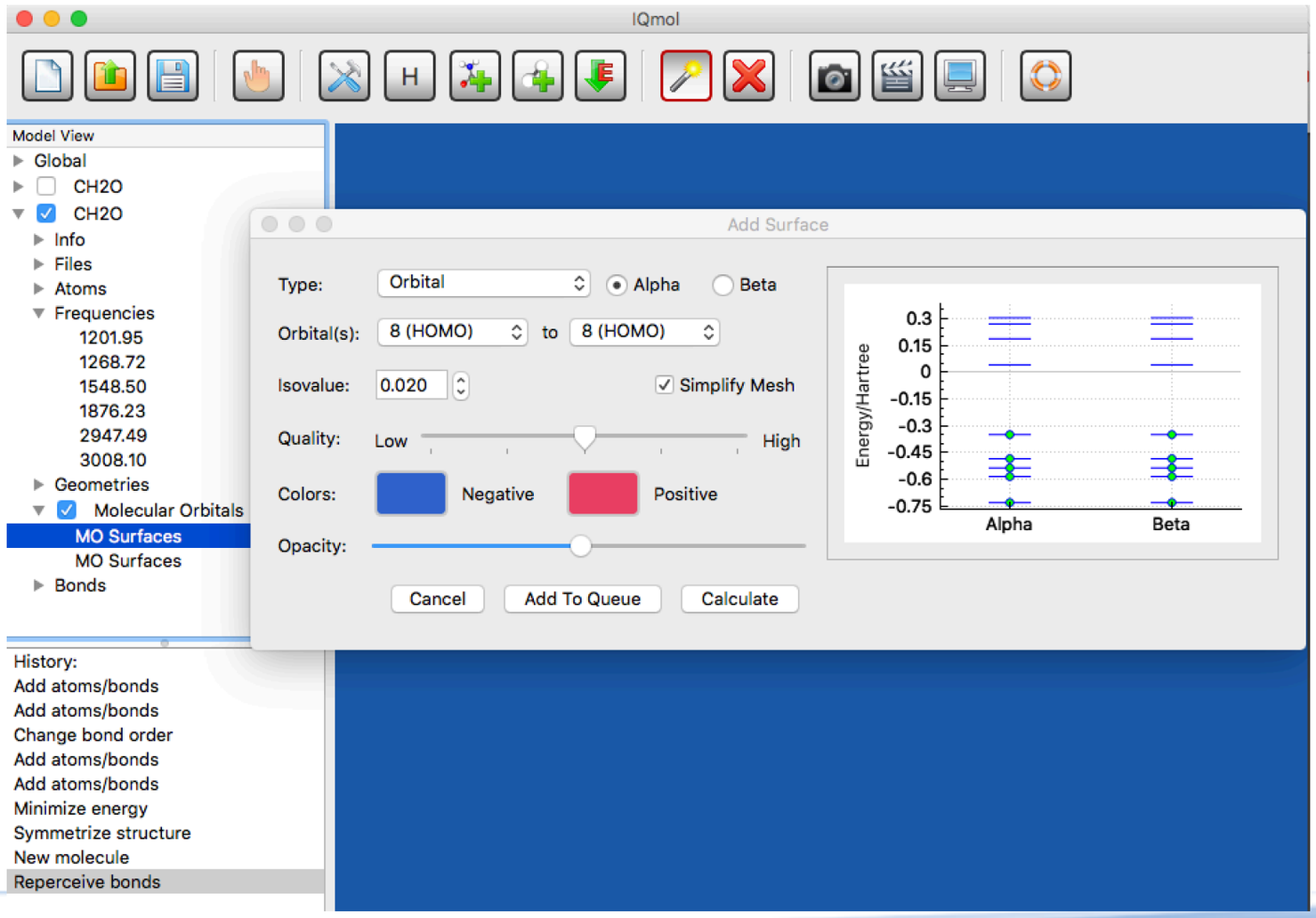






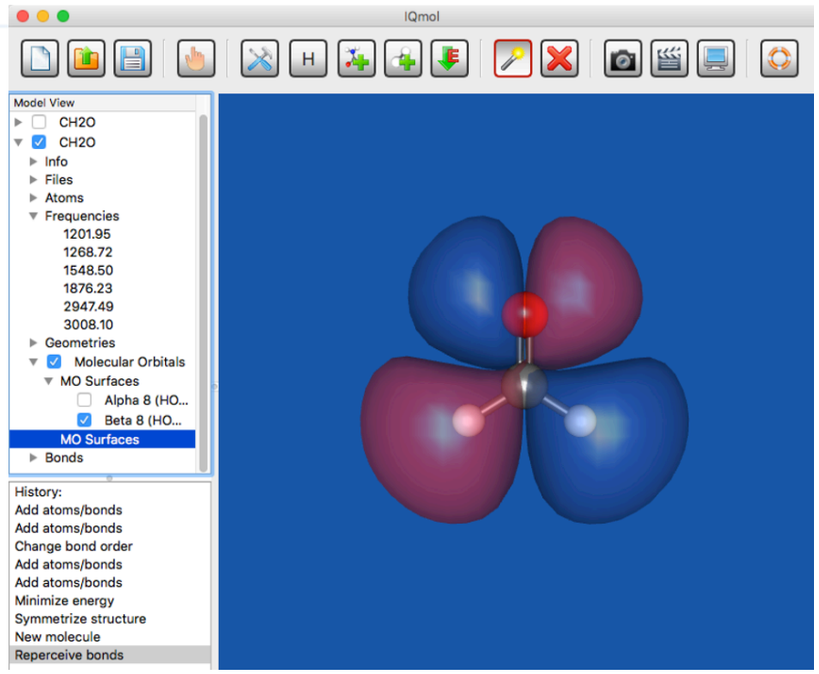
HOMO-LOMO orbitals

- **Must add GUI = 2 in the $ rem section** (IQmol does it by default)
- Open **.Fchk** file to see Orbitals, Density, Spin density and so on.
- Click at **MO Surfaces** and a window will pop up



HOMO-LOMO orbitals

- Select Orbital
- Select the relevant orbital (default: HOMO)
- Select the quality you want
- Click calculate



- Click the arrow next to **Surfaces** to see the orbitals one by one by clicking the checkbox of the corresponding orbital (do not forget to uncheck the old one)
- Use Manipulation Mode to better see the orbital
- To save the screen: **File —> Save Picture**