Introduction to Schrodinger's Software

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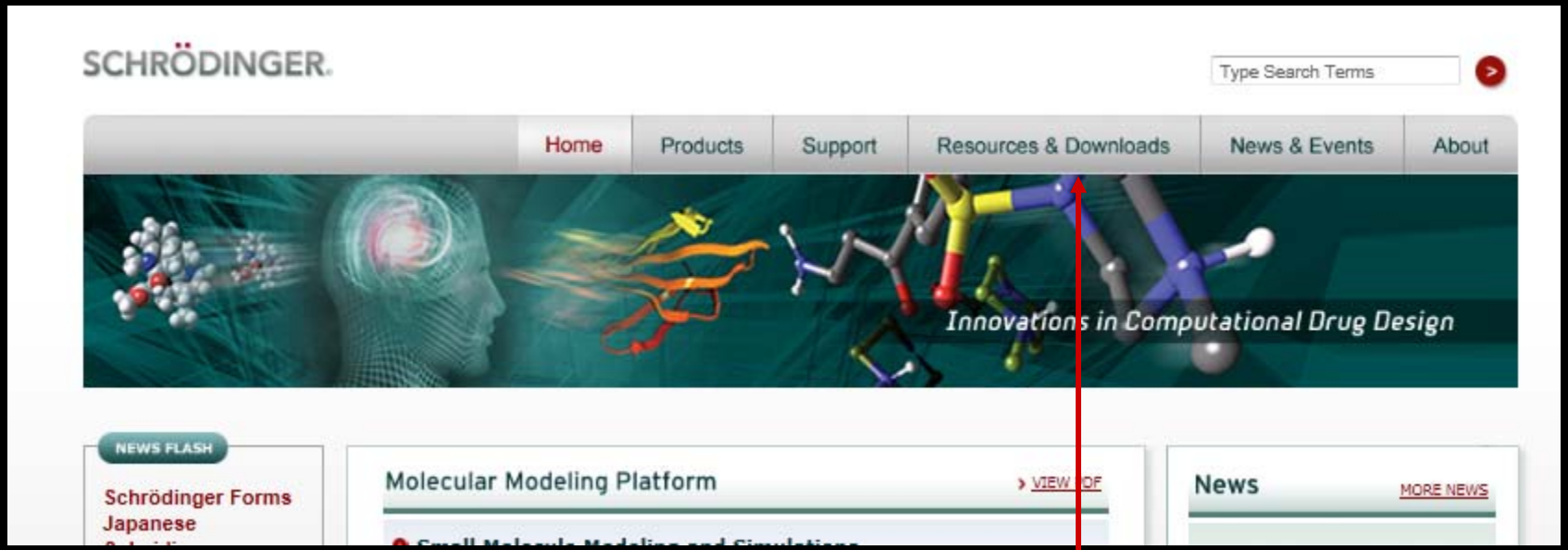
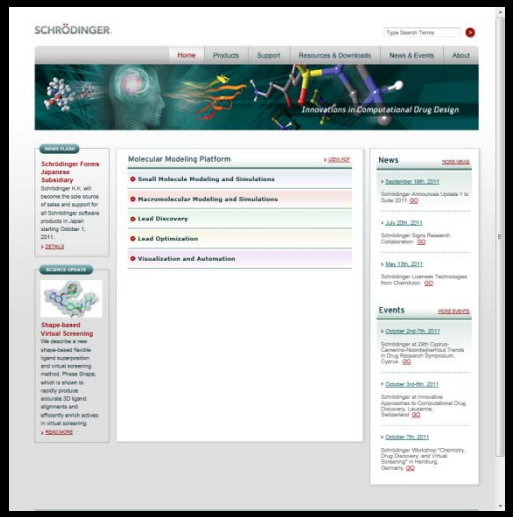
Center for Drug Design
University of Minnesota
MSI Fall Tutorial 2011

Outline

- Software
- Usage

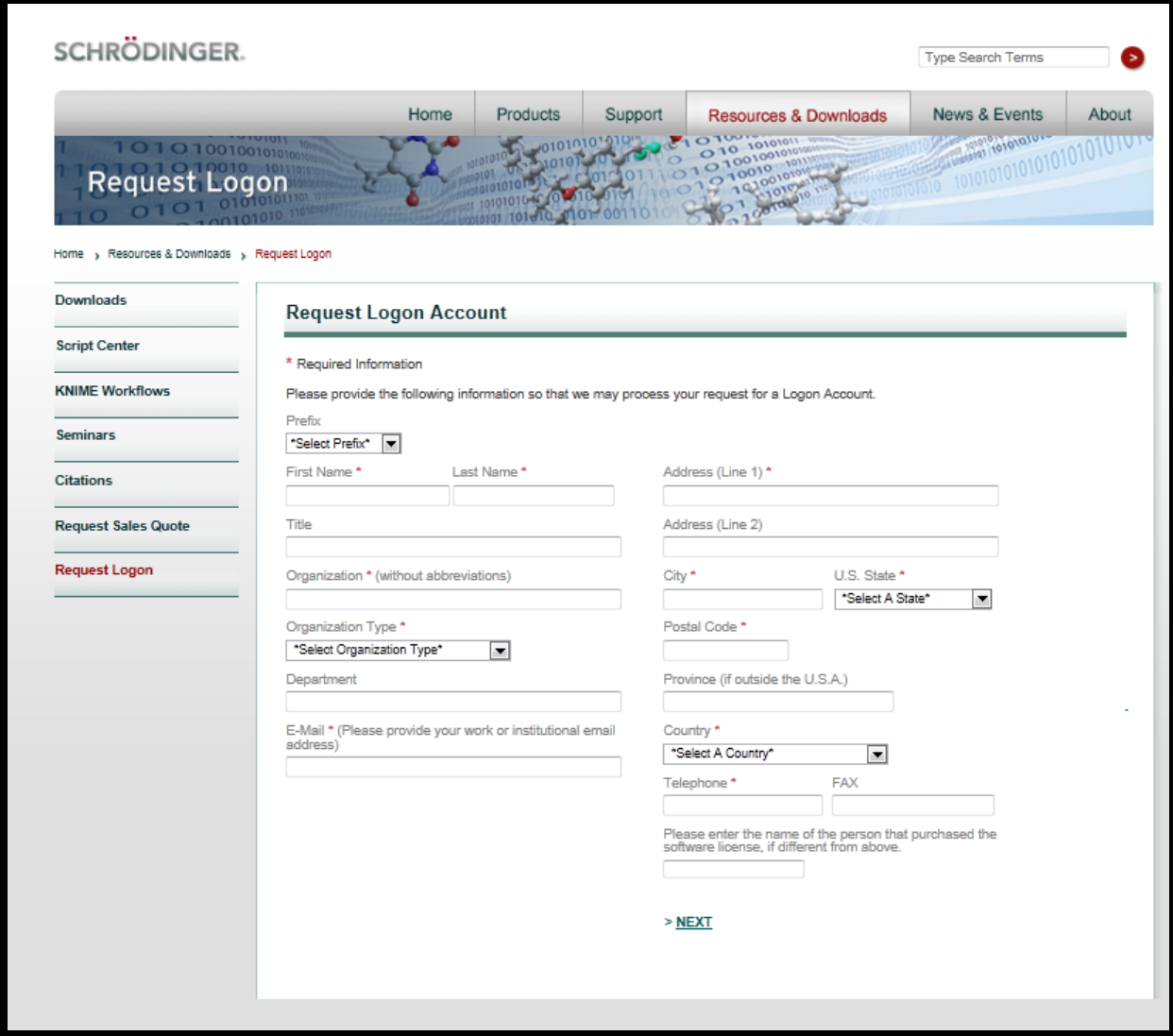
www.schrodinger.com





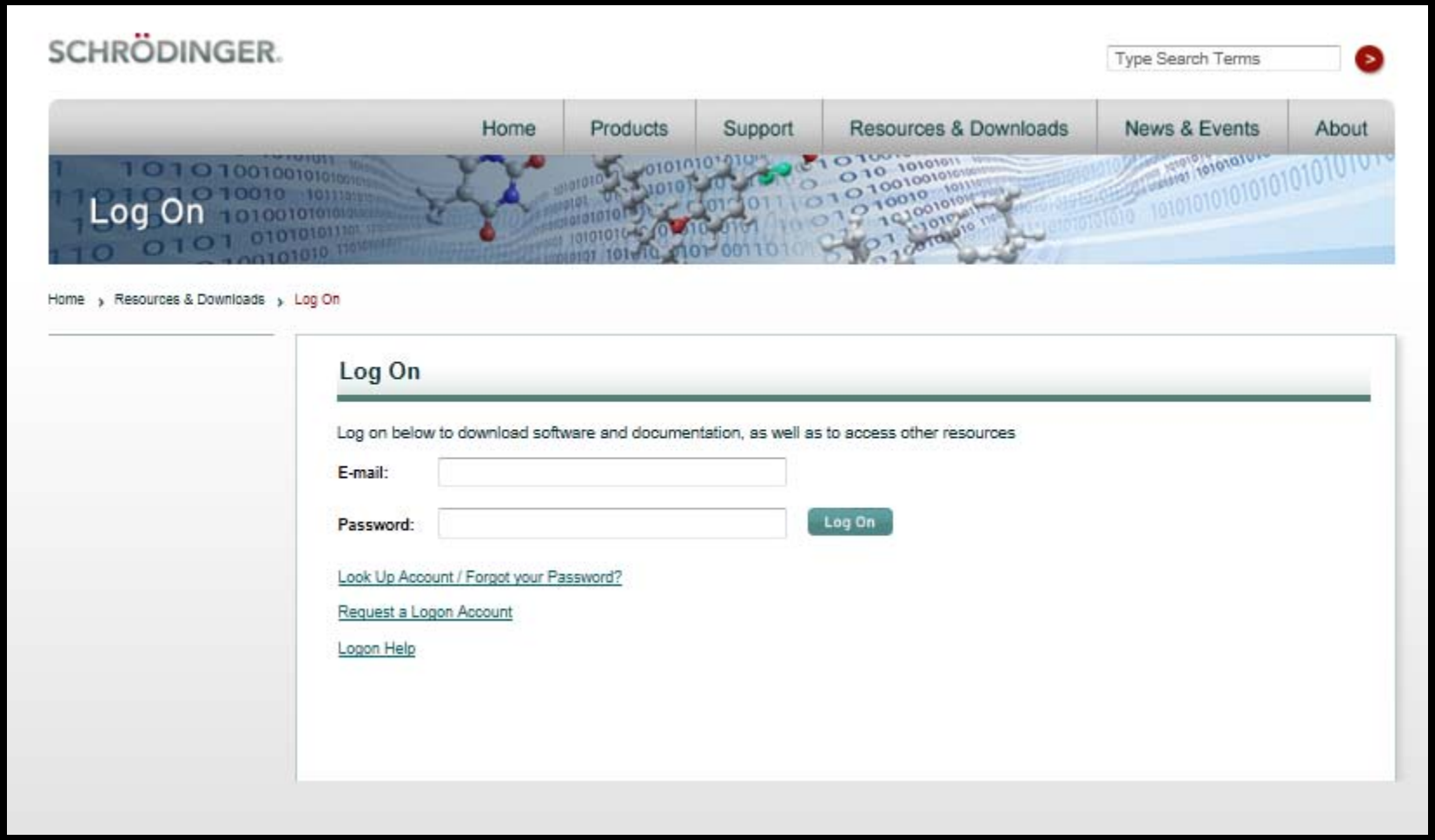
Create you own log in
to download documentation
and tutorials

Registering



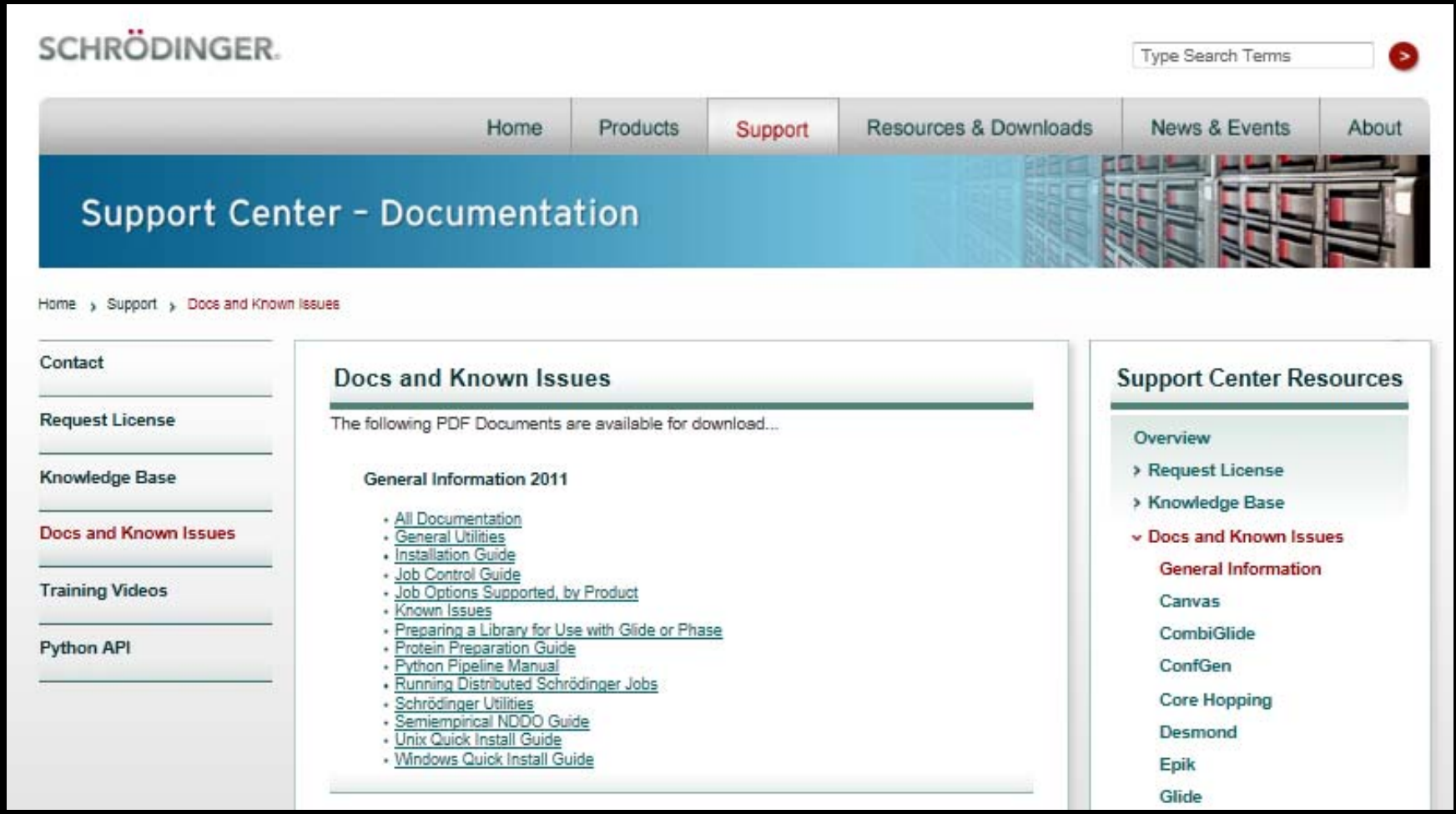
http://www.schrodinger.com/UserInformation.php

Log on



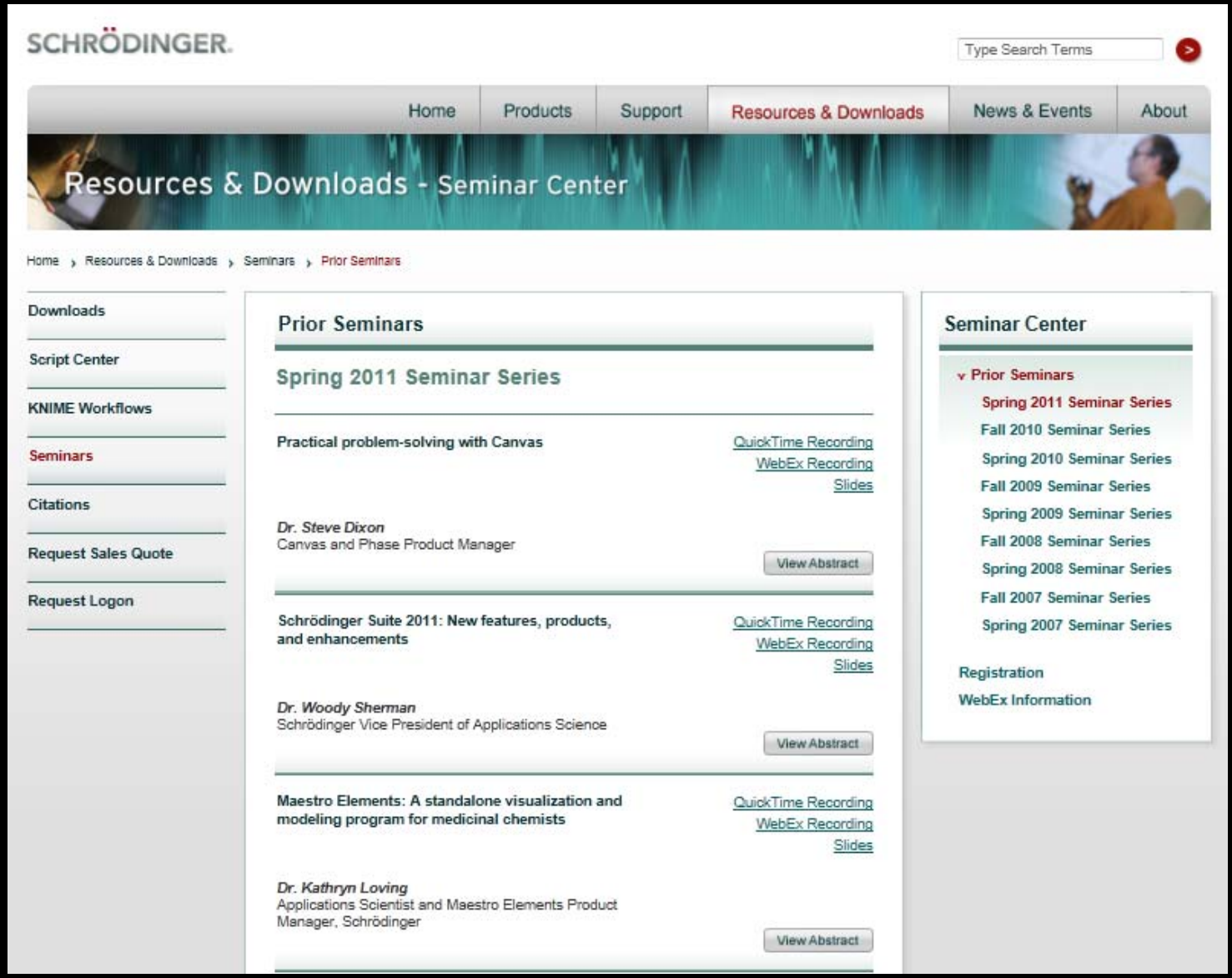
http://www.schrodinger.com/CustomerLogon.php

Documentation



http://www.schrodinger.com/supportdocs/18/

Other presentations



http://www.schrodinger.com/seminarprior/19/

On-line support

help@schrodinger.com

Software

CombiGlide – Combinatorial Library Design

Glide – Ligand Docking

Impact – Molecular Dynamics Simulation

Induced Fit – Ligand Docking

Jaguar – Quantum Mechanics

Liaison – Predicts Binding Affinity

LigPrep – 2D to 3D Ligand Conversion Tool

Software

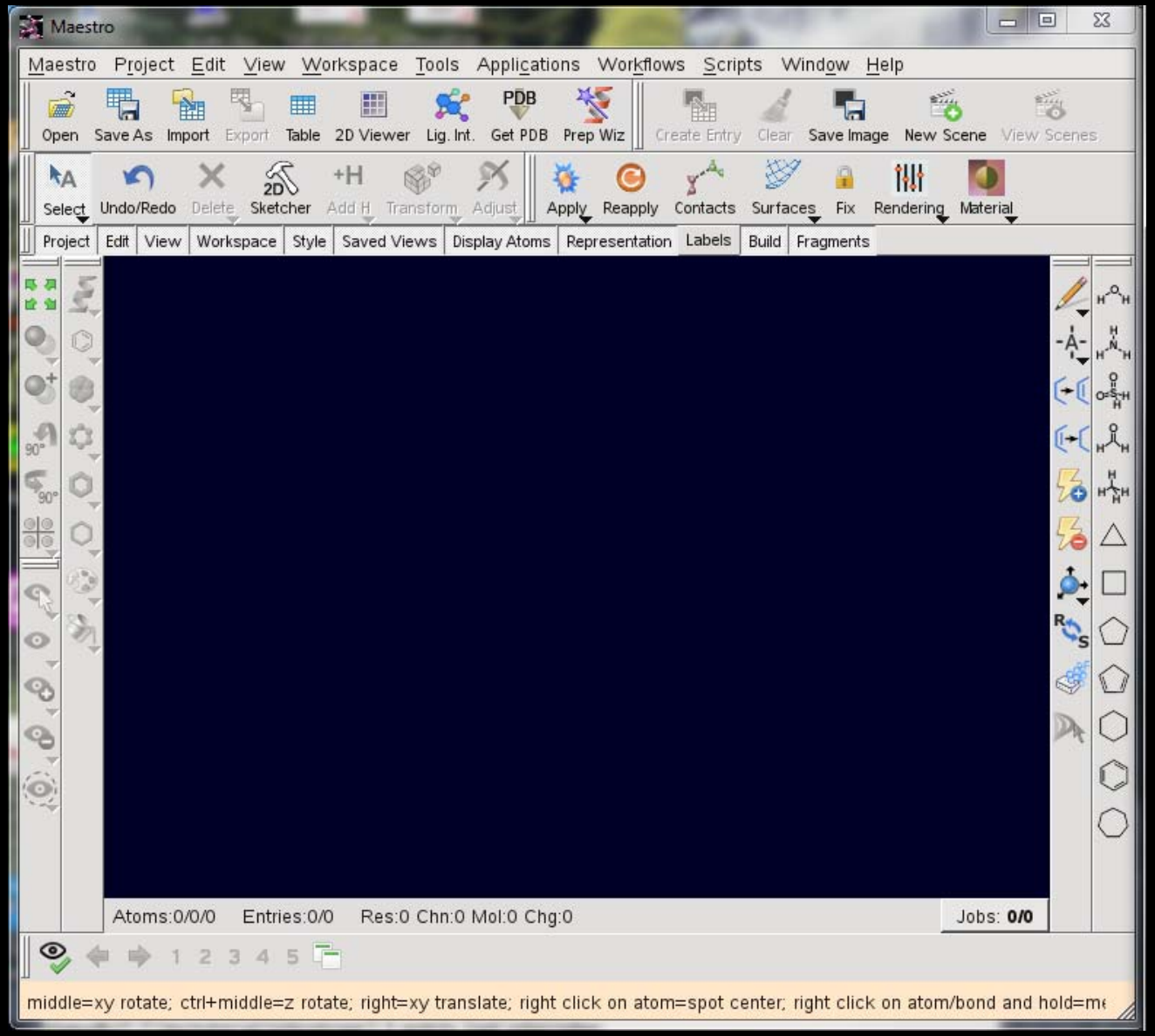
- MacroModel – Molecular Modeling
- Maestro – Graphical User Interface
- Phase – Pharmacophore Modeling
- Prime – Protein Structure Prediction
- QikProp – ADME Properties
- Qsite – Reaction Mechanism (QM/MM)
- Strike – Structural Activity Relationship

Running Maestro

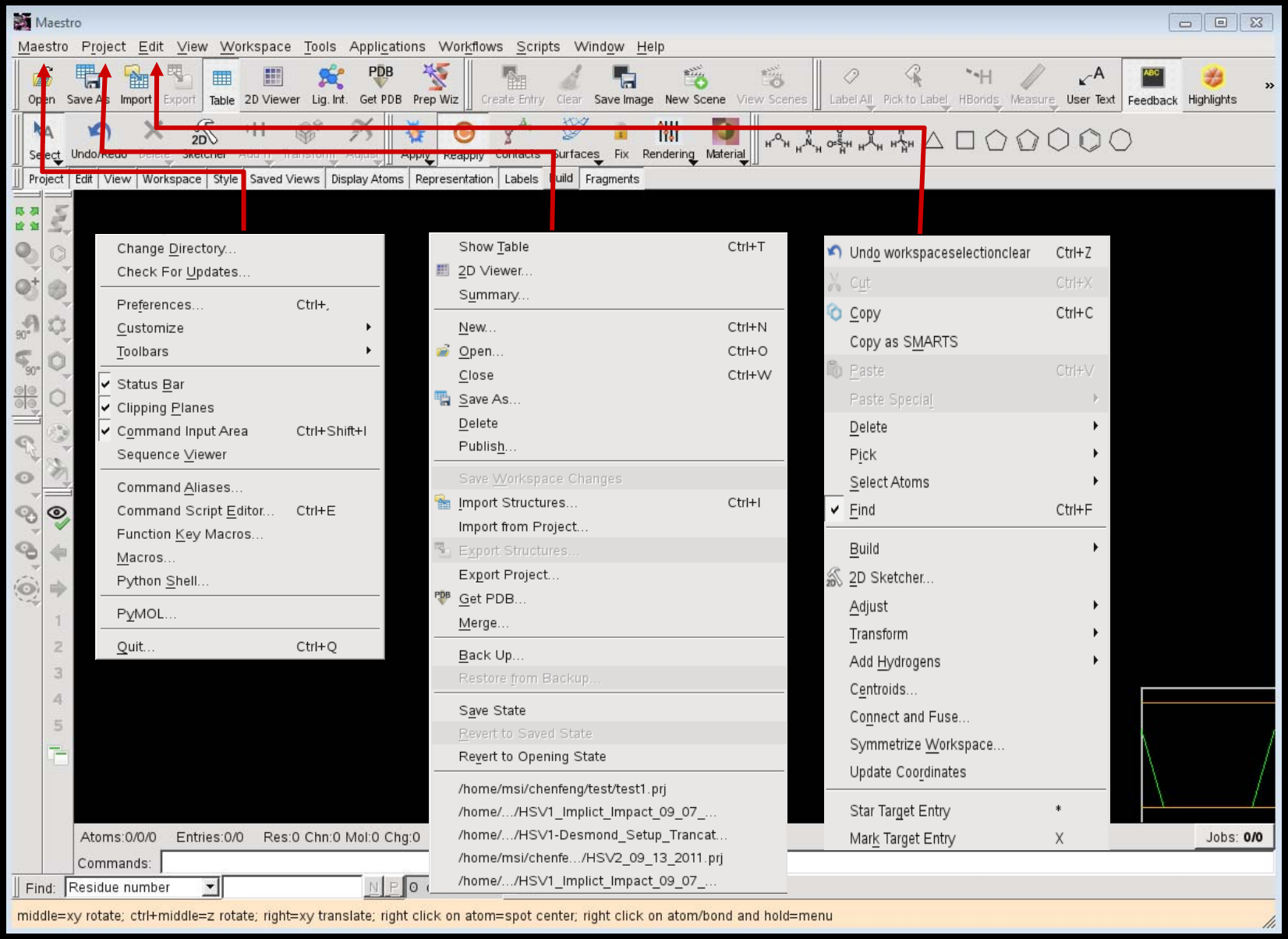
module load schrodinger

maestro

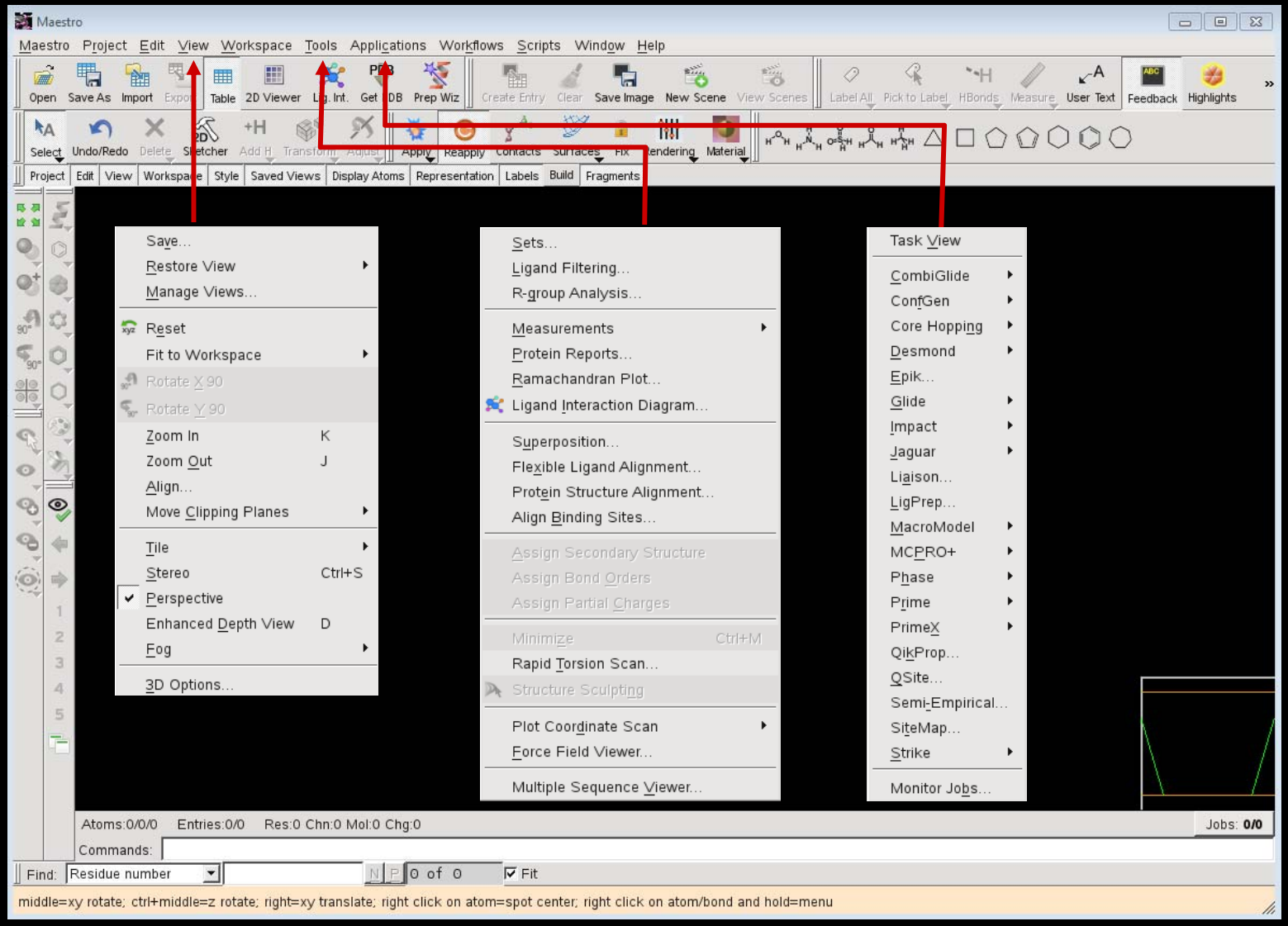
Maestro


Maestro
Maestro Project Edit View Workspace Tools Applications Workflows Scripts Window Help
Open Save As Import Export Table 2D Viewer Lig. Int. Get PDB Prep Wiz
Create Entry Clear Save Image New Scene View Scenes
Select Undo/Redo Delete Sketcher Add H Transform Adjust
Apply Reapply Contacts Surfaces Fix Rendering Material
Project Edit View Workspace Style Saved Views Display Atoms Representation Labels Build Fragments
Atoms:0/0/0 Entries:0/0 Res:0 Chn:0 Mol:0 Chg:0
Jobs: 0/0
1 2 3 4 5
middle=xy rotate; ctrl+middle=z rotate; right=xy translate; right click on atom=spot center; right click on atom/bond and hold=me

Maestro Pull-downs



Maestro Pull-downs



You and Your Mouse

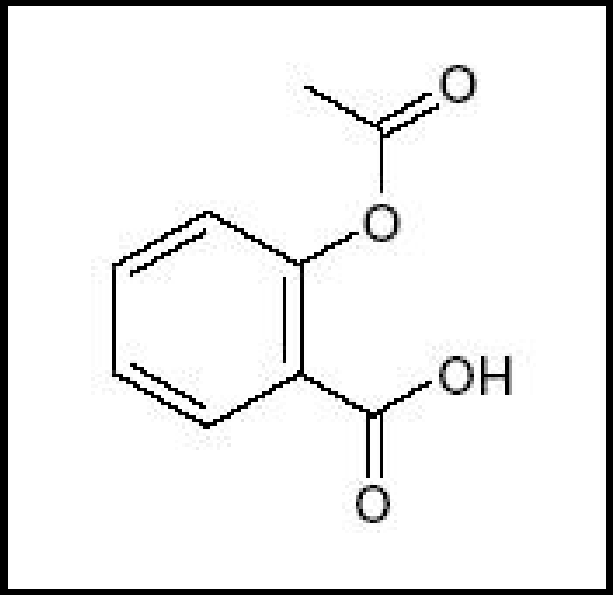
Left button click on atom to select atom. Hold down left button and drag to select a group of atoms

Hold down middle button and move the mouse to rotate

Hold down right button and move the mouse to translate

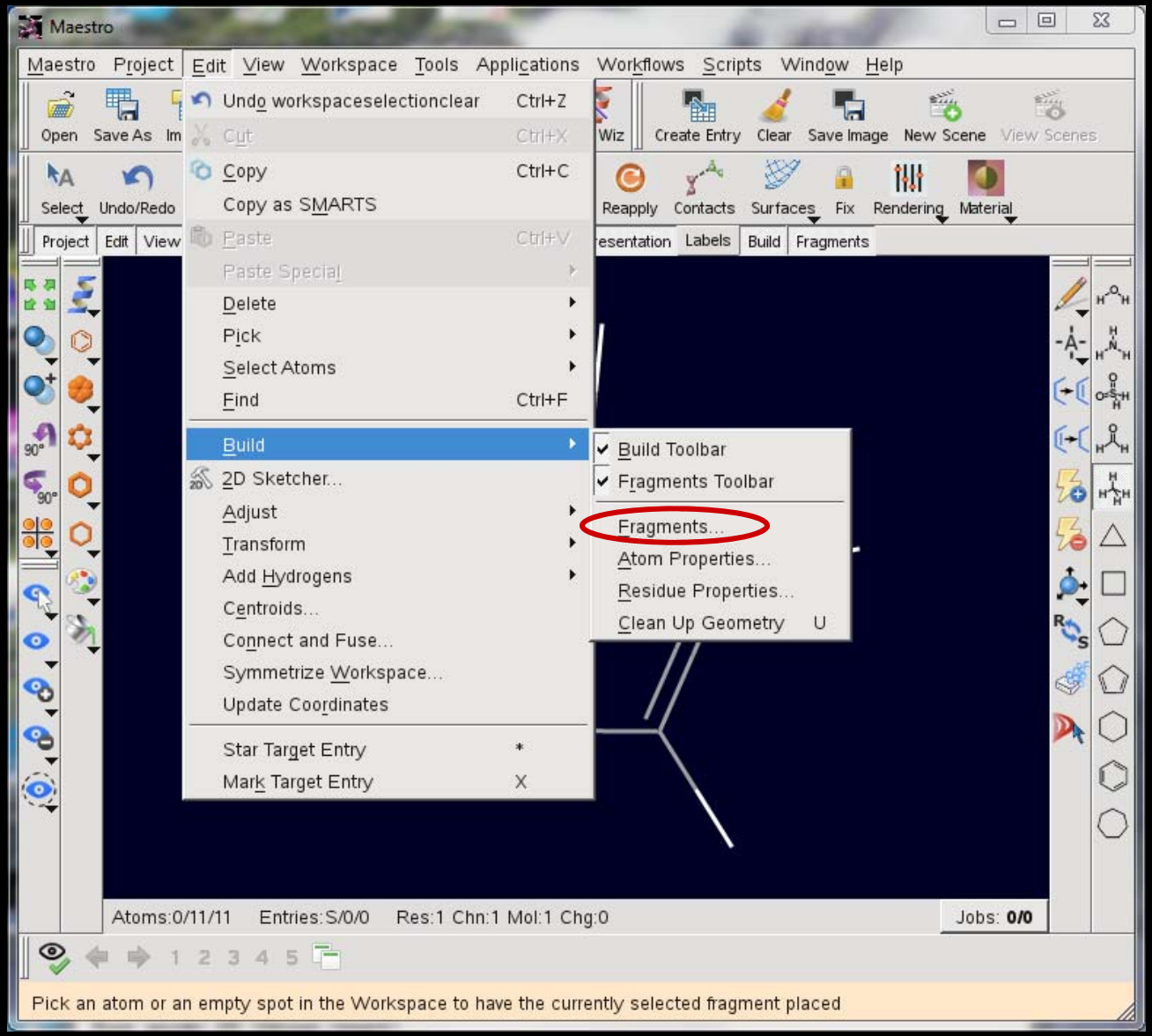
Hold down left and right buttons together and move the mouse to zoom

Sketch Molecules

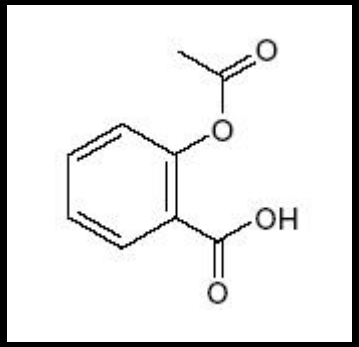


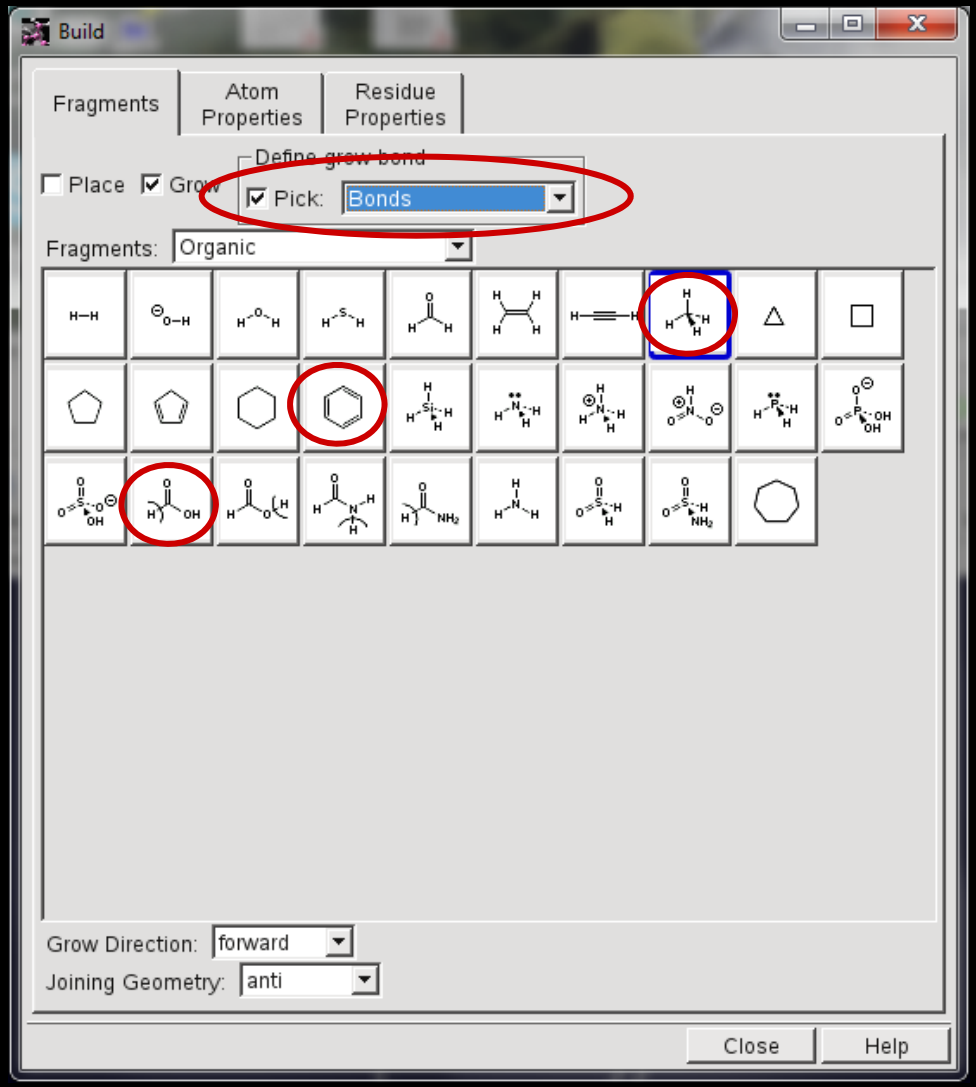
Aspirin or acetylsalicylic acid

Sketch Molecules

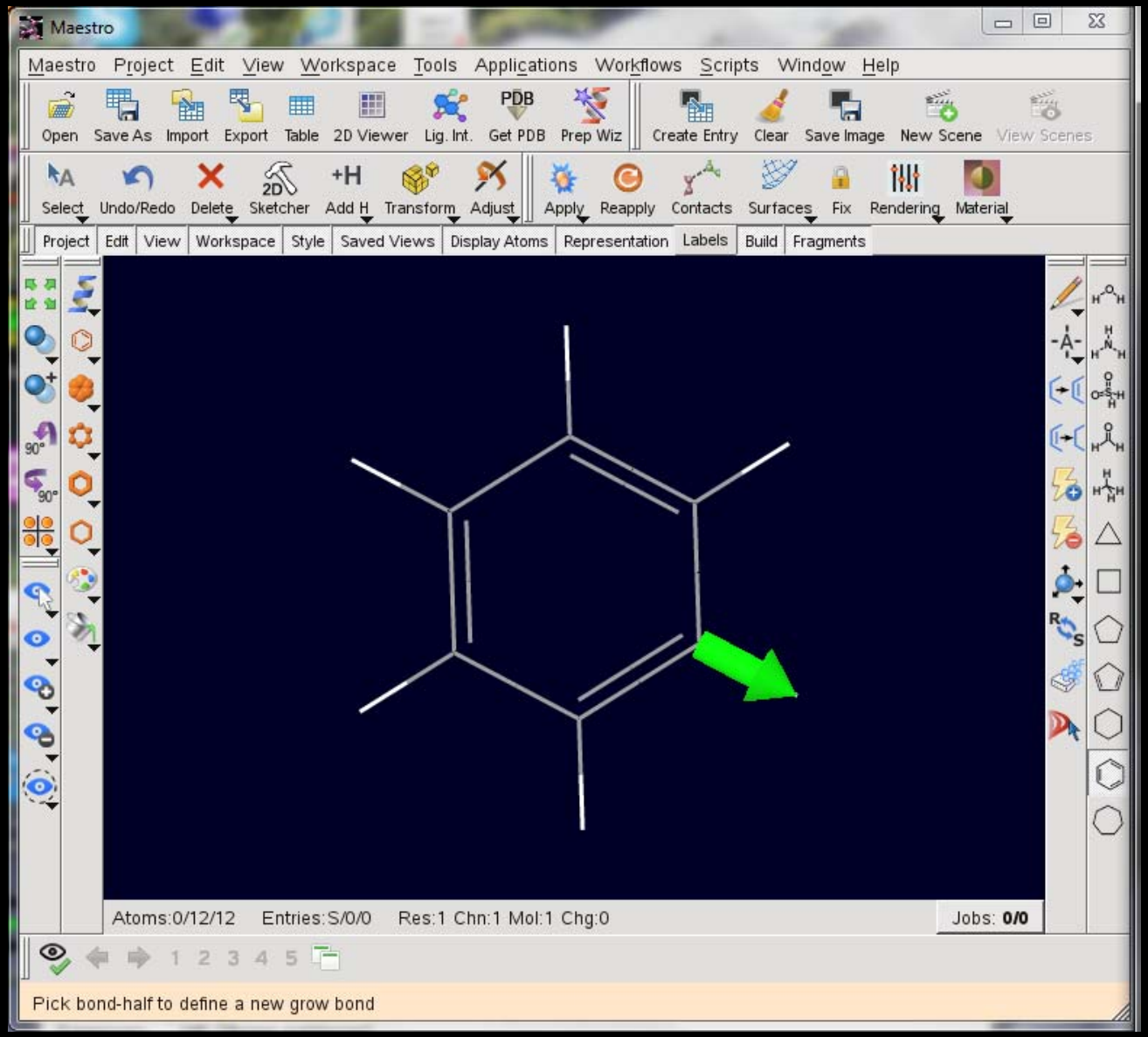


Sketch Molecules

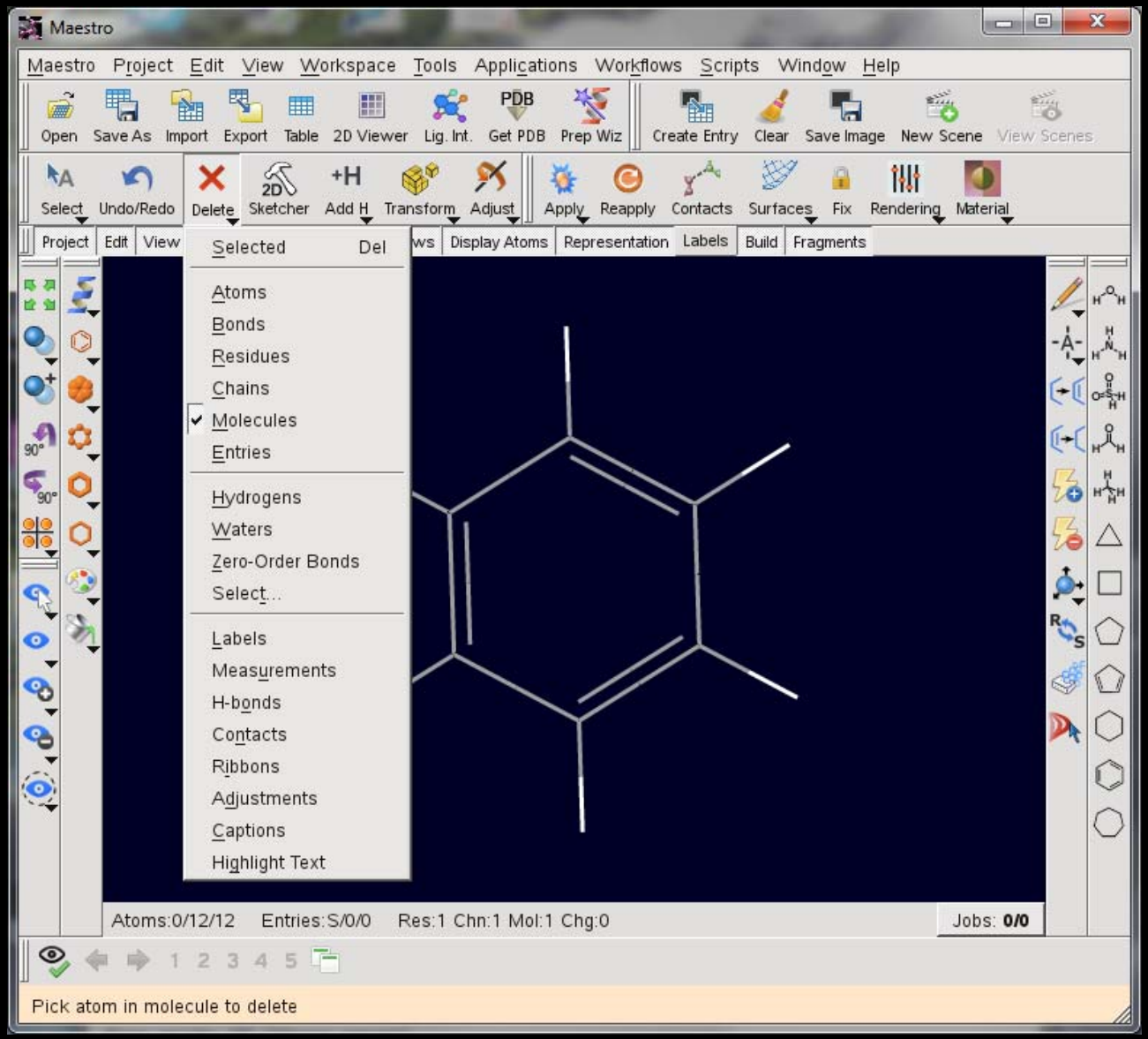




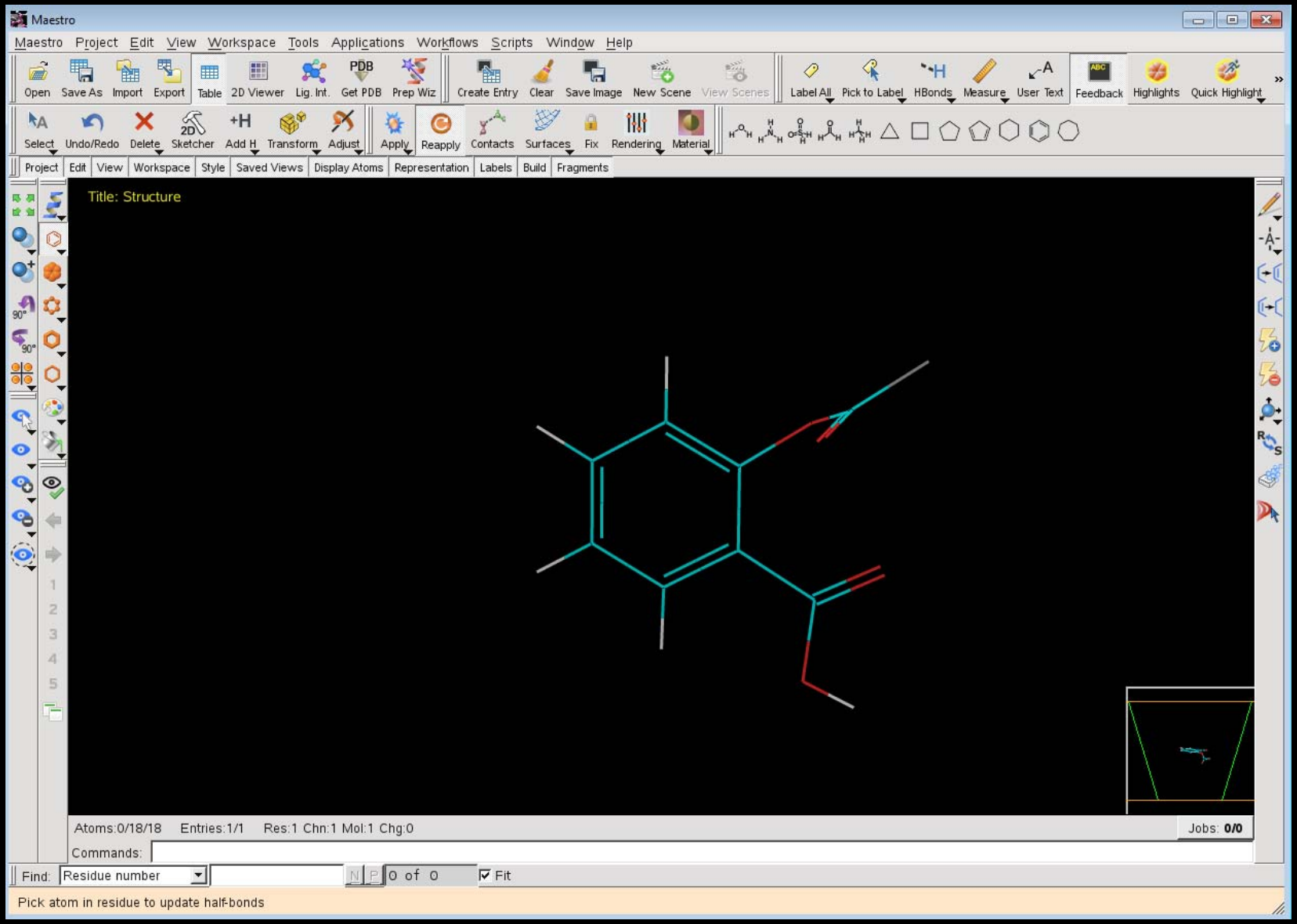
Sketch Molecules



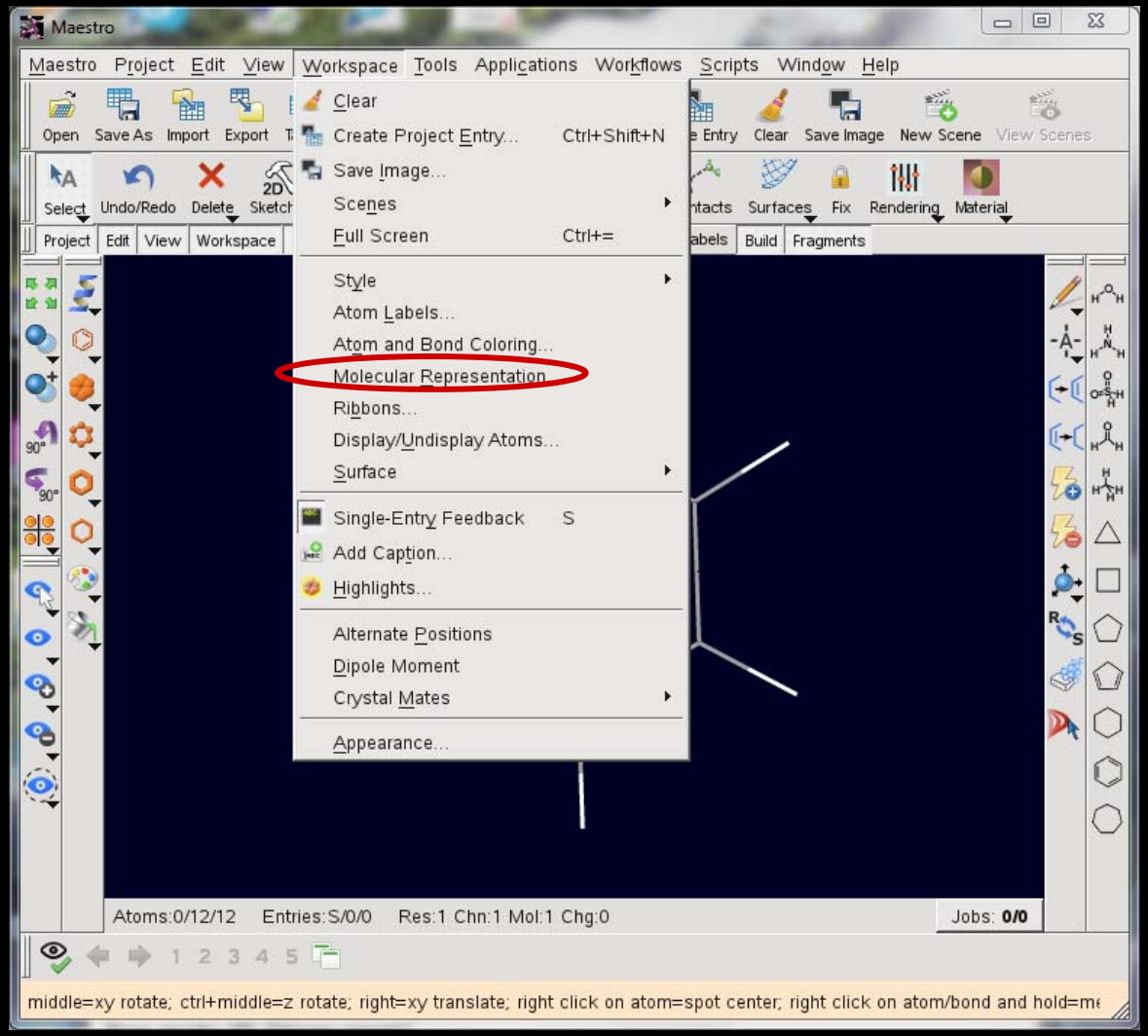
Delete Atoms or Molecules



Sketch Molecules

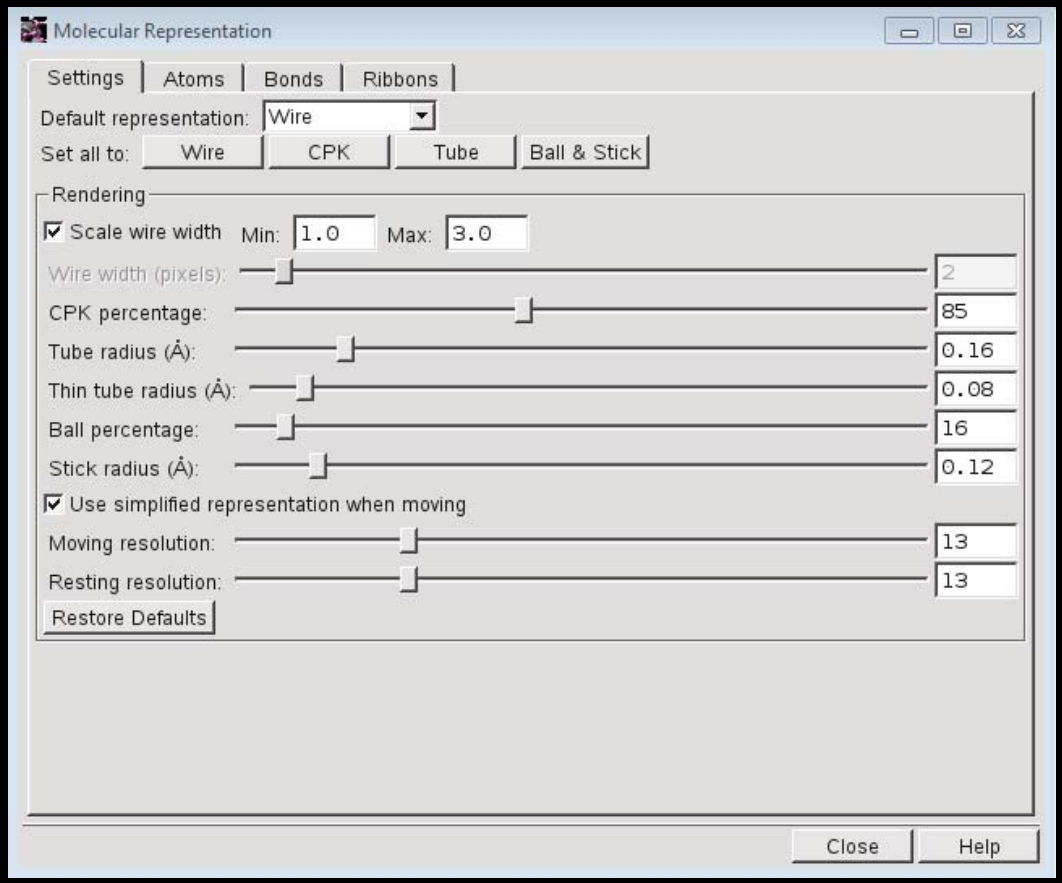


Molecular Representation



Workspace / Molecular Representation

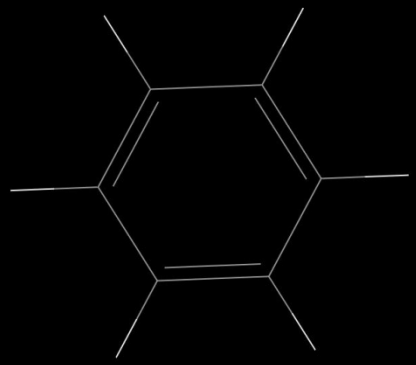
Molecular Representation



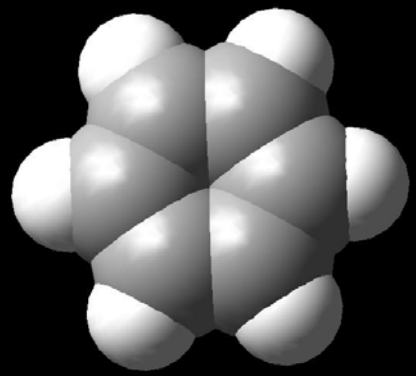
Workspace / Molecular Representation

Molecular Representation

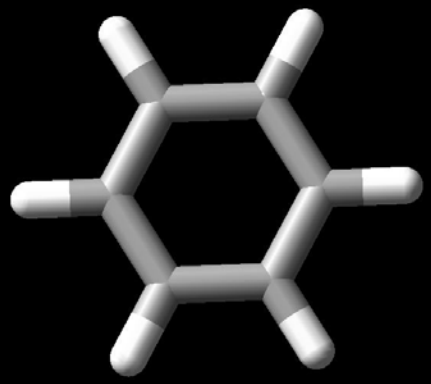
Wire



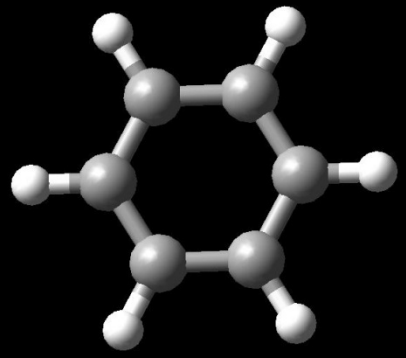
CPK



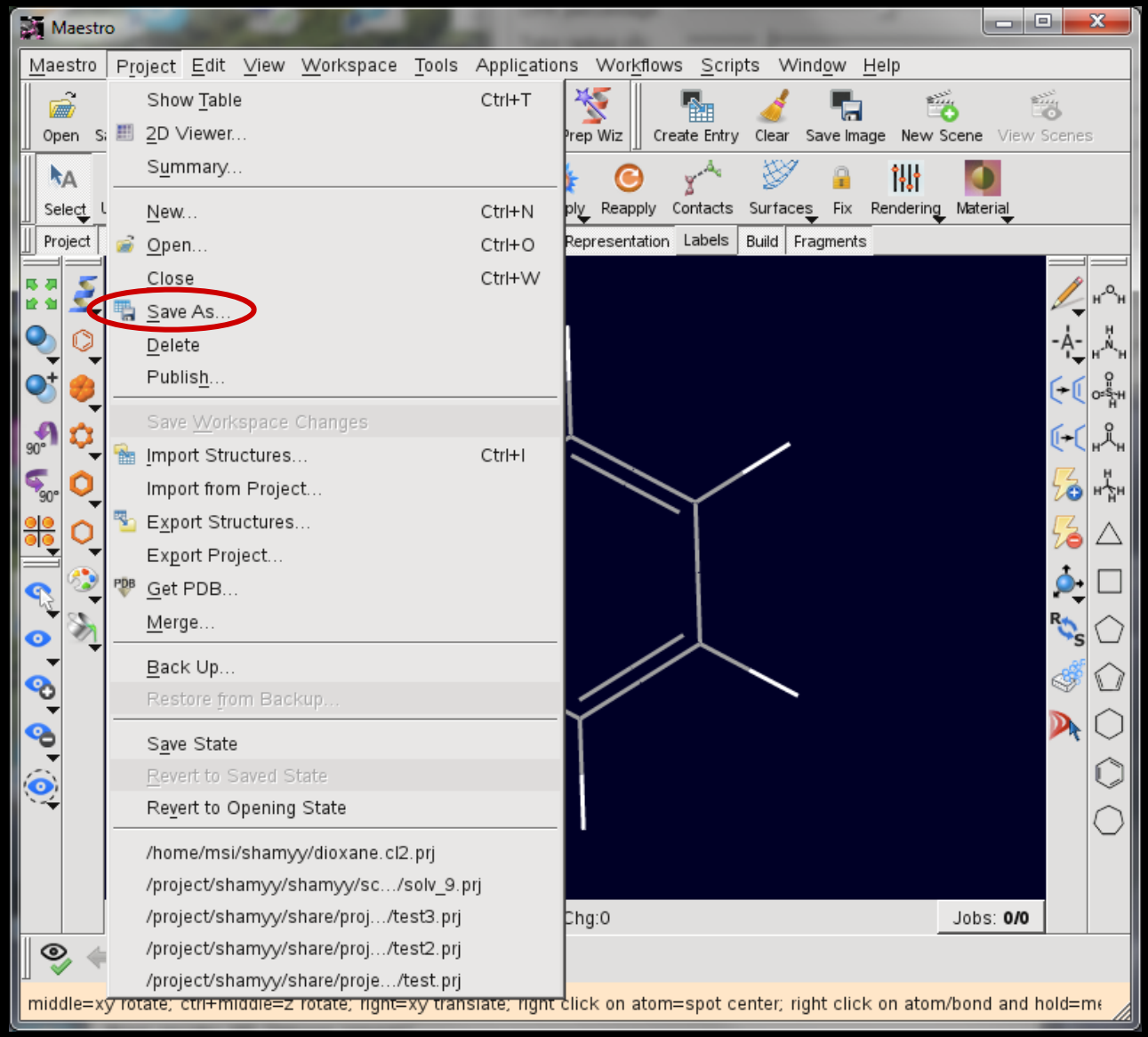
Tube



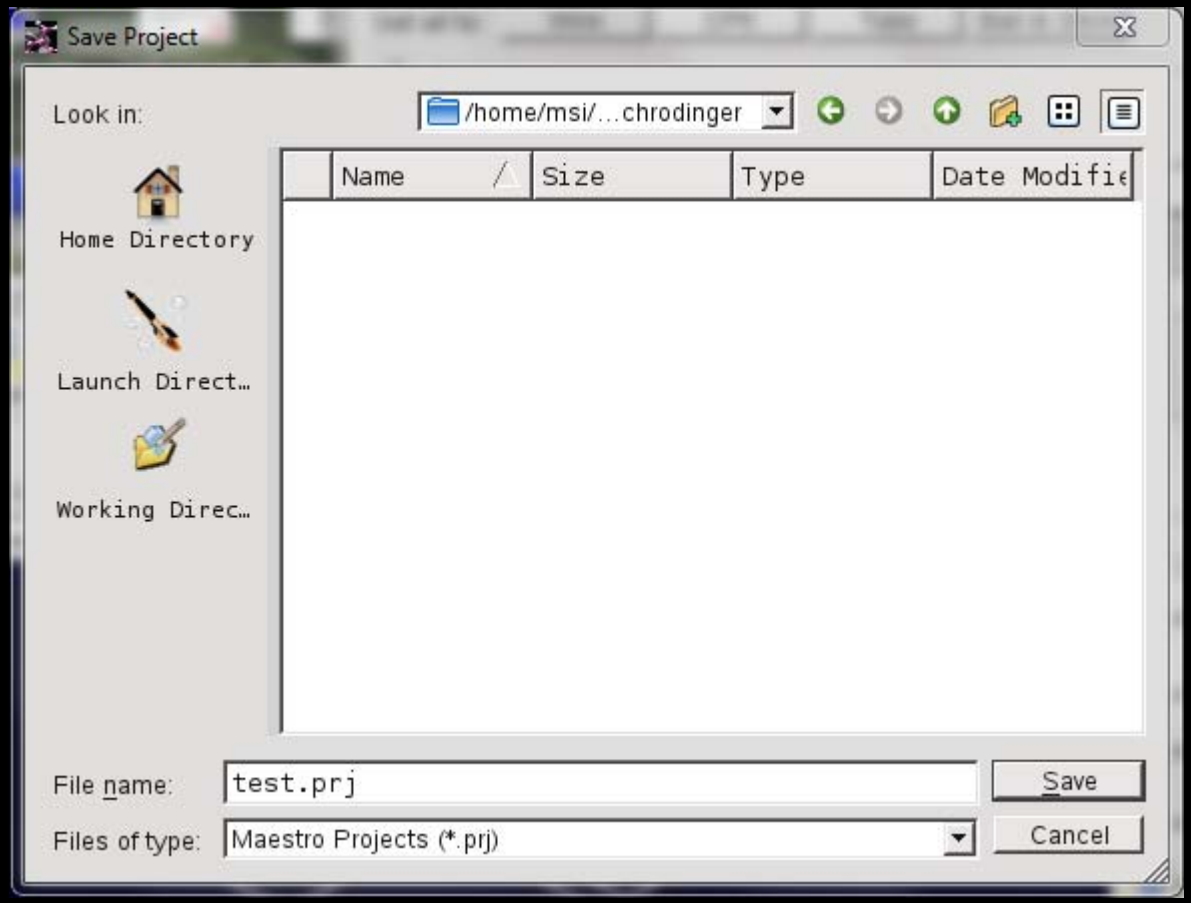
Ball &
Stick



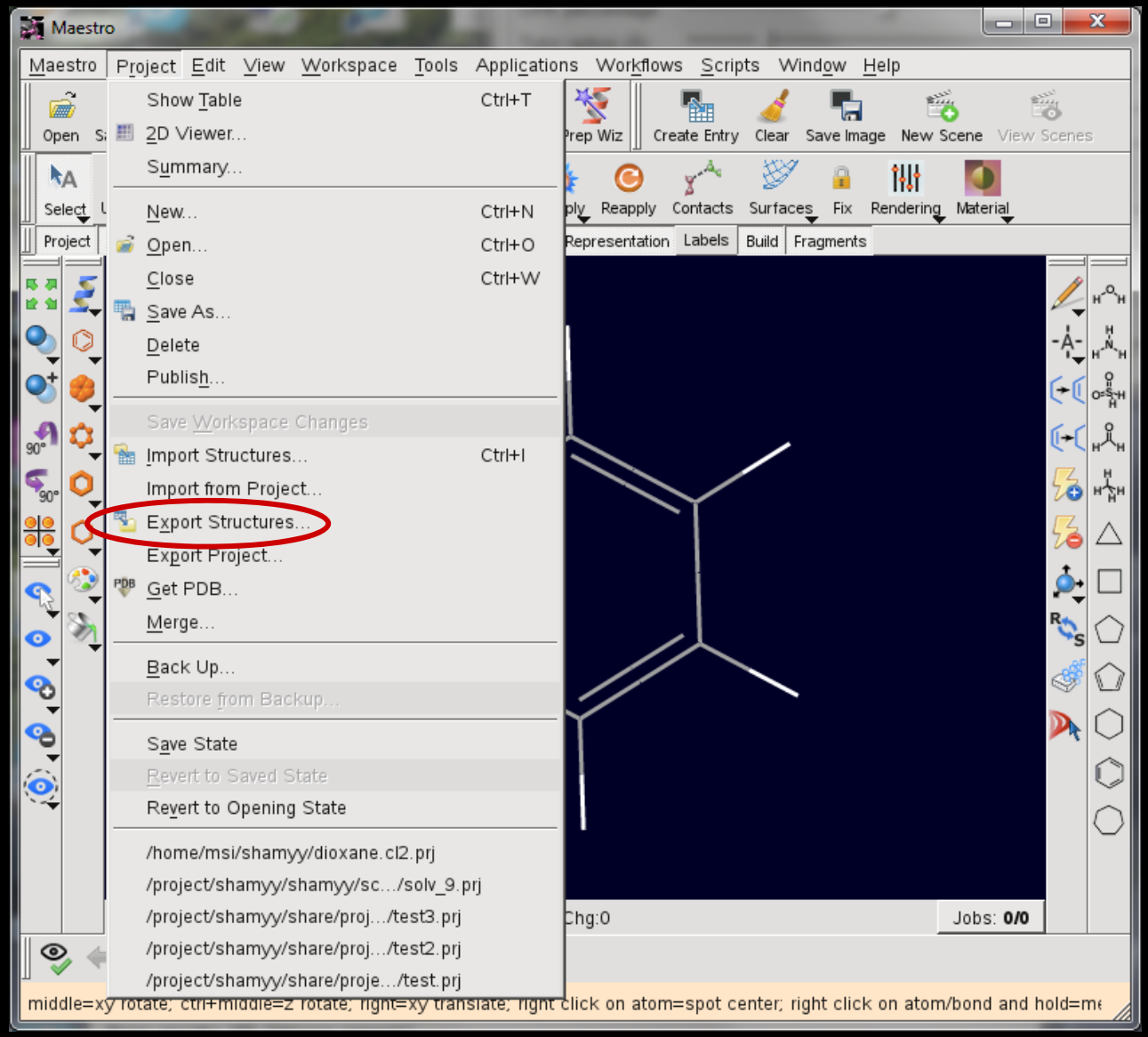
Saving Project



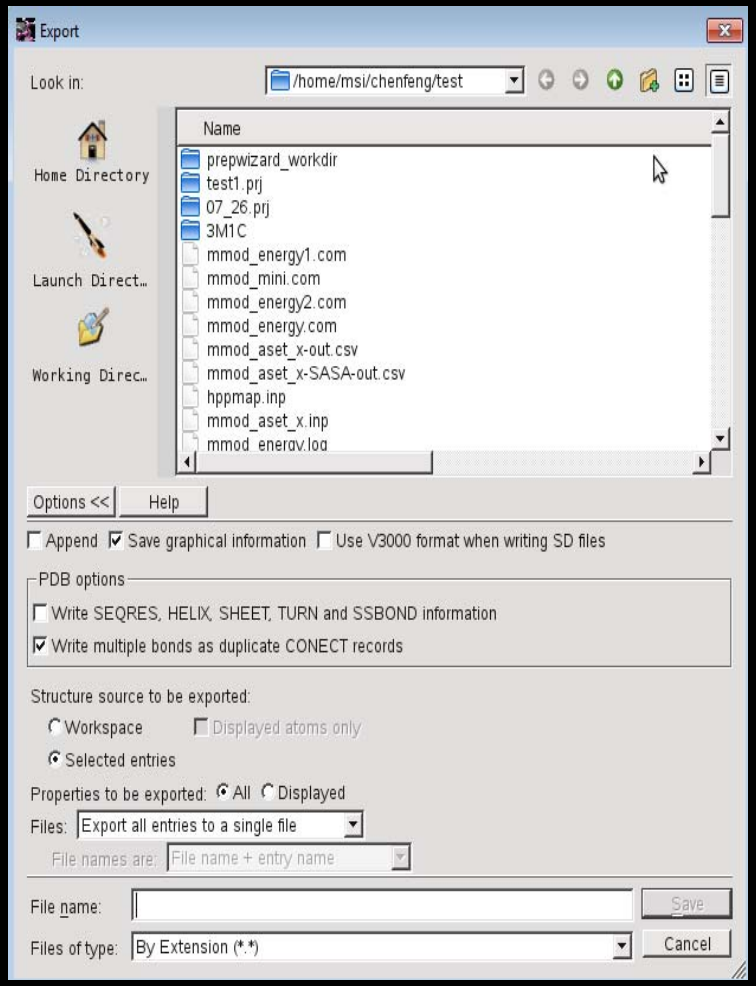
Saving Project



Exporting Structures



Export Structures



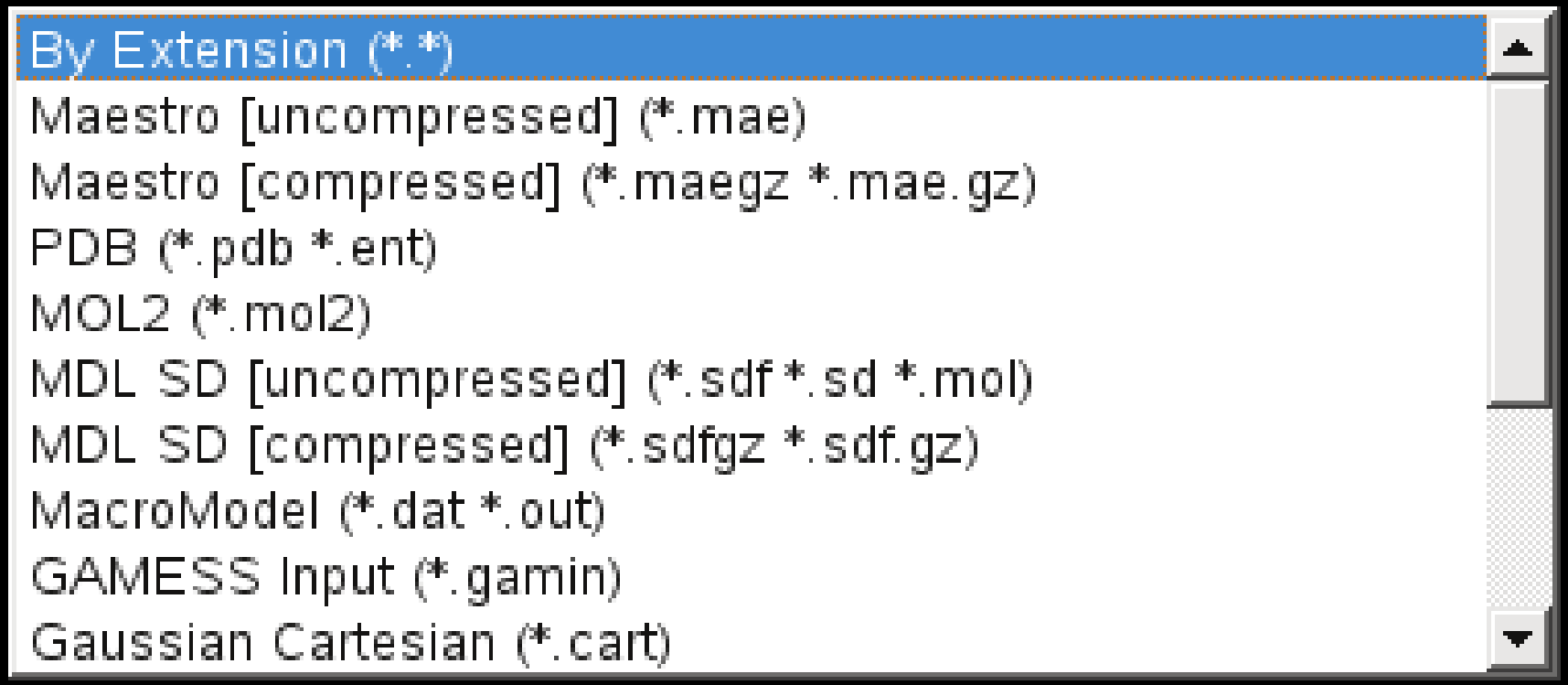
Project / Export Structures

Format: Maestro

Save graphic information: on

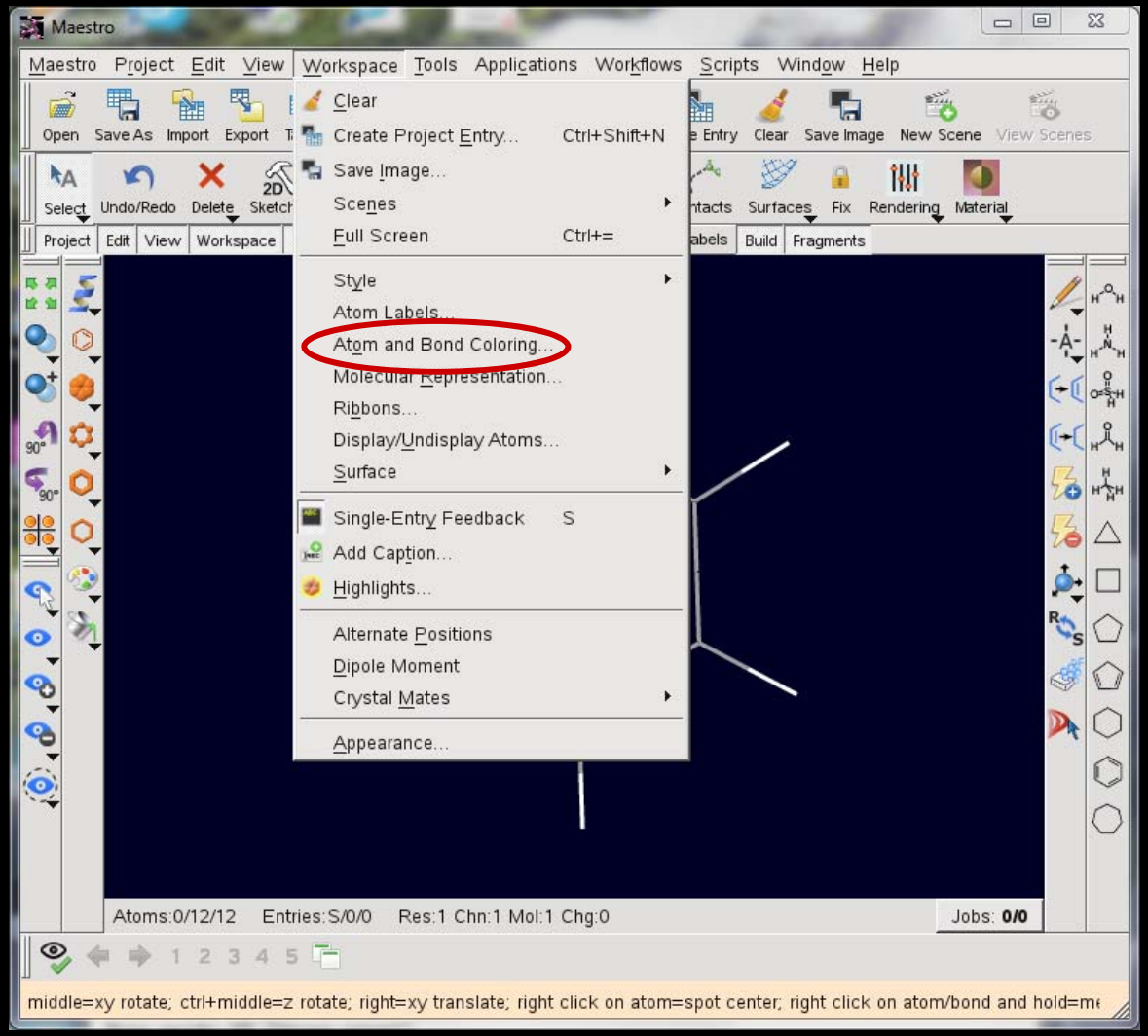
Export

Other Formats



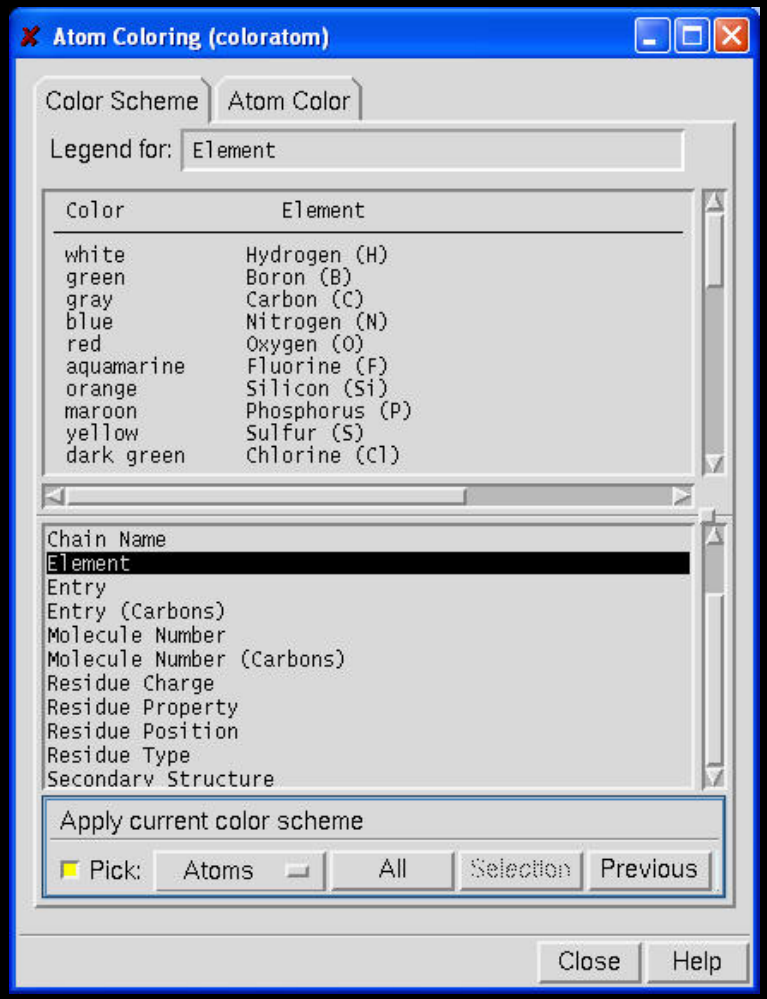
And more …..

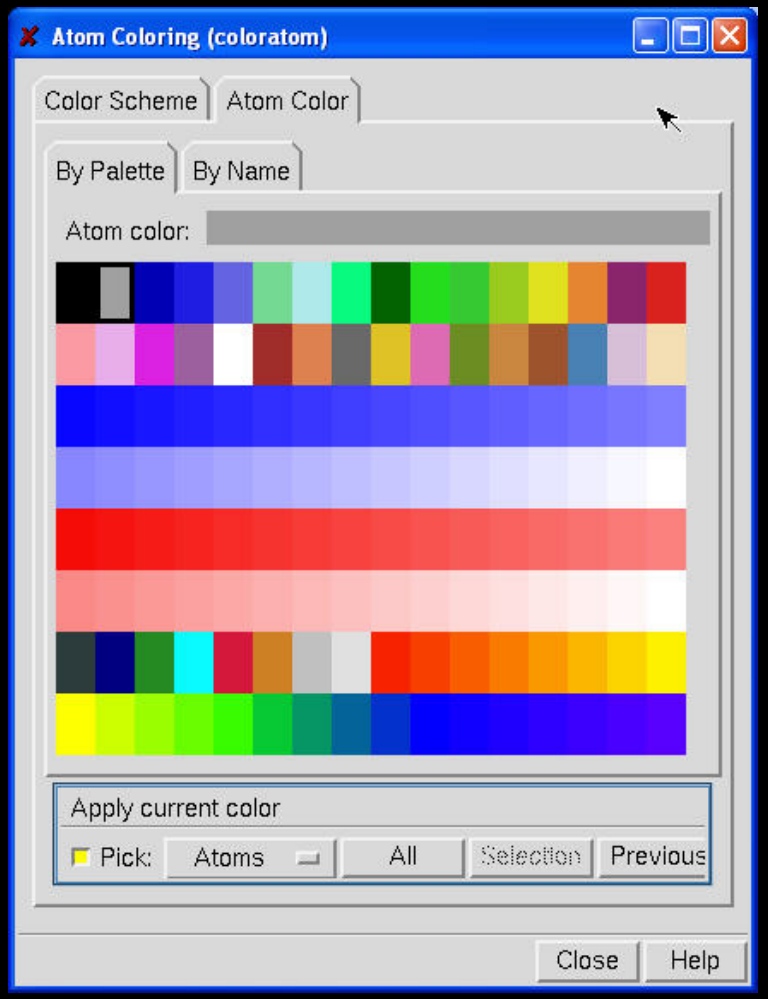
Coloring Atoms



Workspace / Atom Coloring

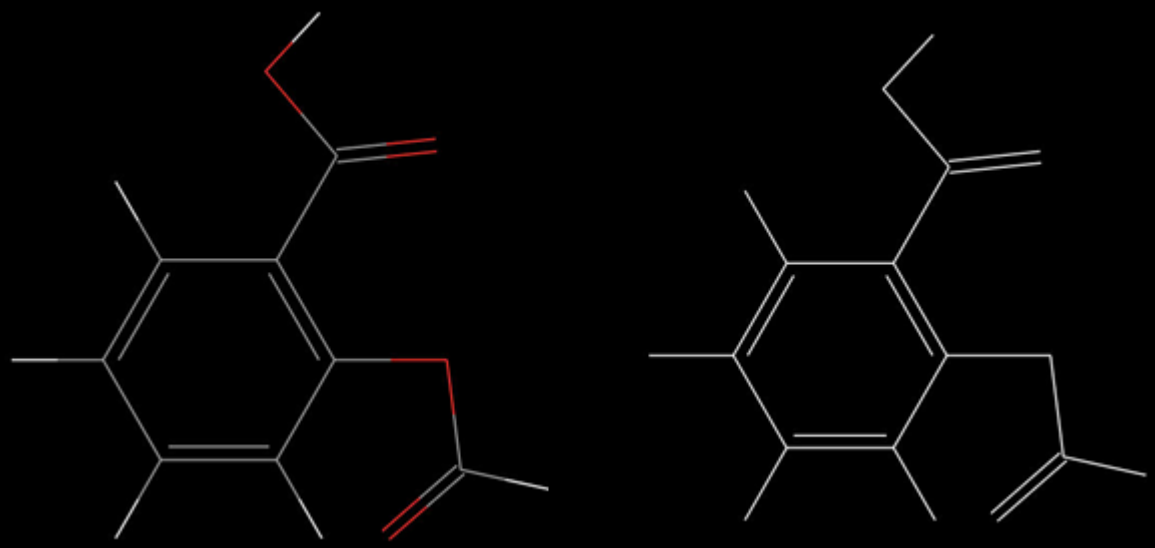
Coloring Atoms



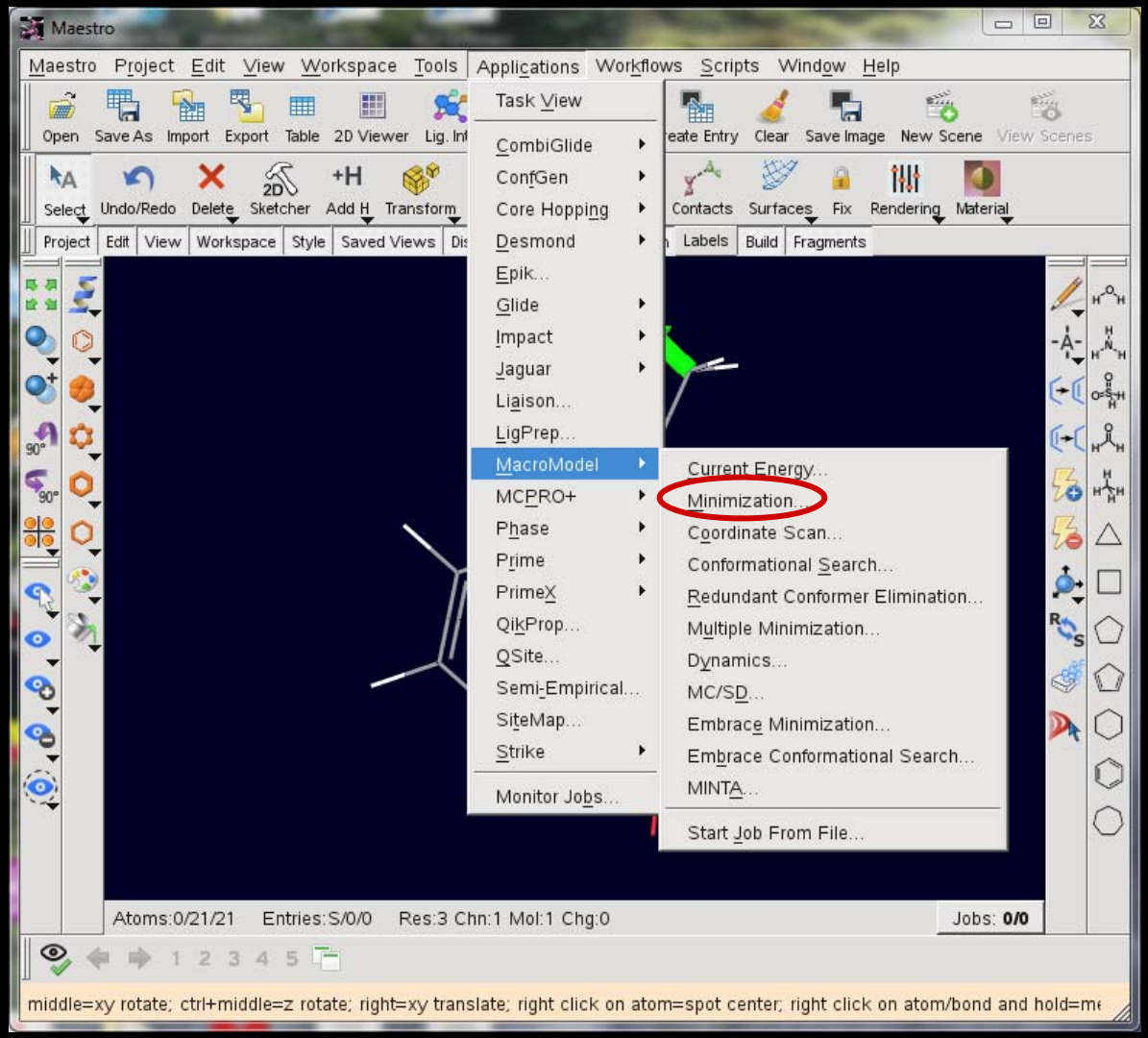


Workspace / Atom Bonding Coloring

Coloring Atoms

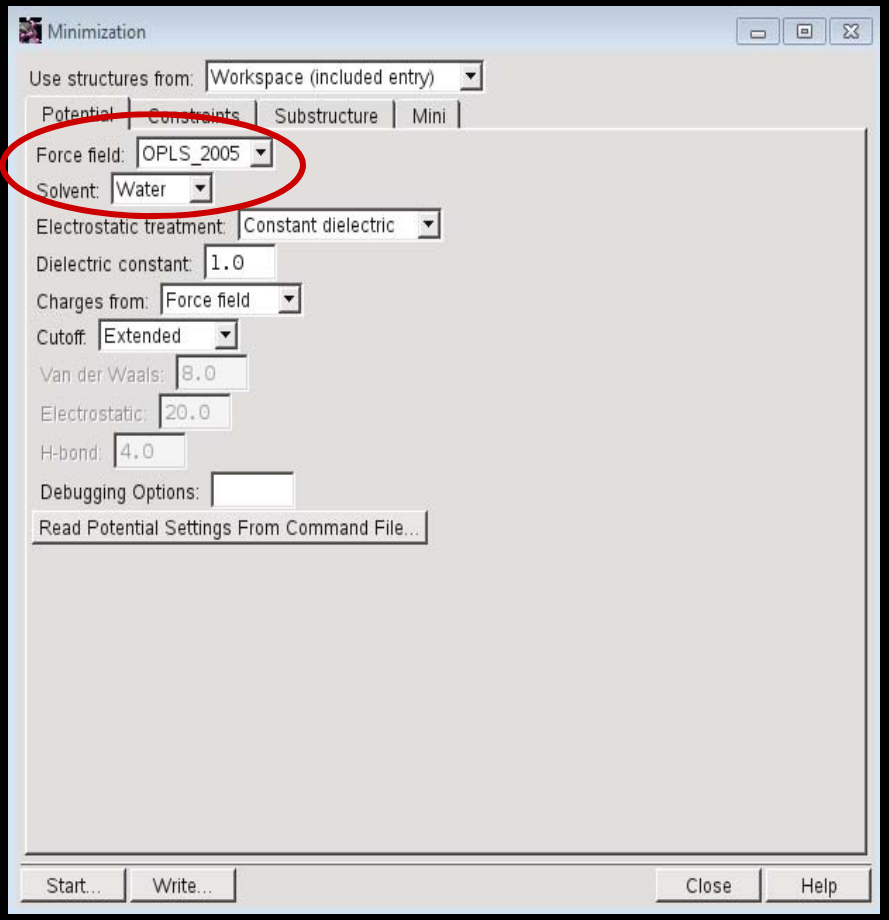


Minimize Structure



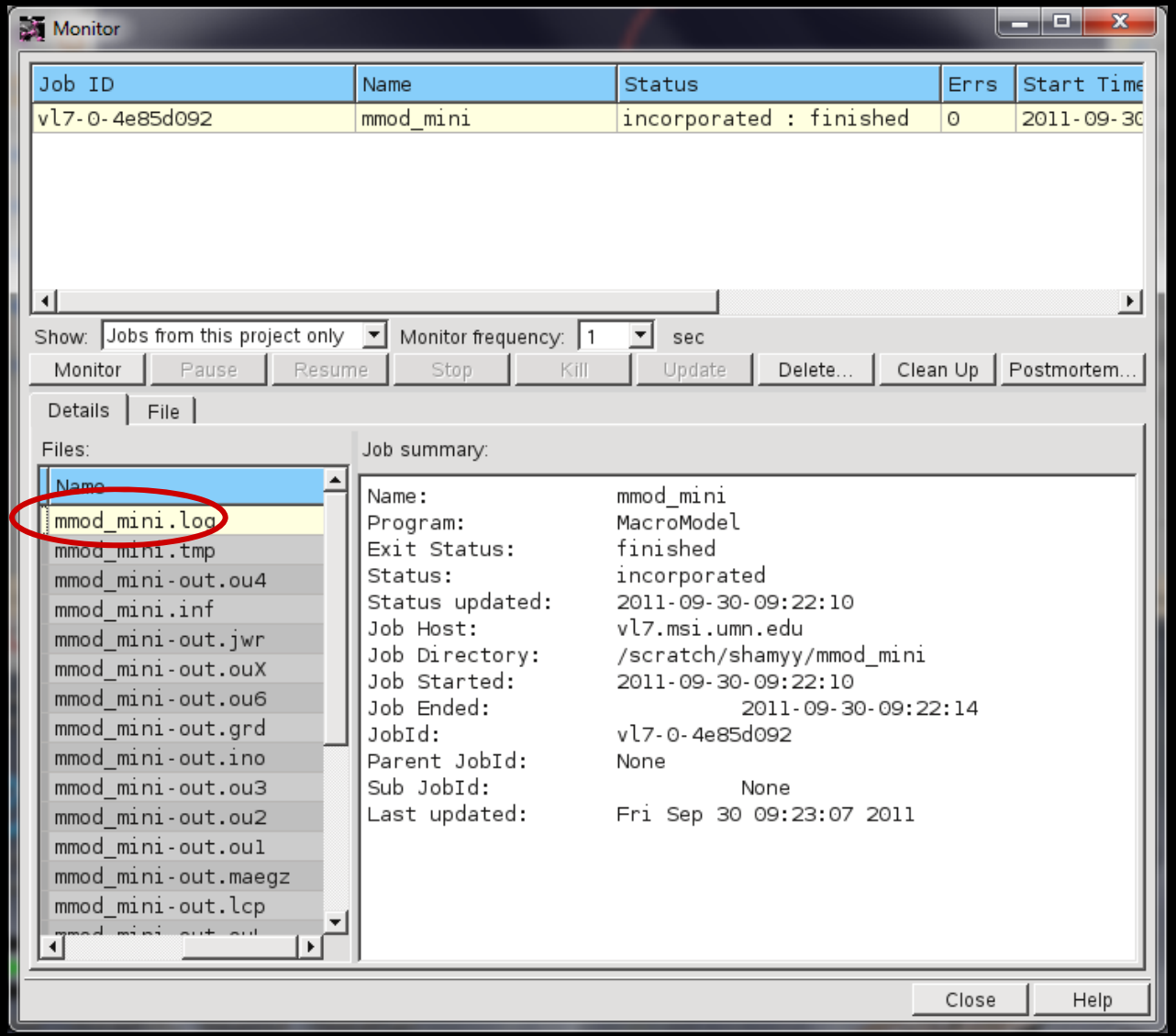
Applications / MacroModel / Minimization

Minimize Structure

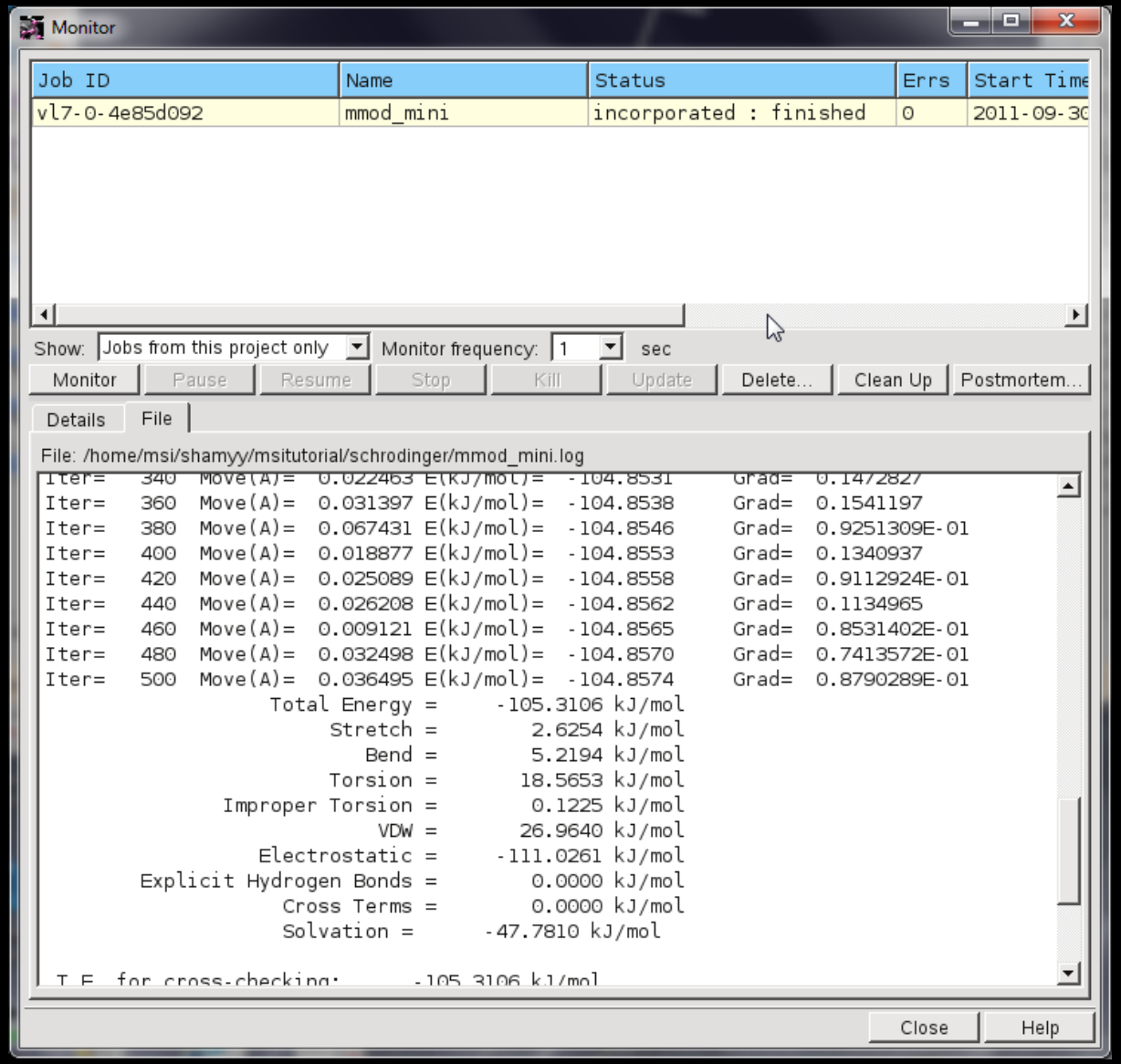


Applications / MacroModel / Minimization

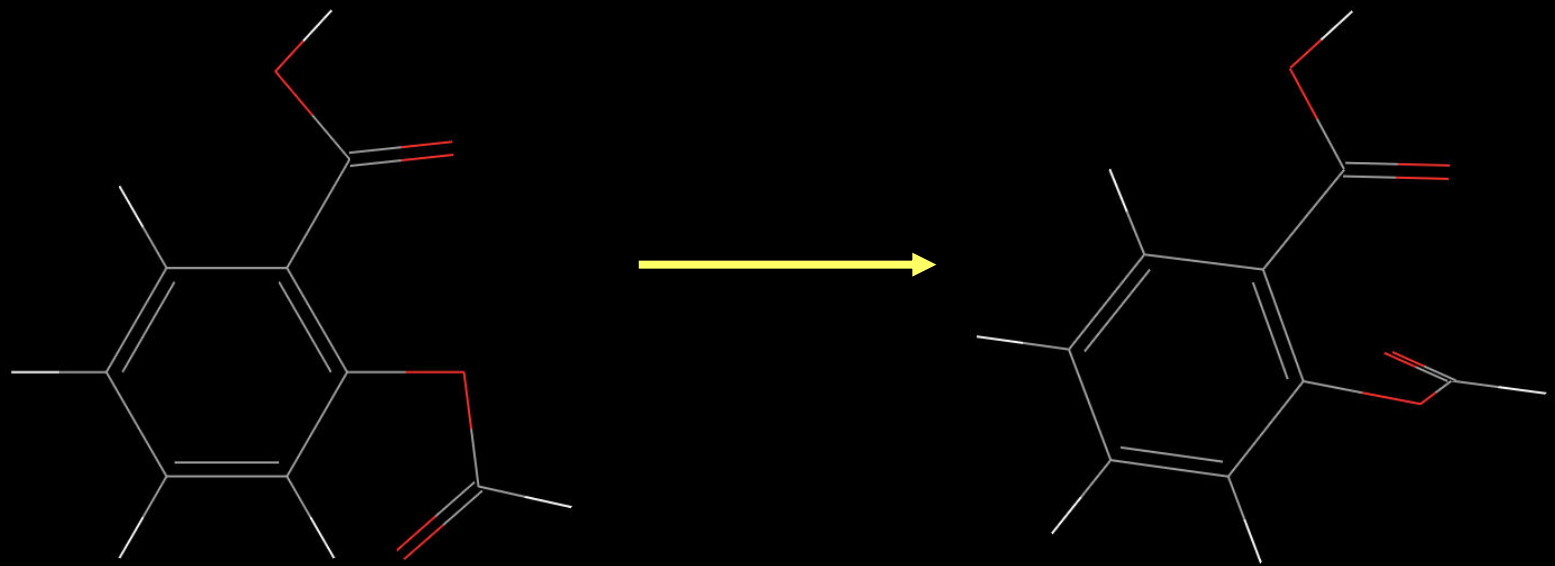
Minimize Structure



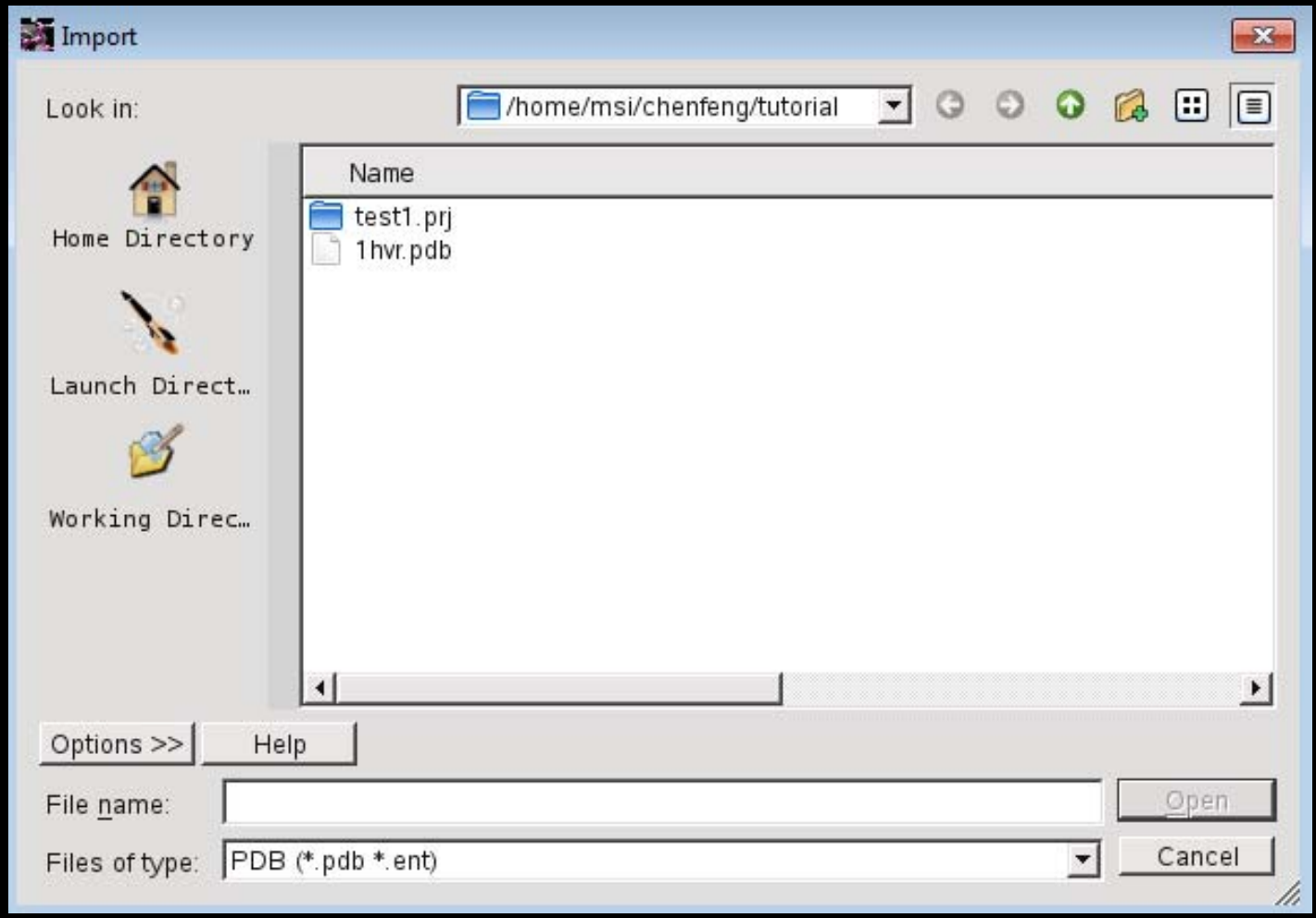
Minimize Structure



Minimized Structure

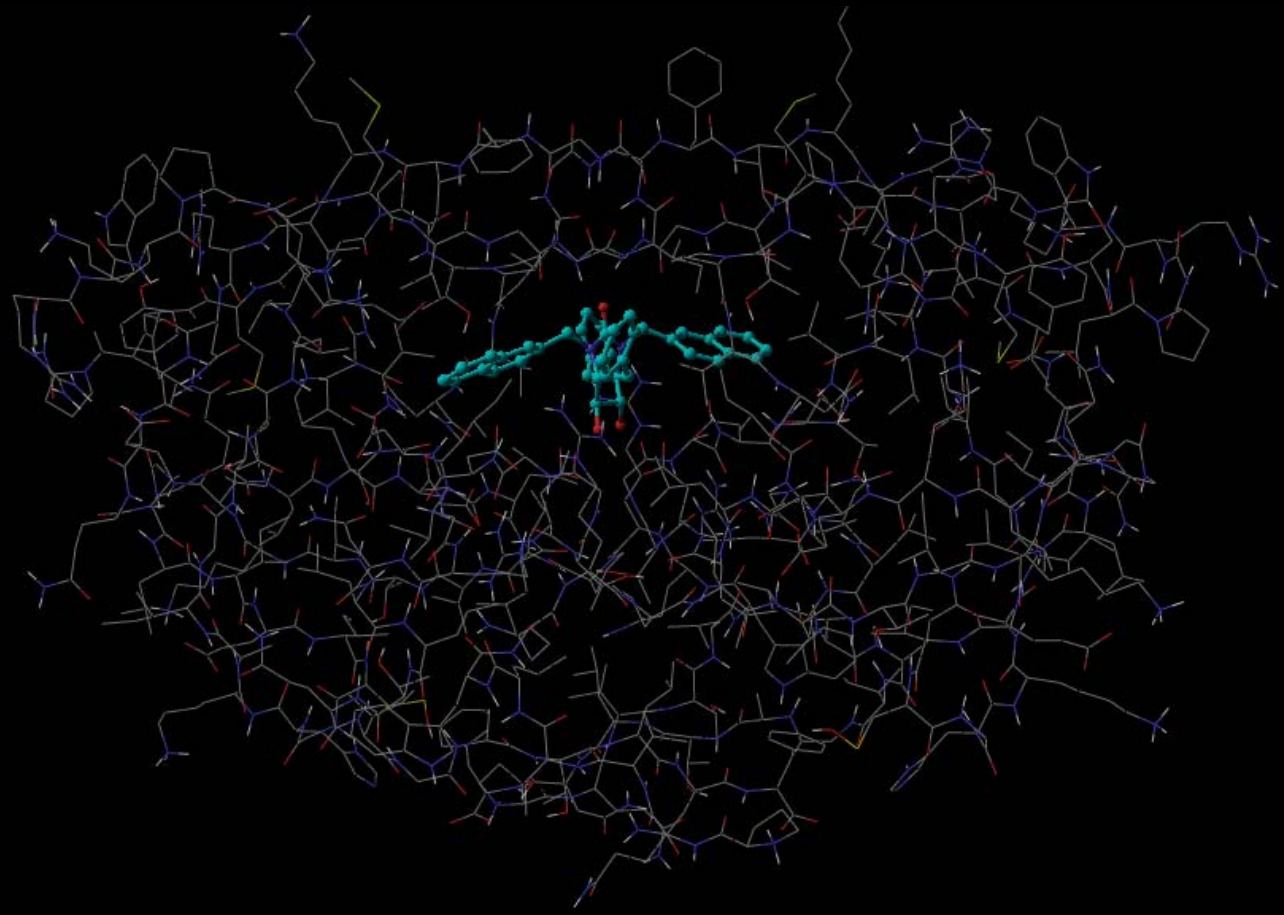


Import PDB file

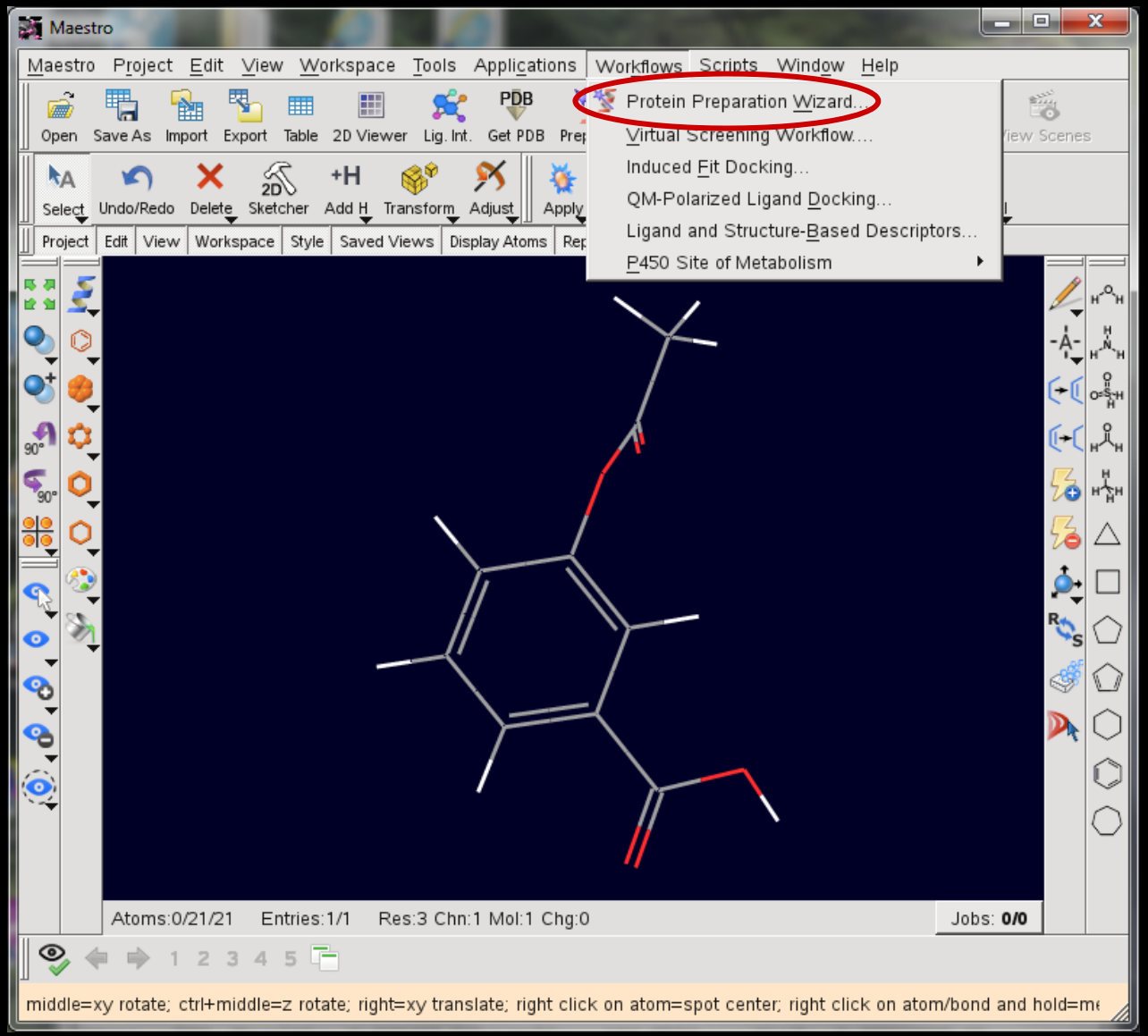


Project / Import Structures

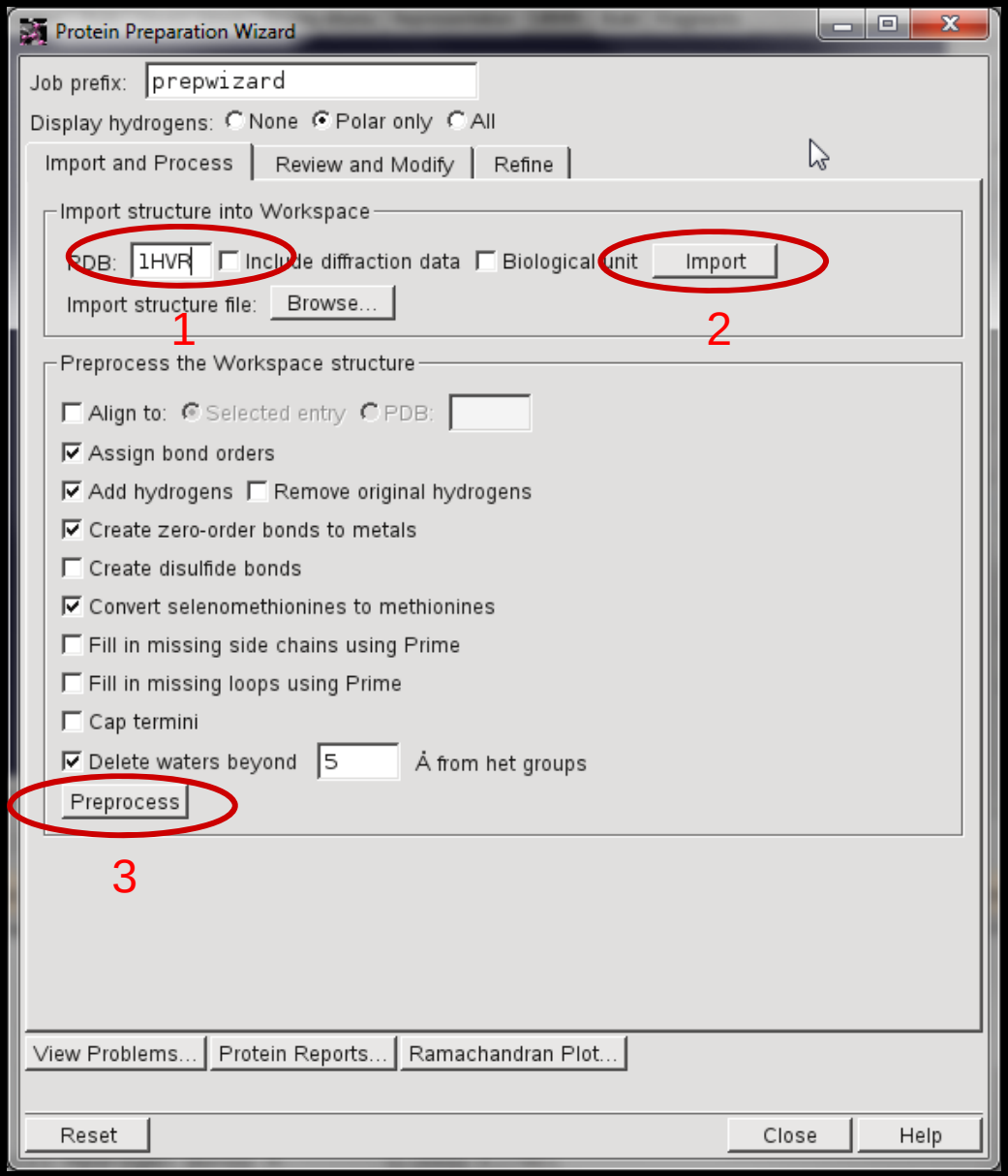
Import PDB file



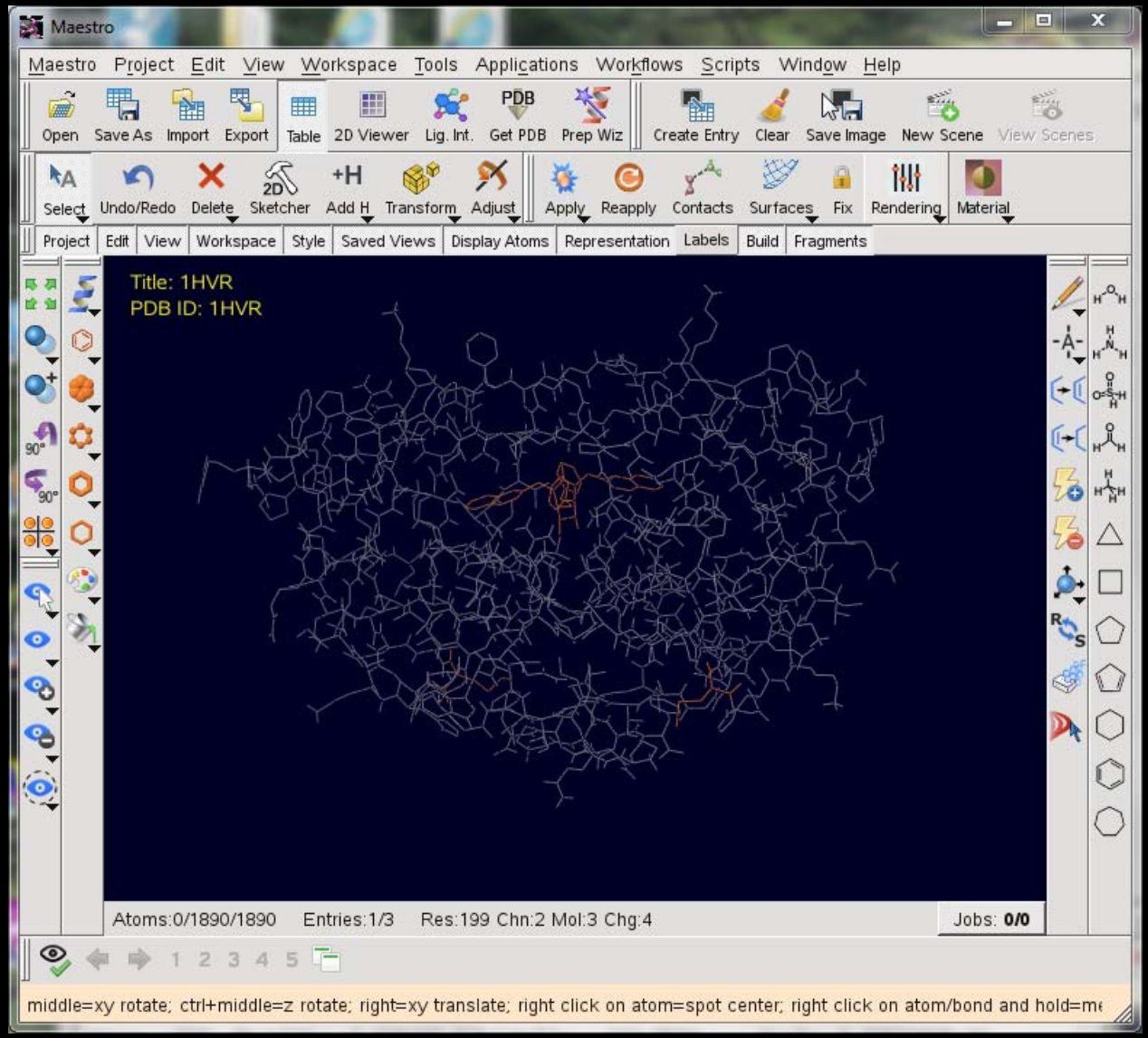
Protein Preparation Wizard



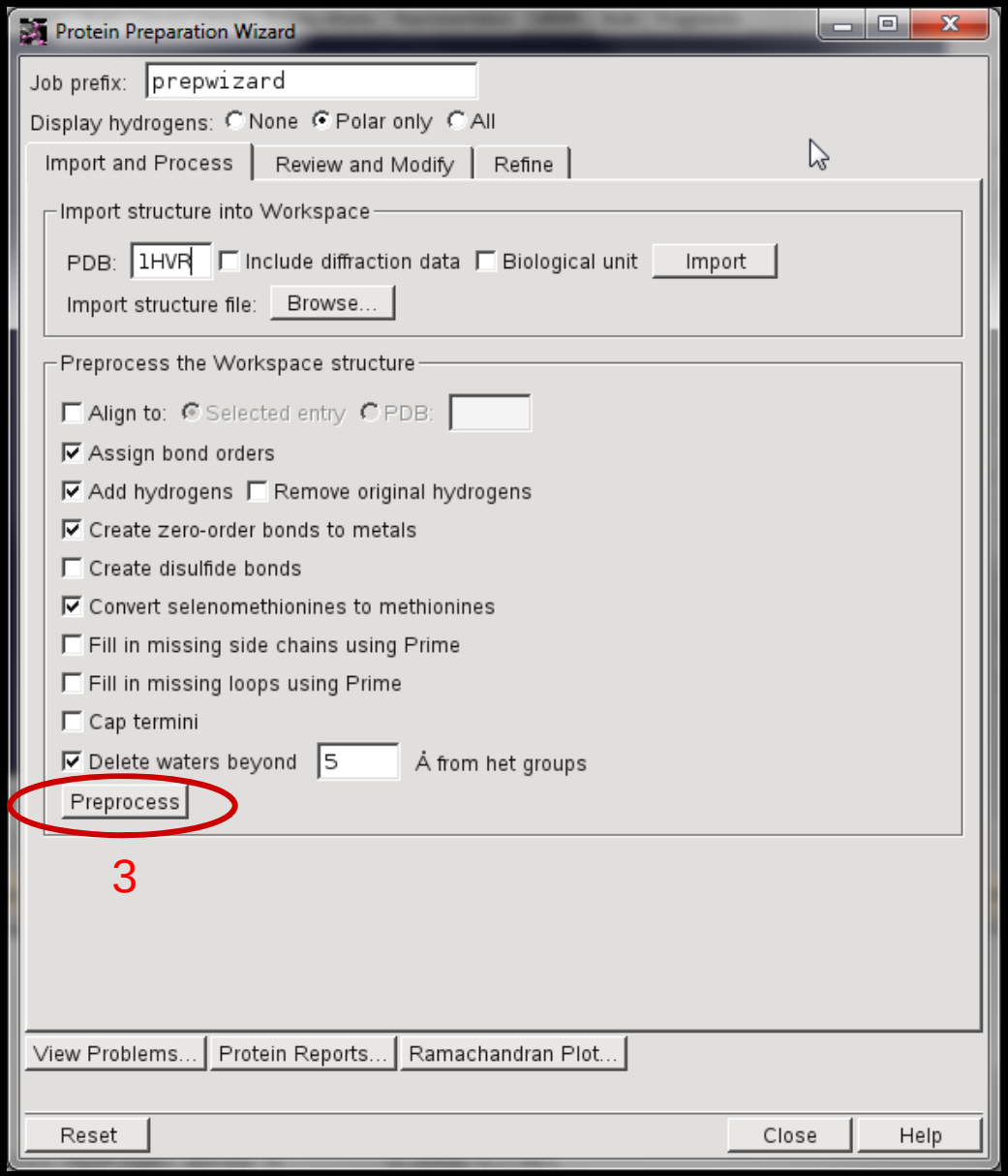
Protein Preparation Wizard



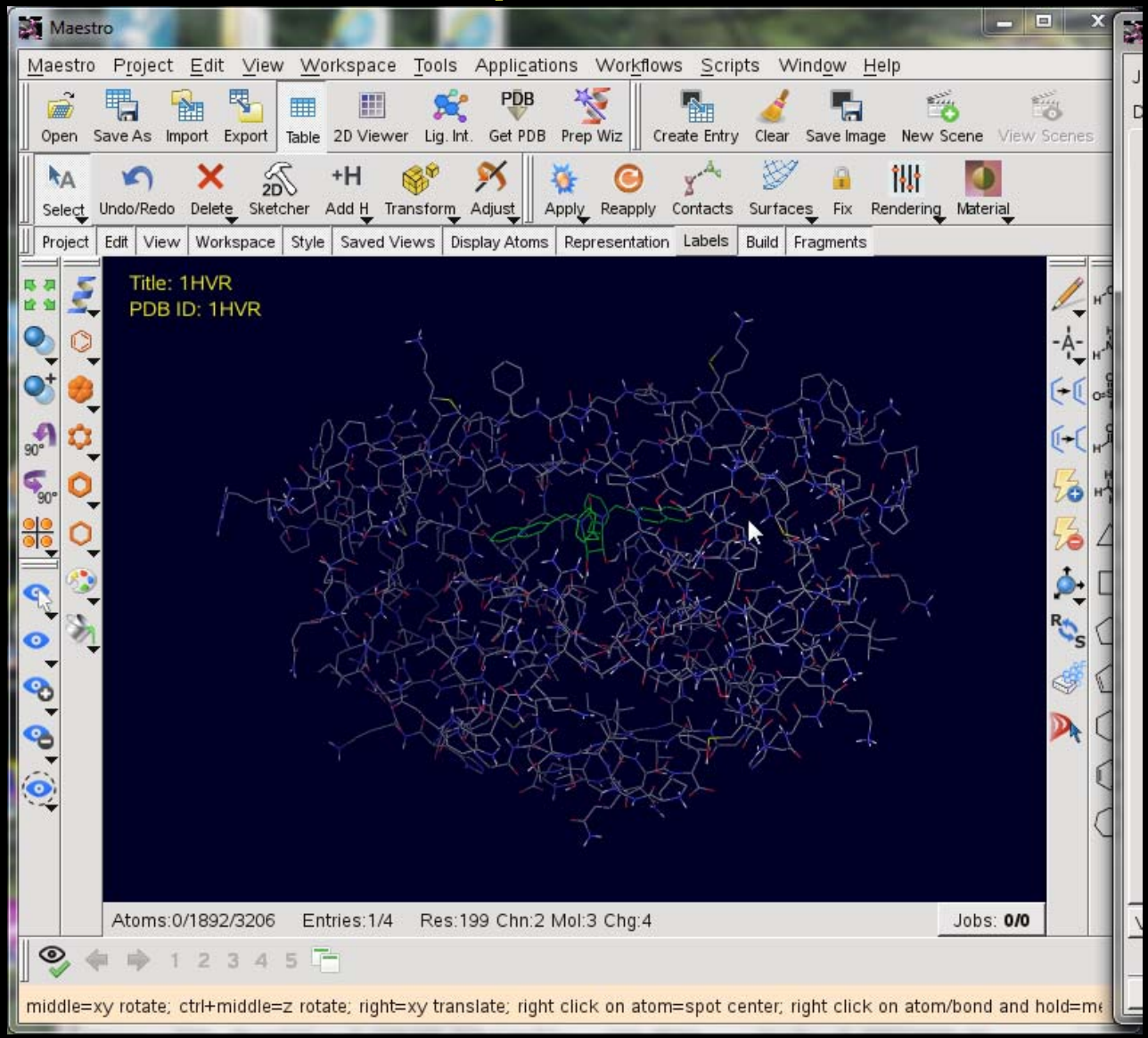
Protein Preparation Wizard



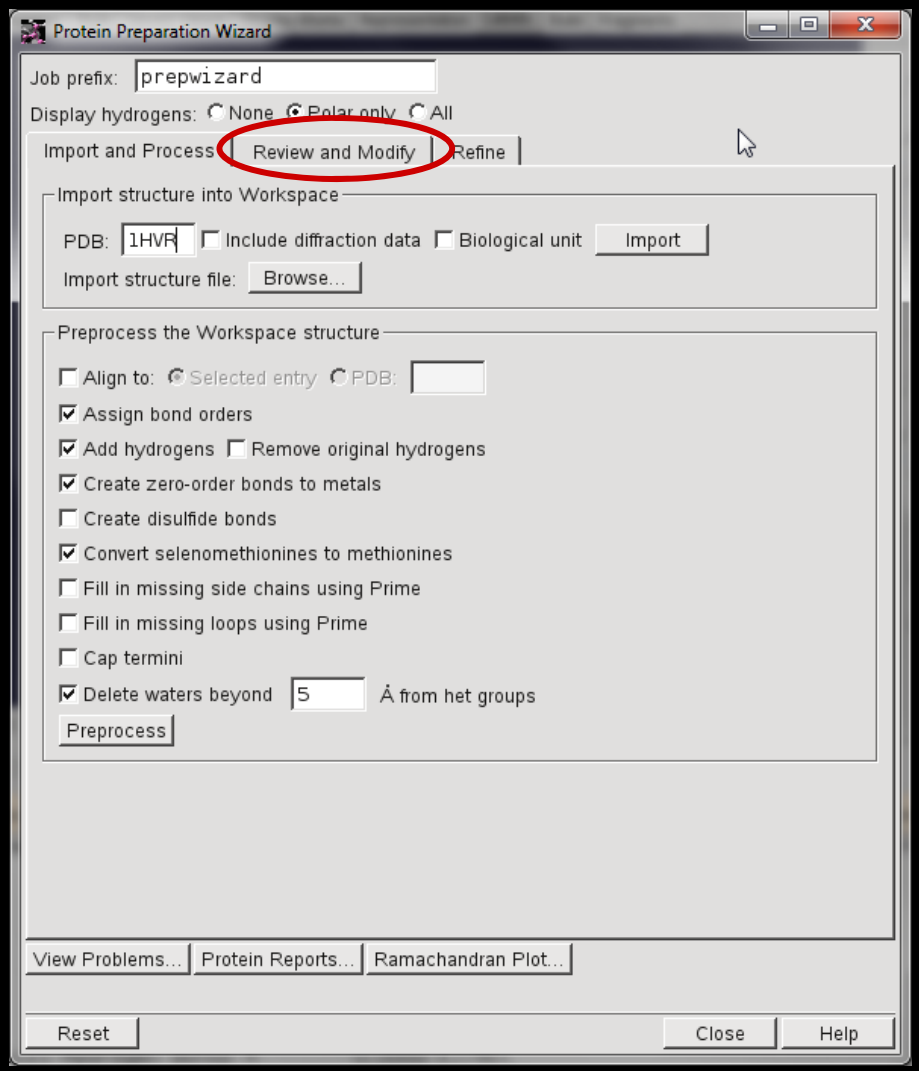
Protein Preparation Wizard

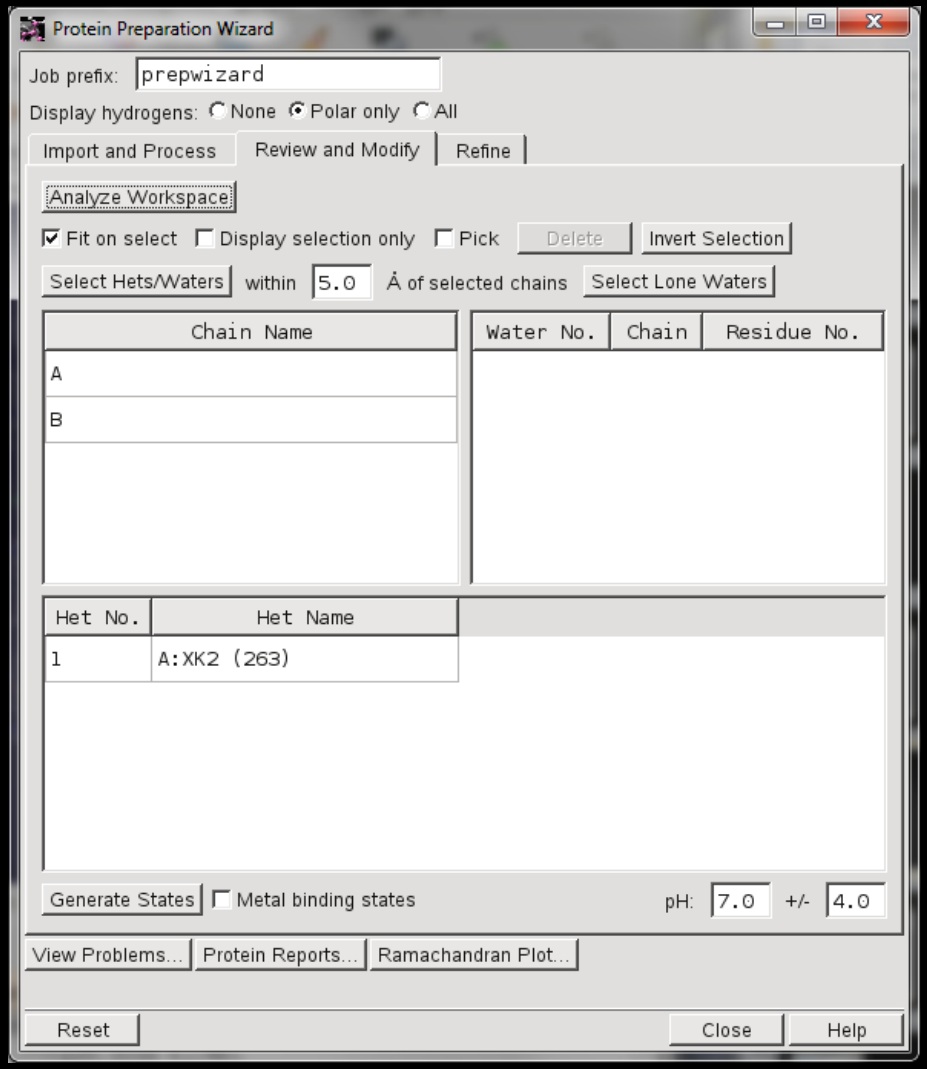


Protein Preparation Wizard

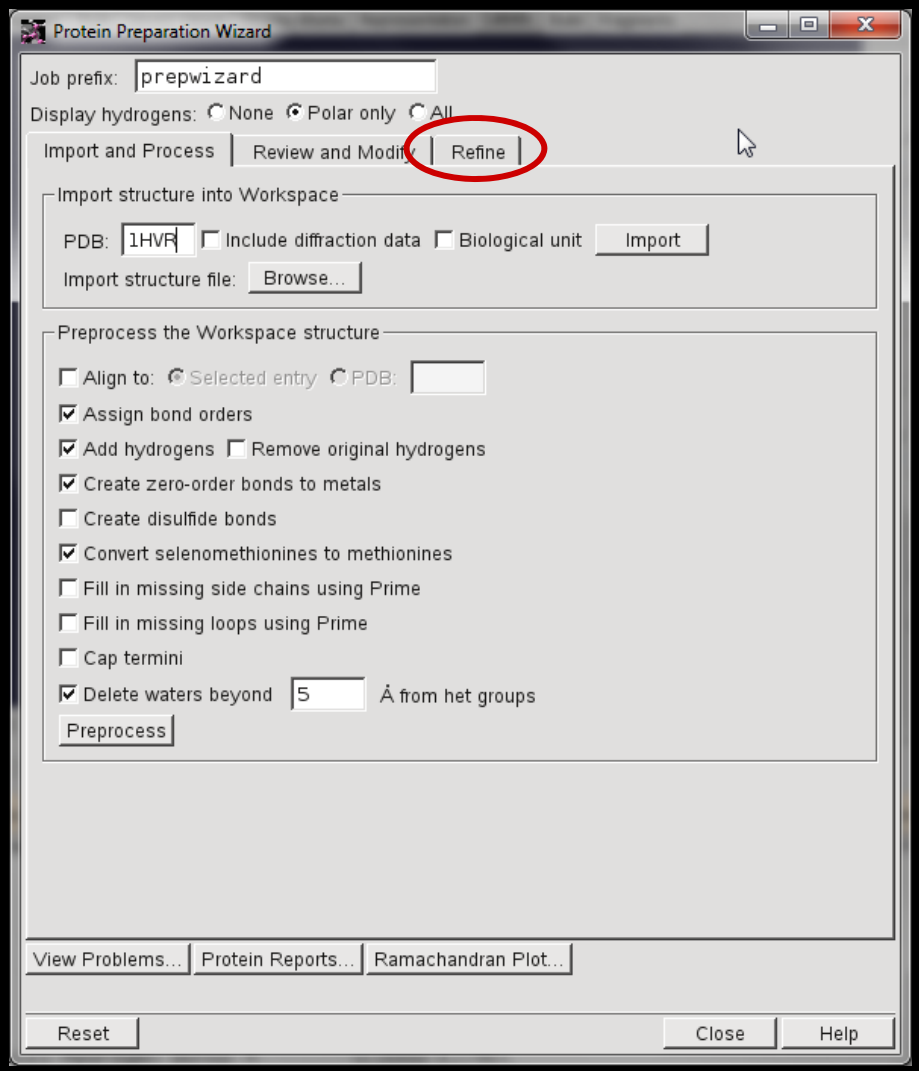


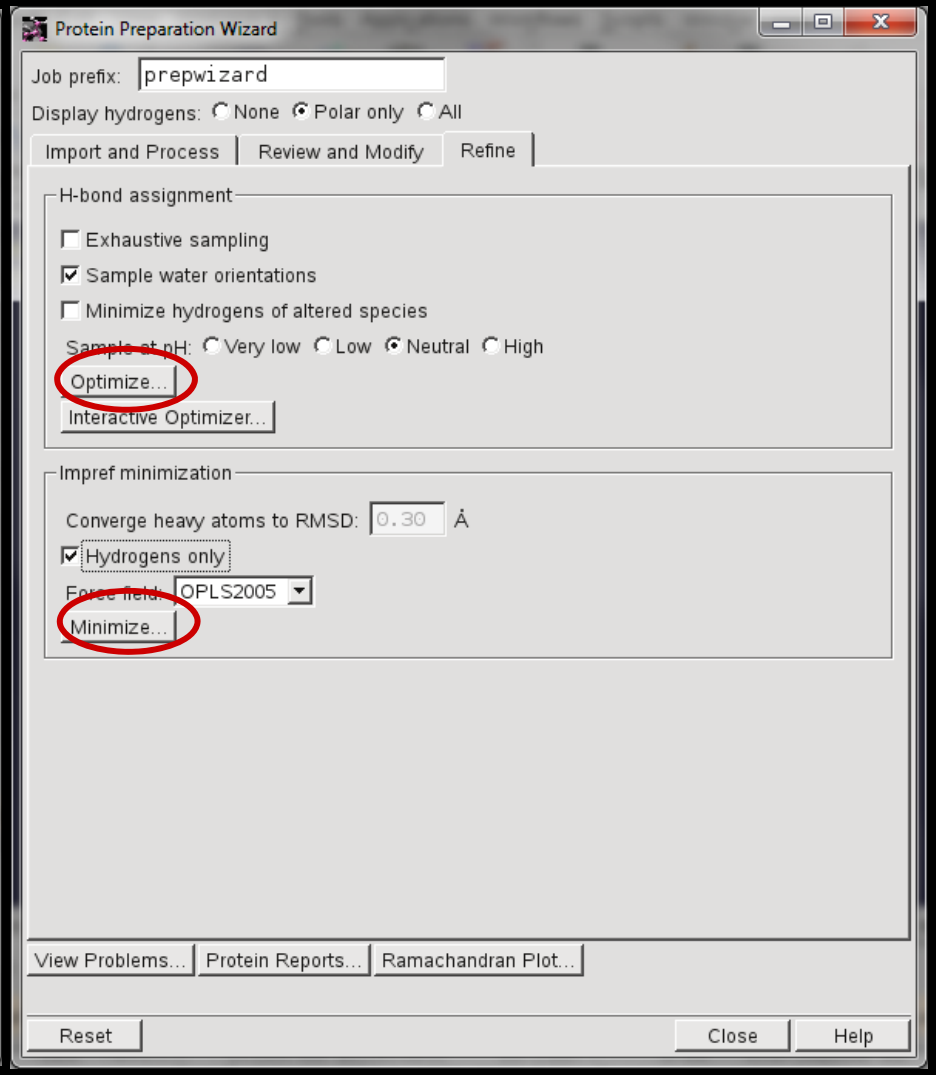
Protein Preparation Wizard



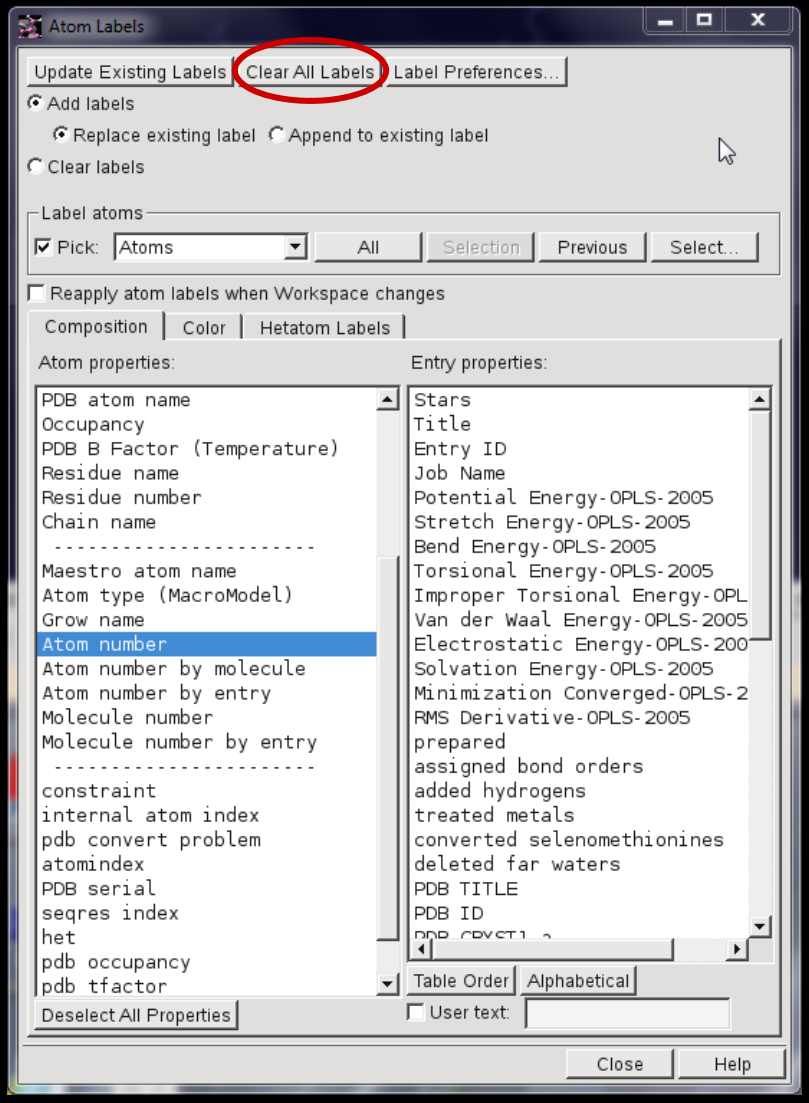


Protein Preparation Wizard



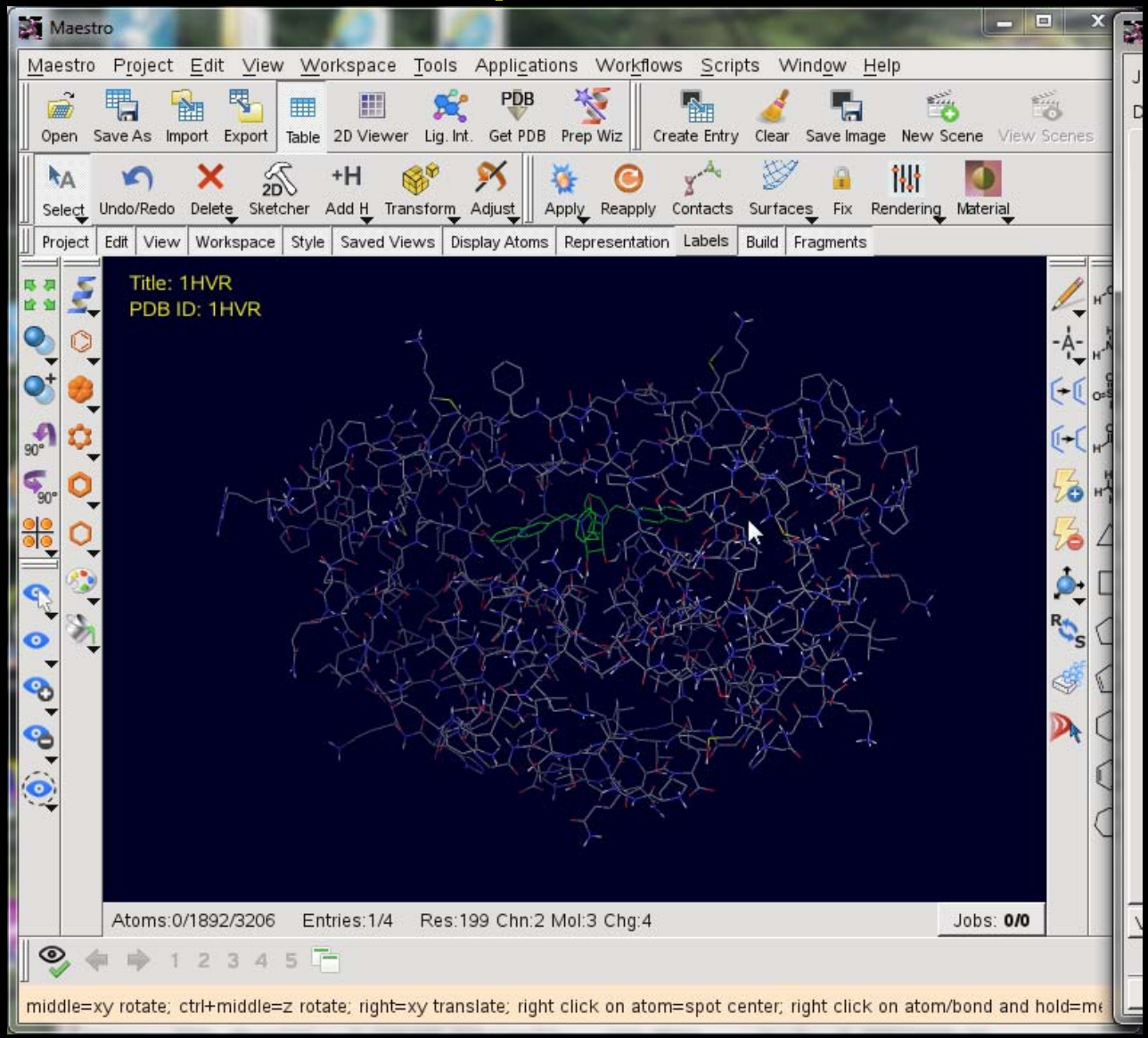


Atom Labels

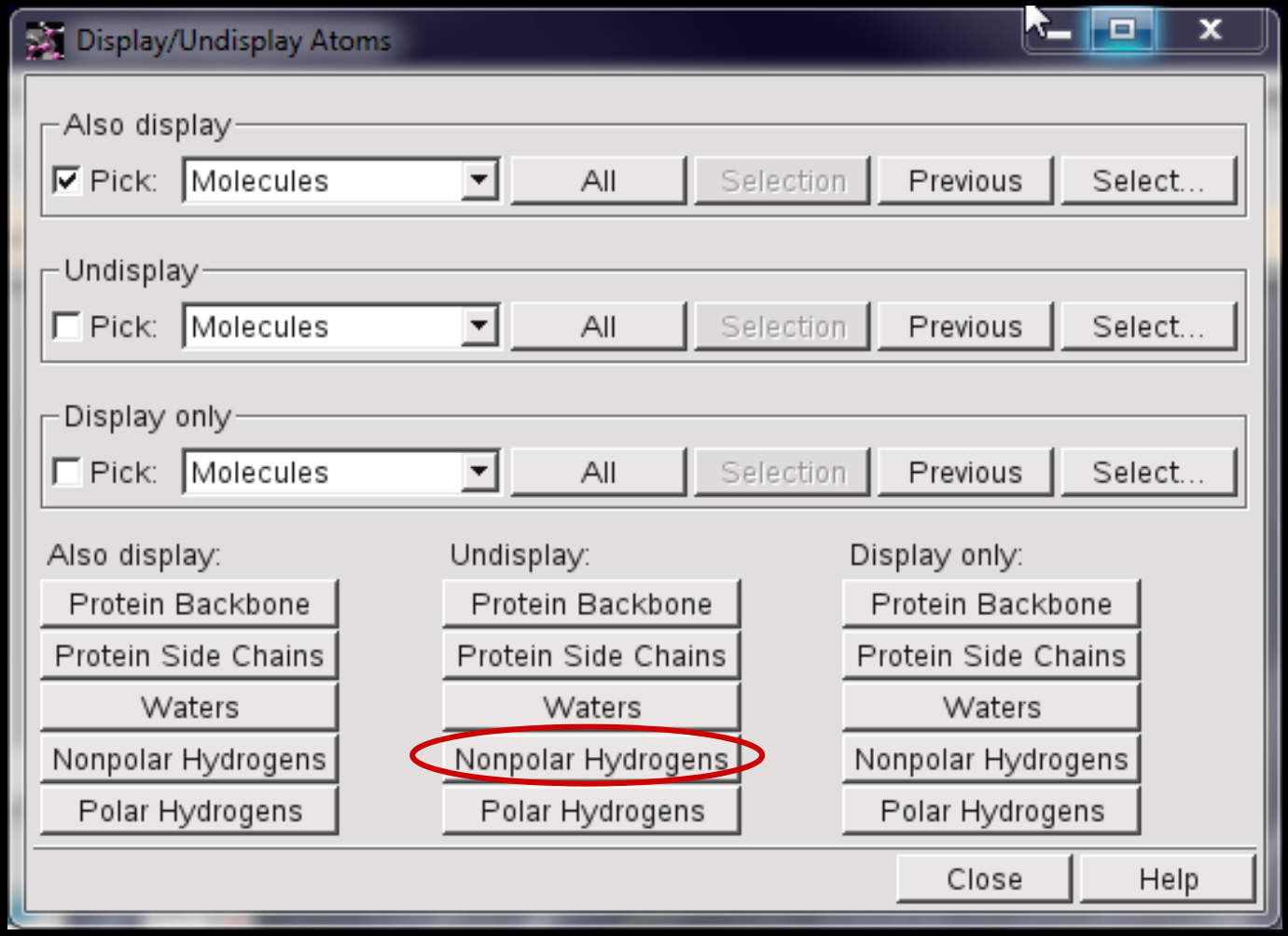


Workspace / Atom Labels

Protein Preparation Wizard

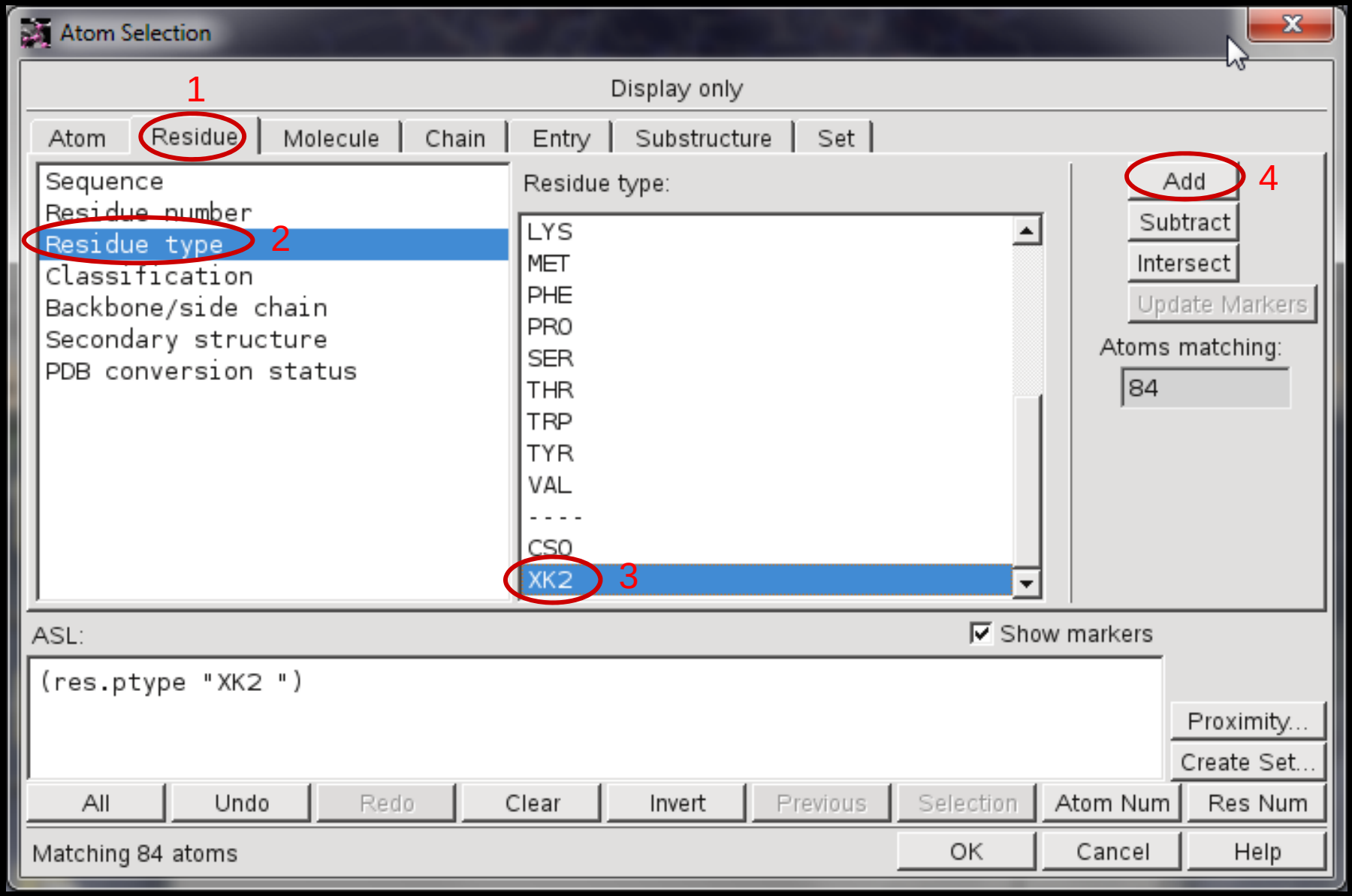


Display / Undisplay

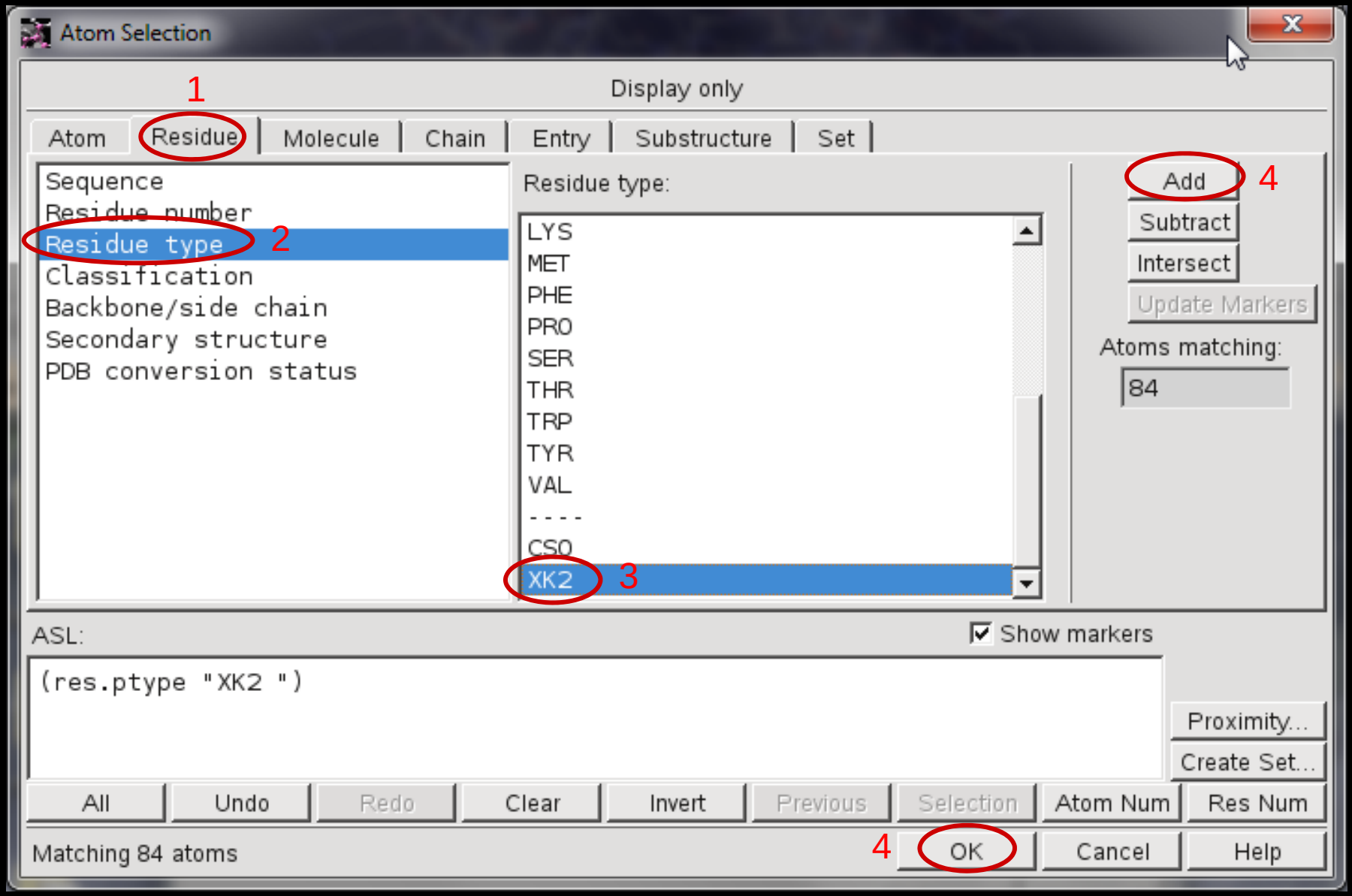


Workspace / Display/Undisplay Atoms

Atom Selection

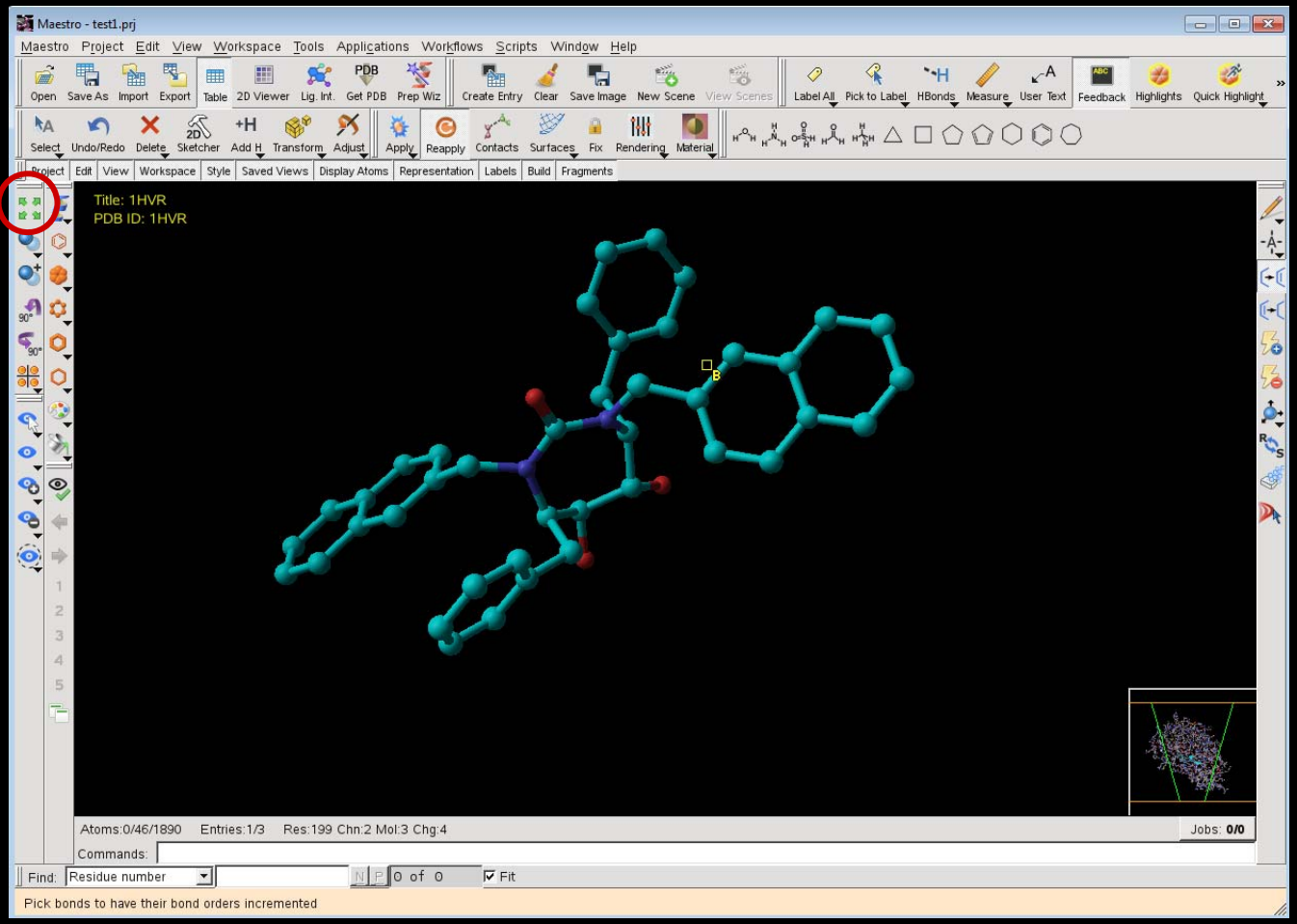


Atom Selection

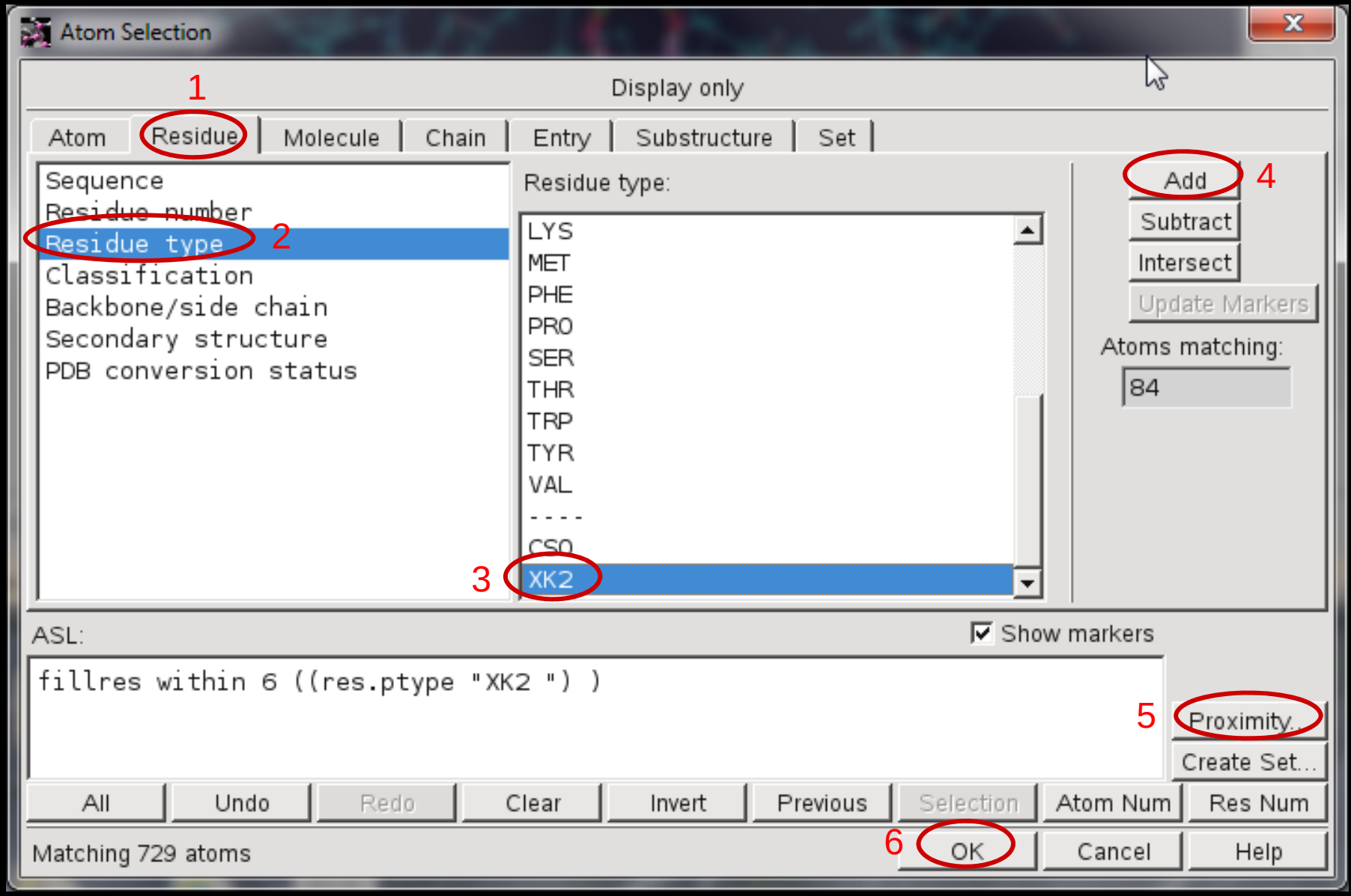


Display / Undisplay

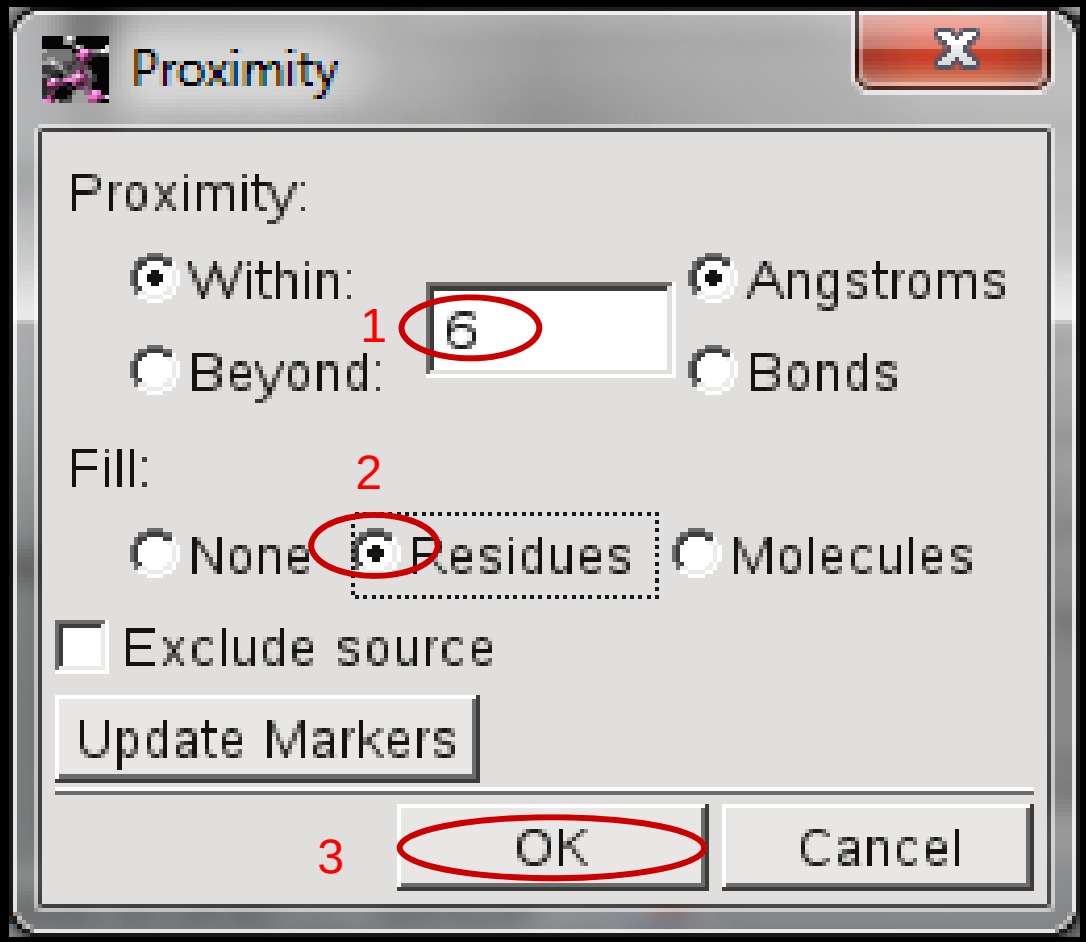
Center



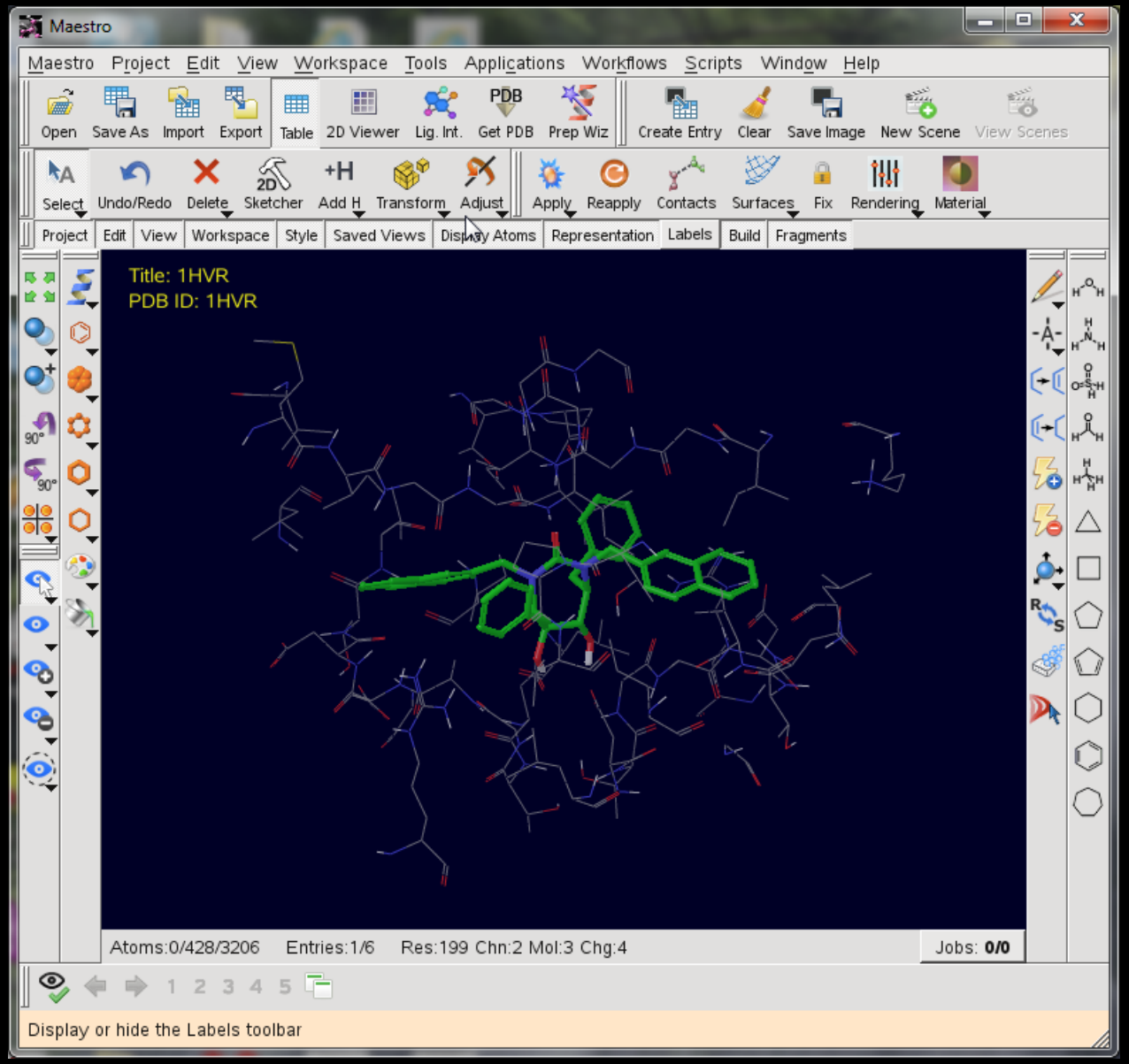
Displaying Binding site



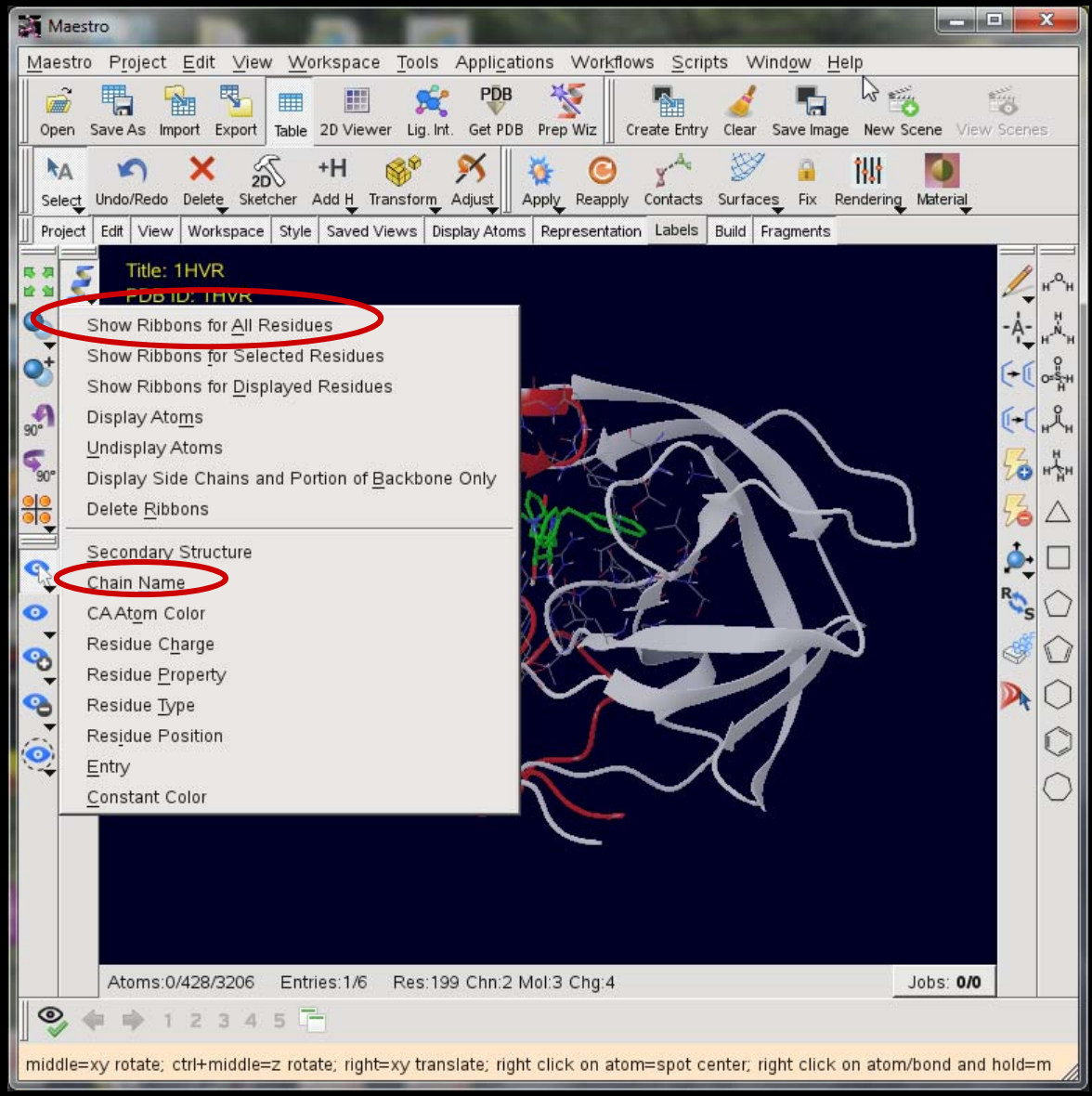
Selecting with “Proximity”



Displaying Binding site



Displaying Ribbons



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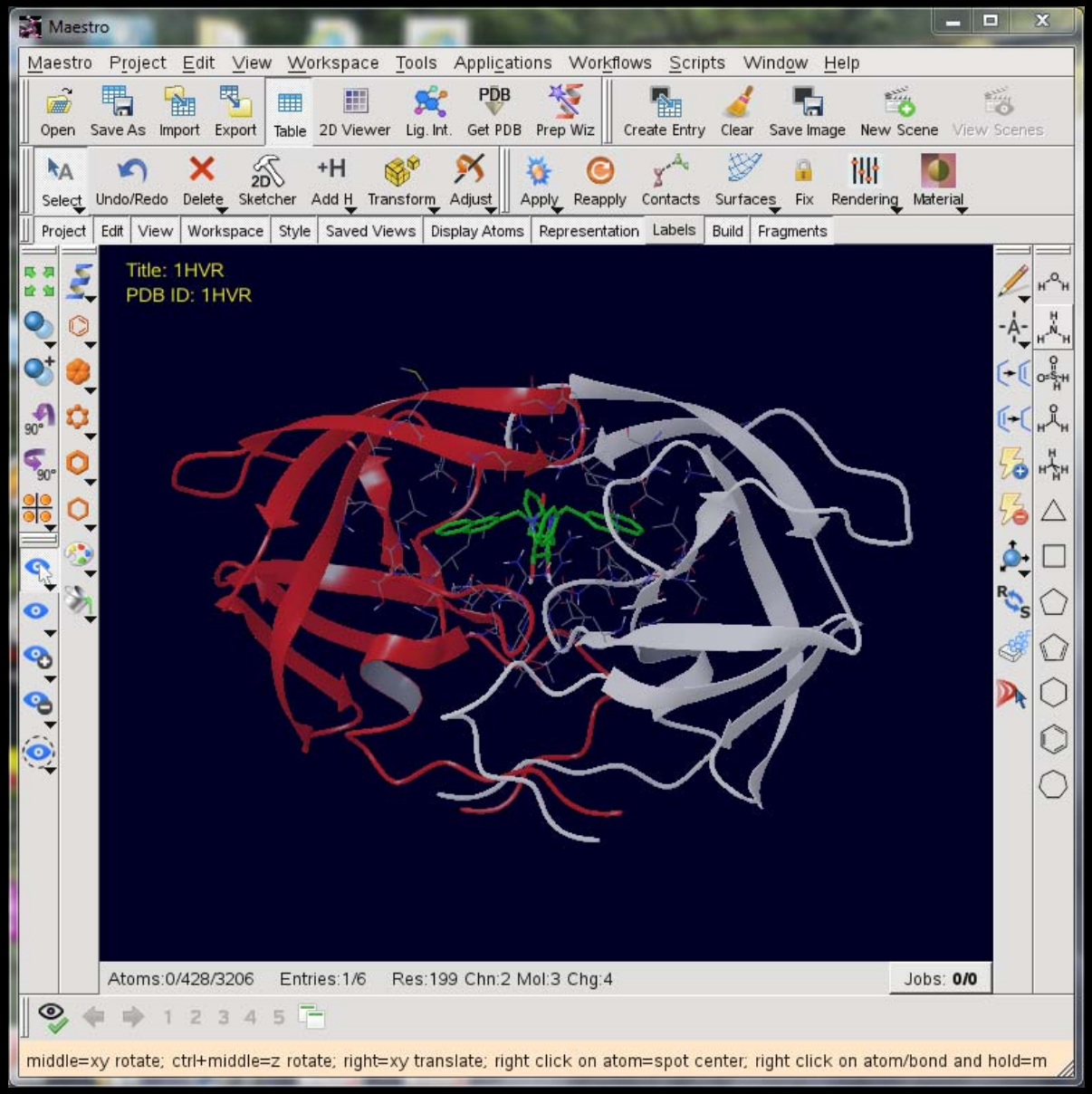
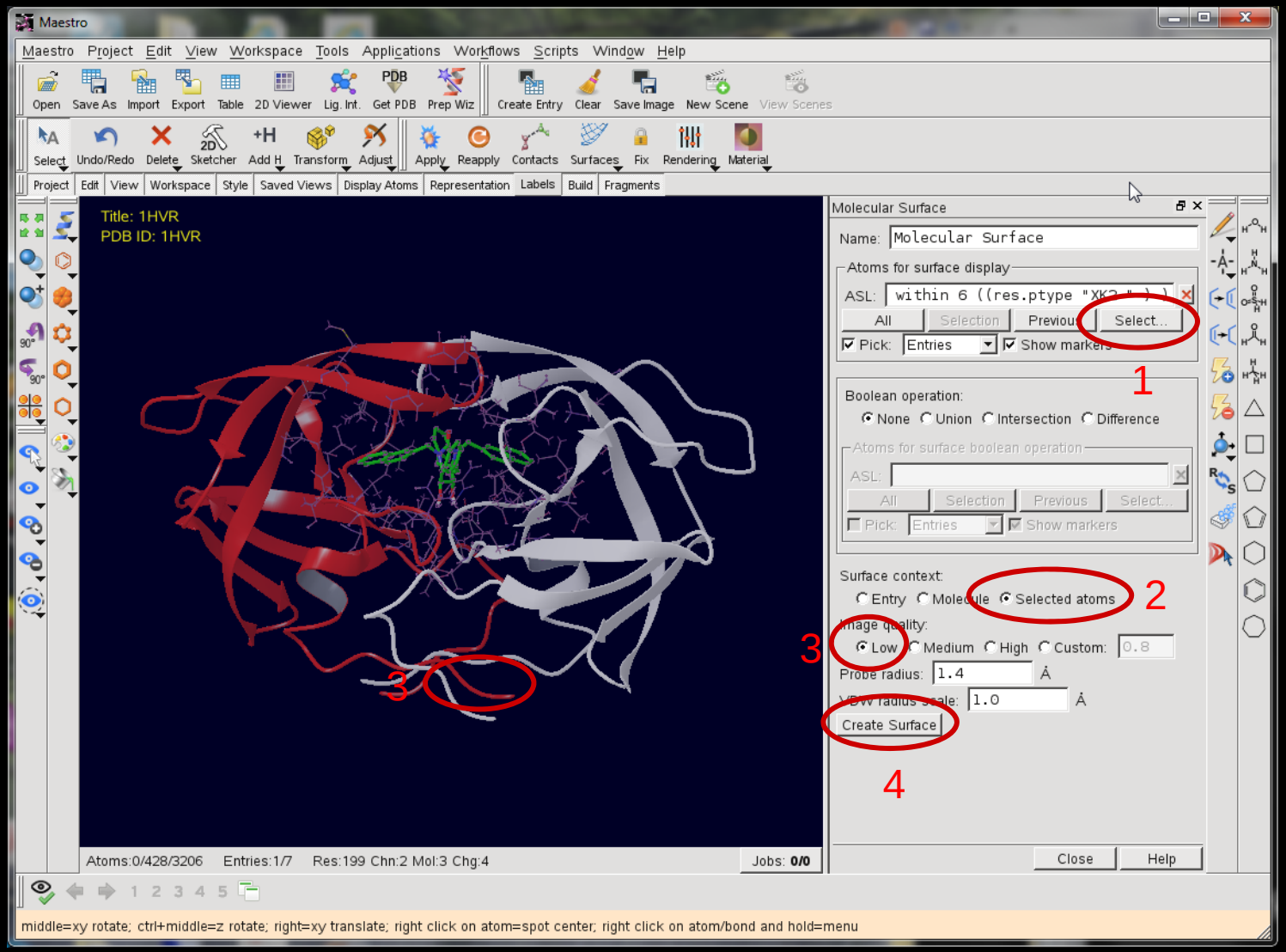
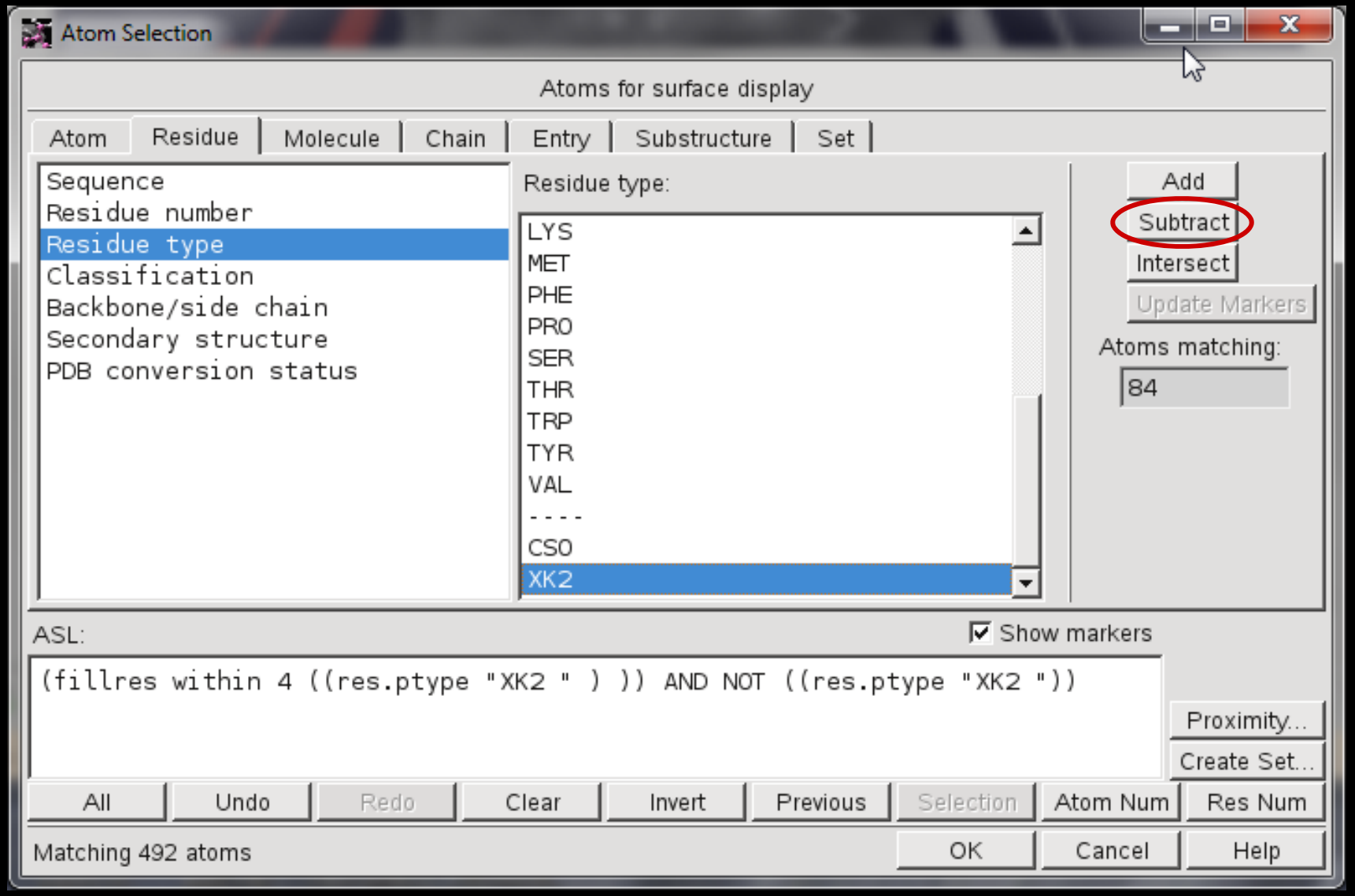


Display Binding Site Surface

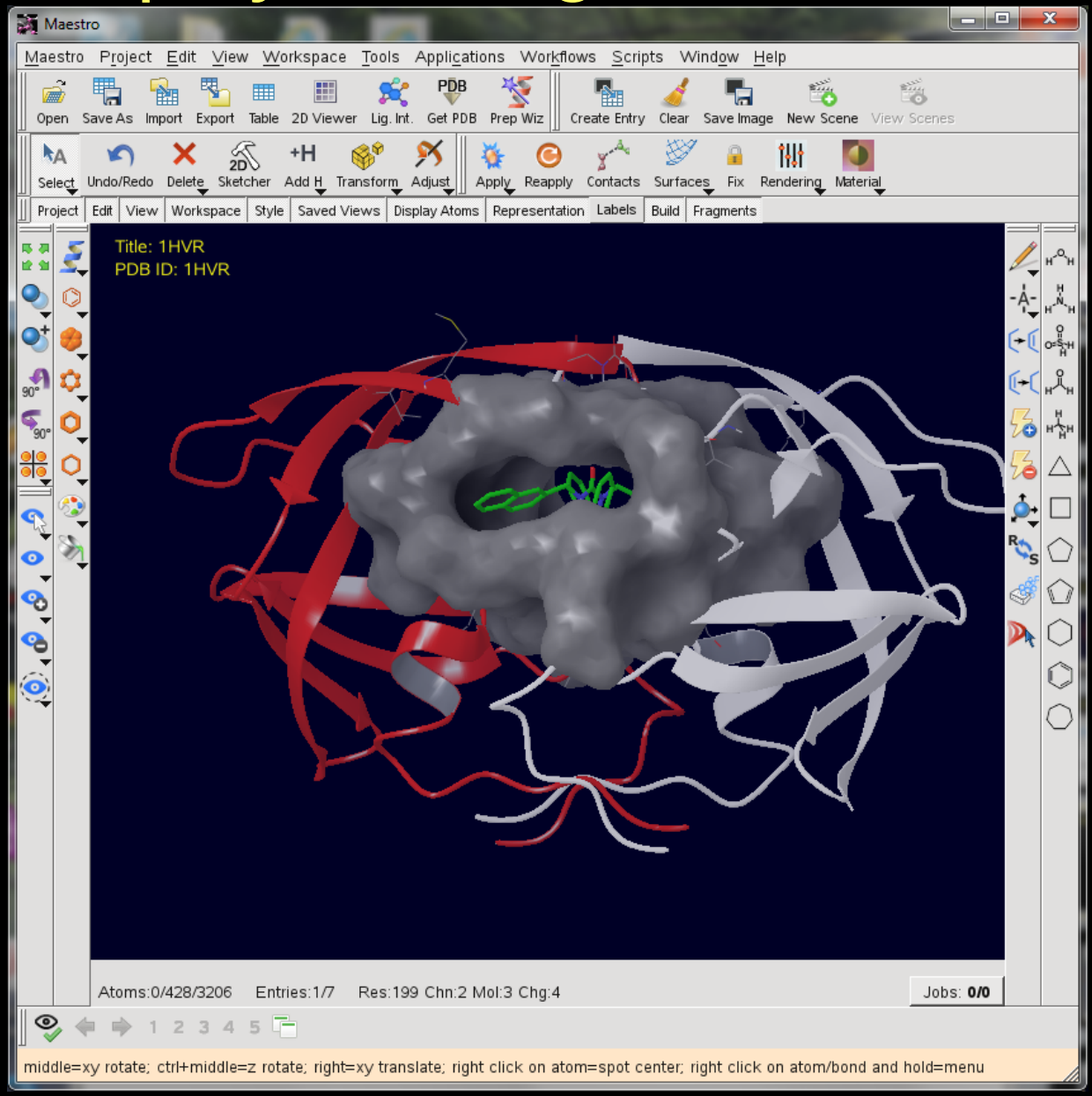


Workspace / Surface / Molecular Surface

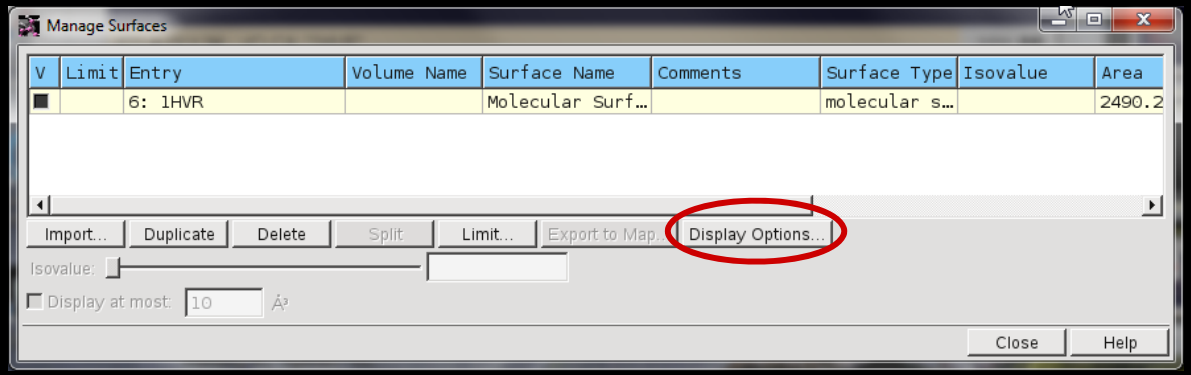
Display Binding Site Surface

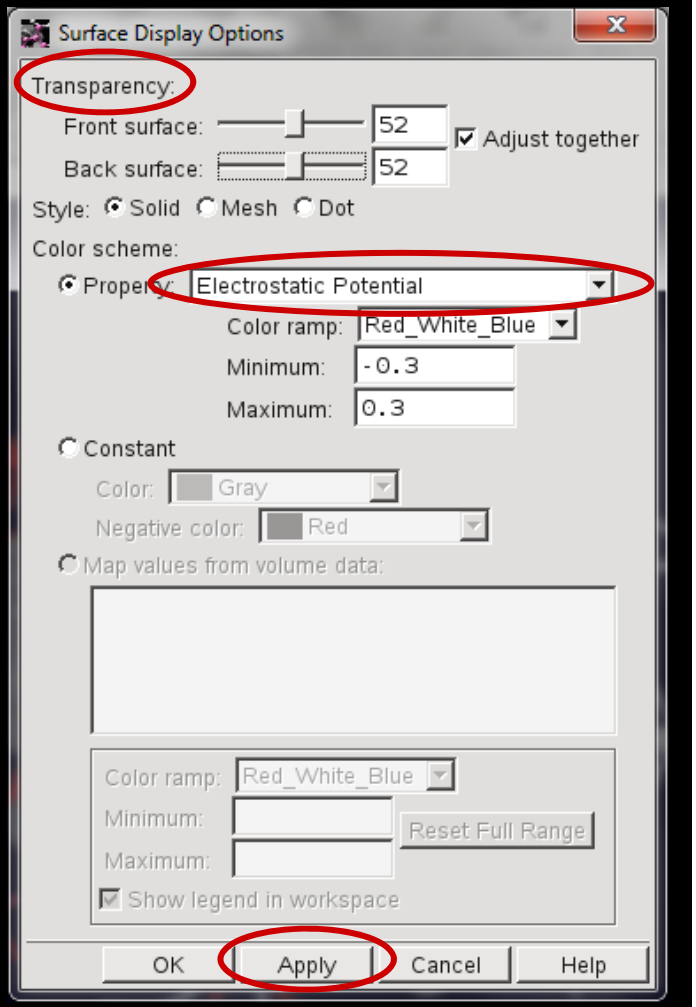


Display Binding Site Surface



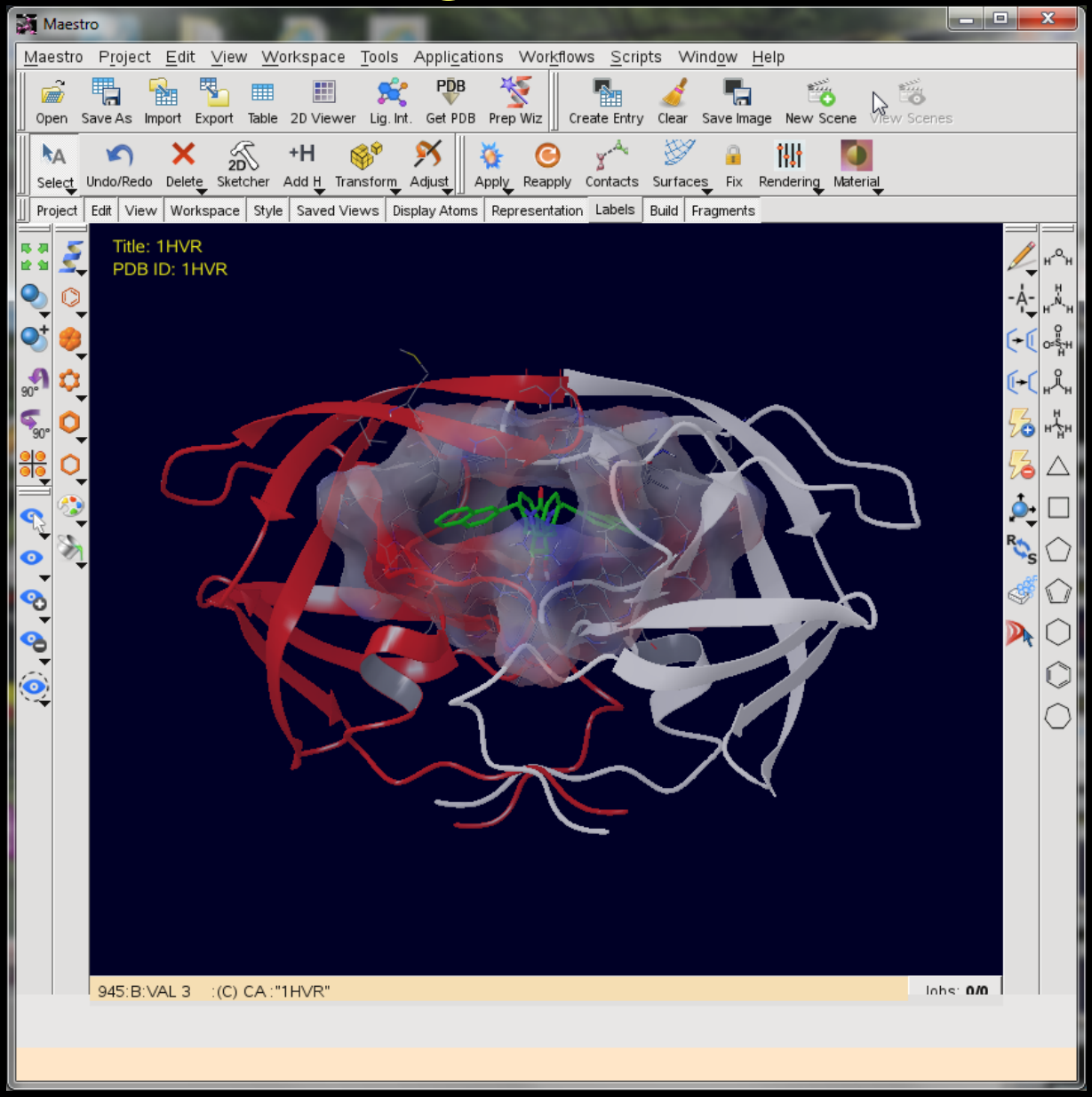
Manage Surfaces



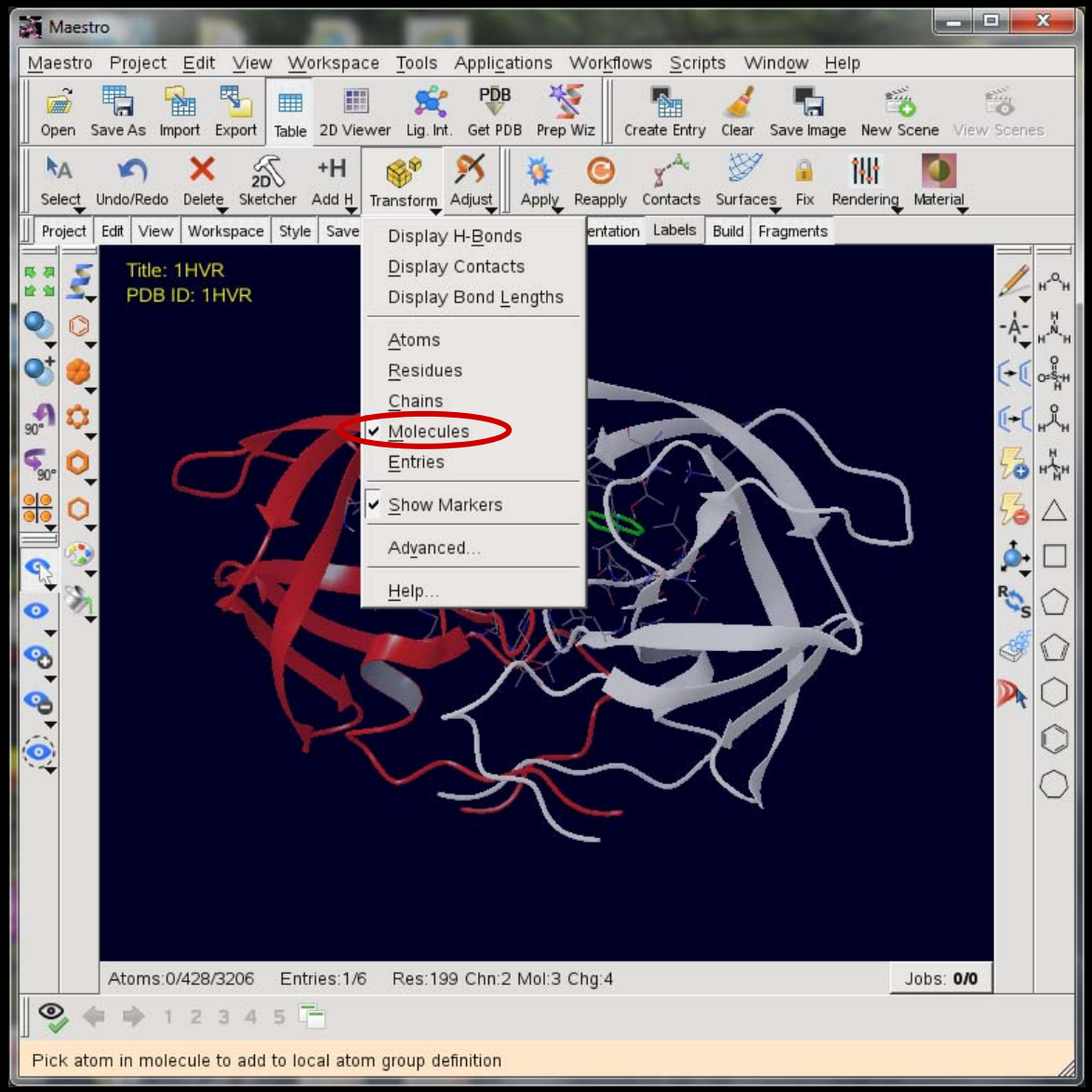


Workspace / Surface / Manage Surfaces

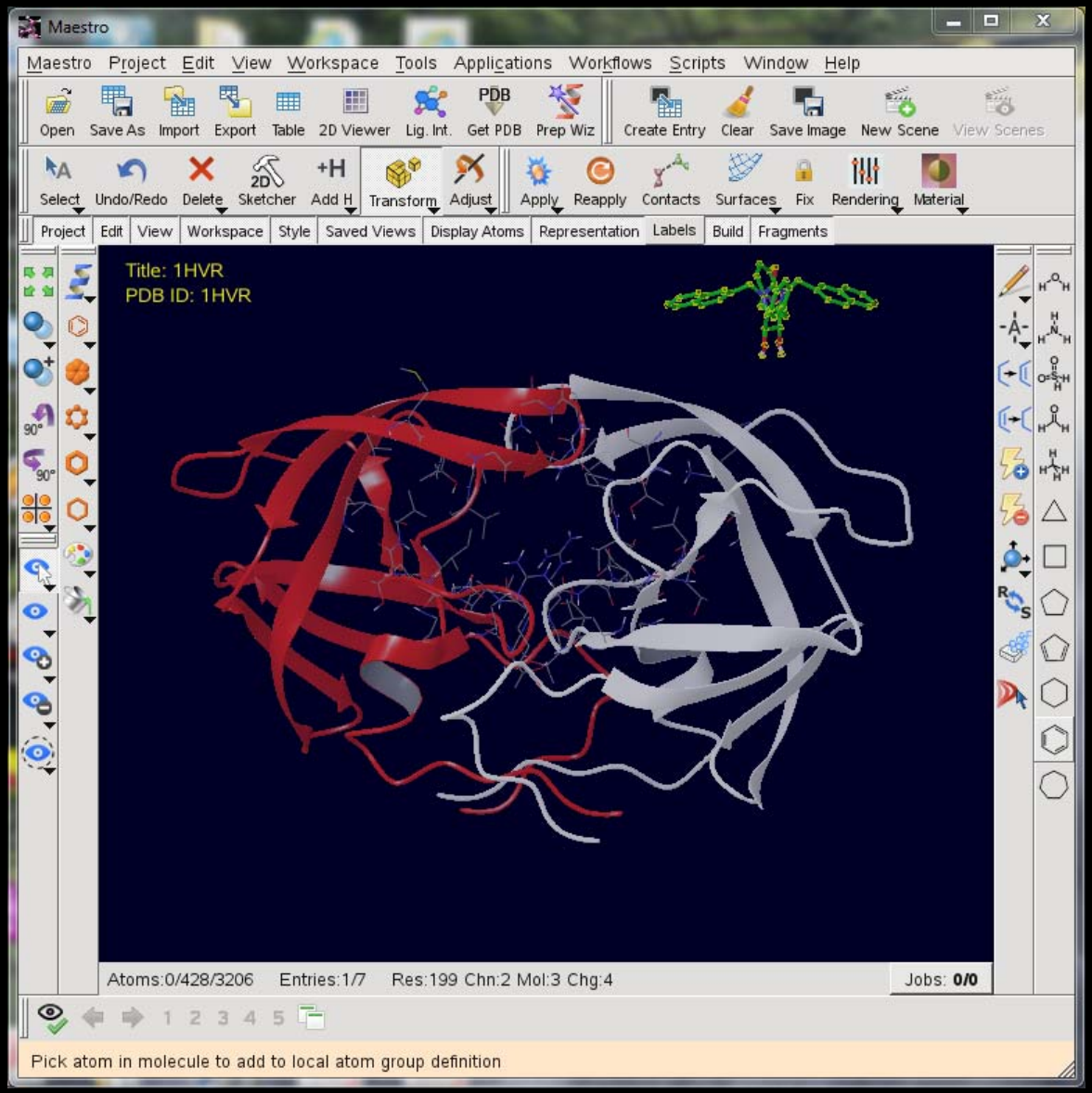
Manage Surfaces



Detach Molecules



Detach Molecules



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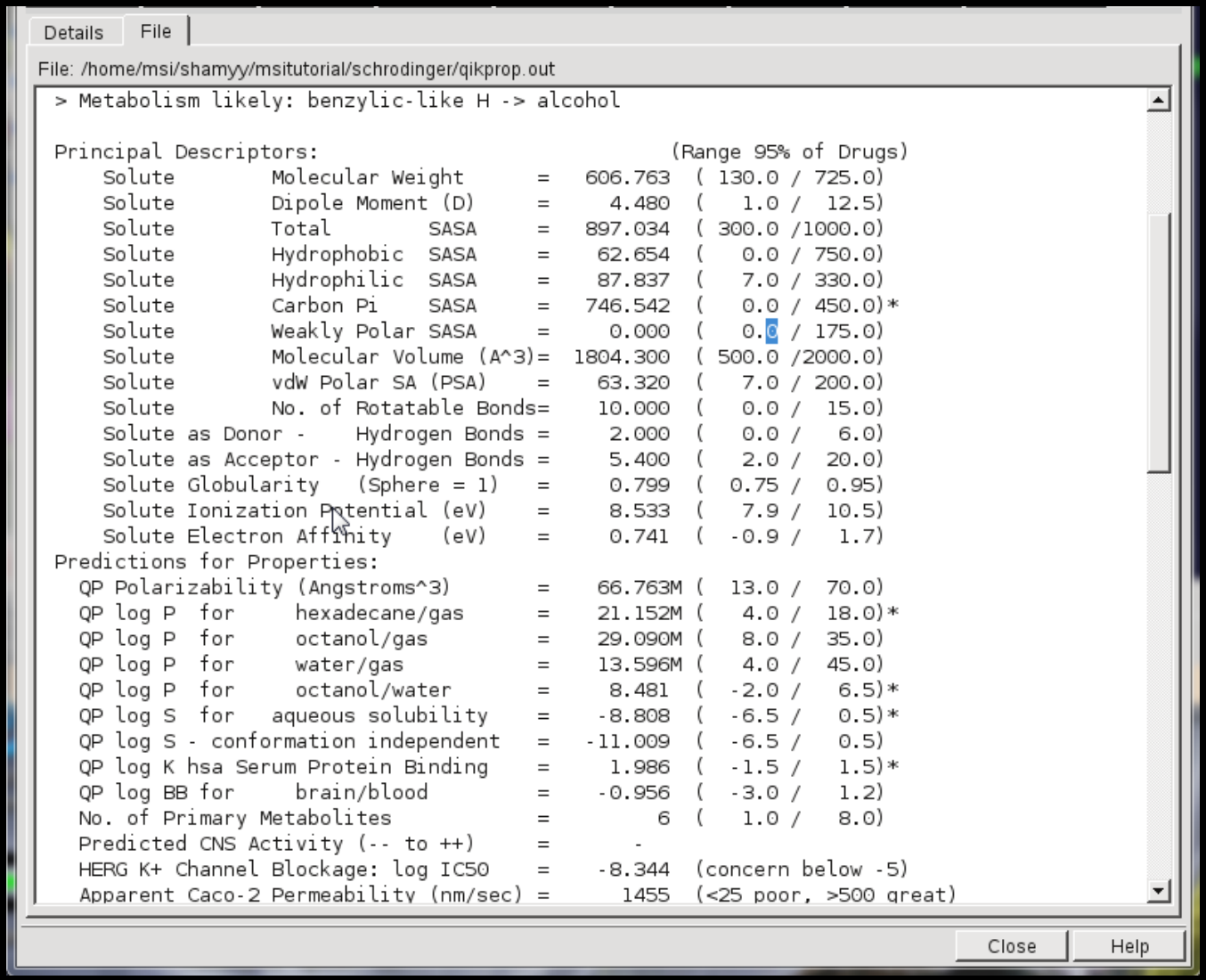
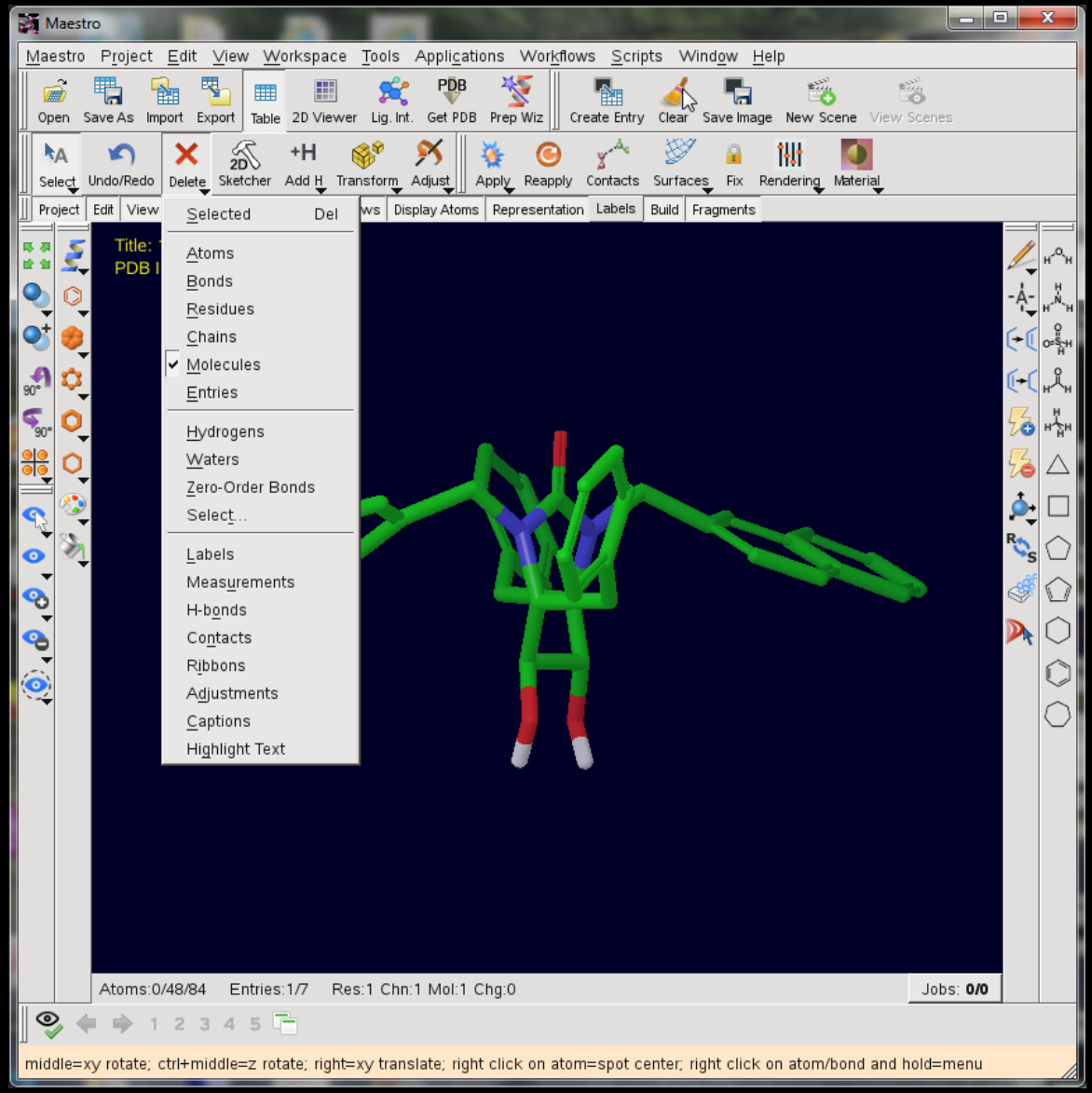
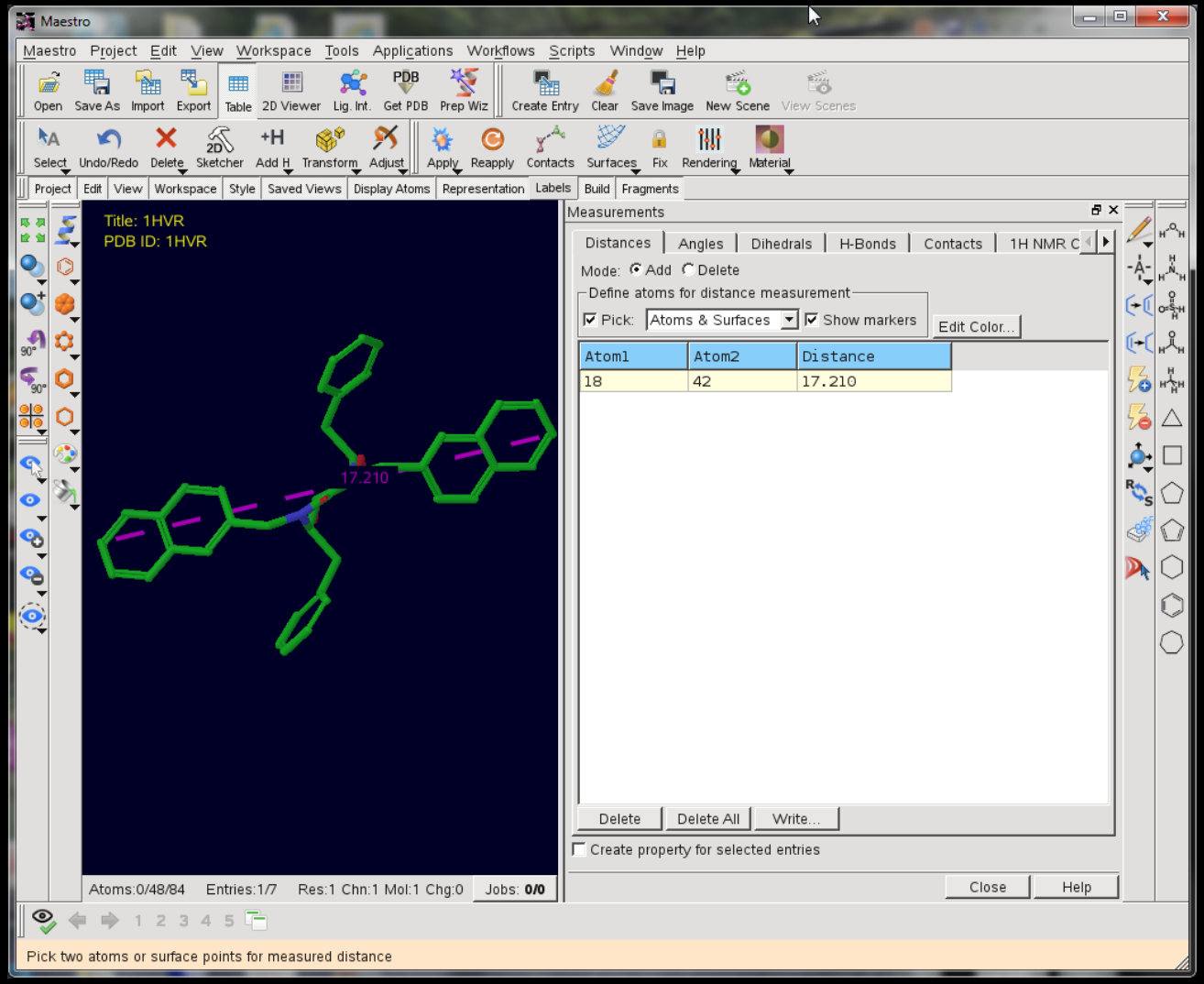


Delete Molecules

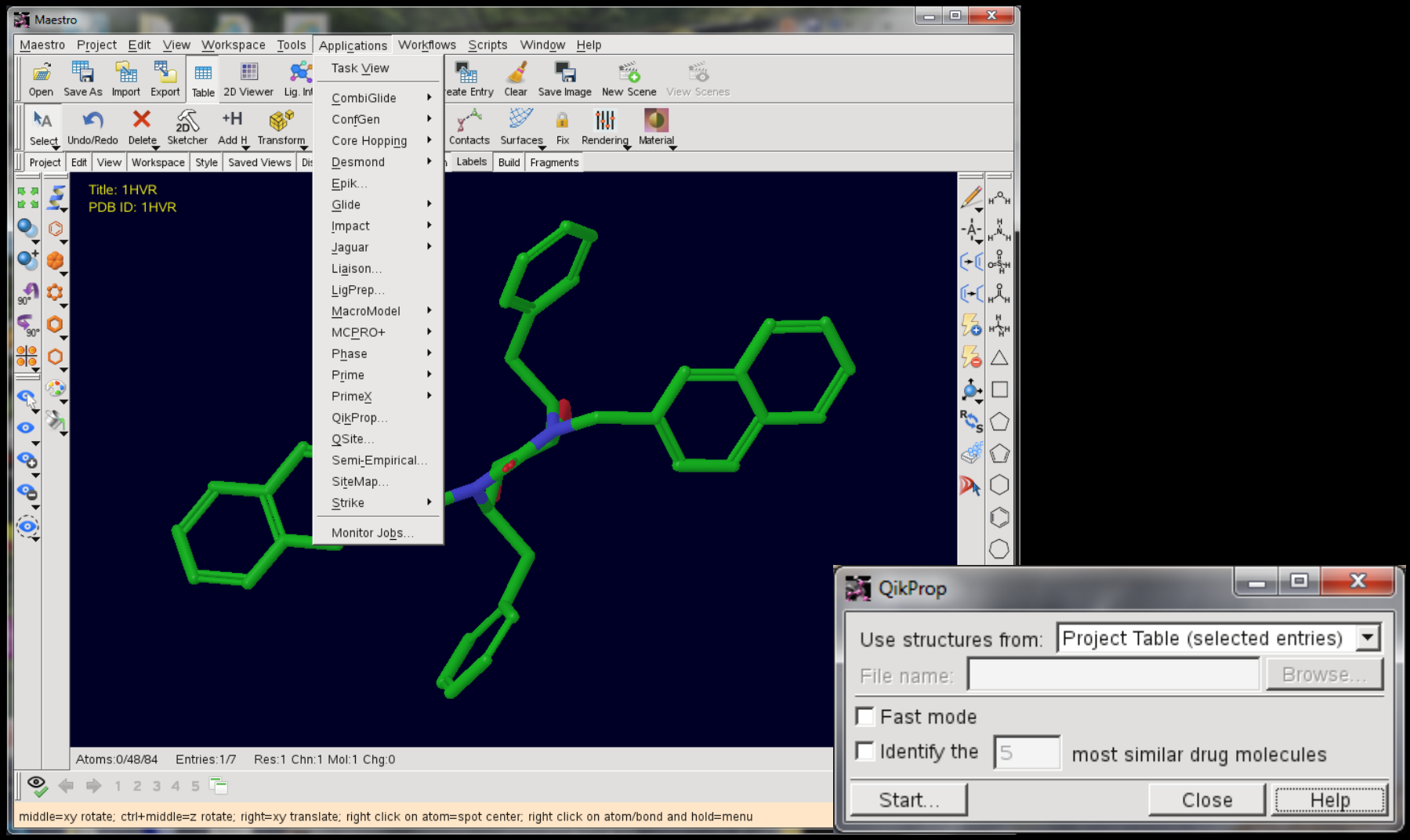


Measure



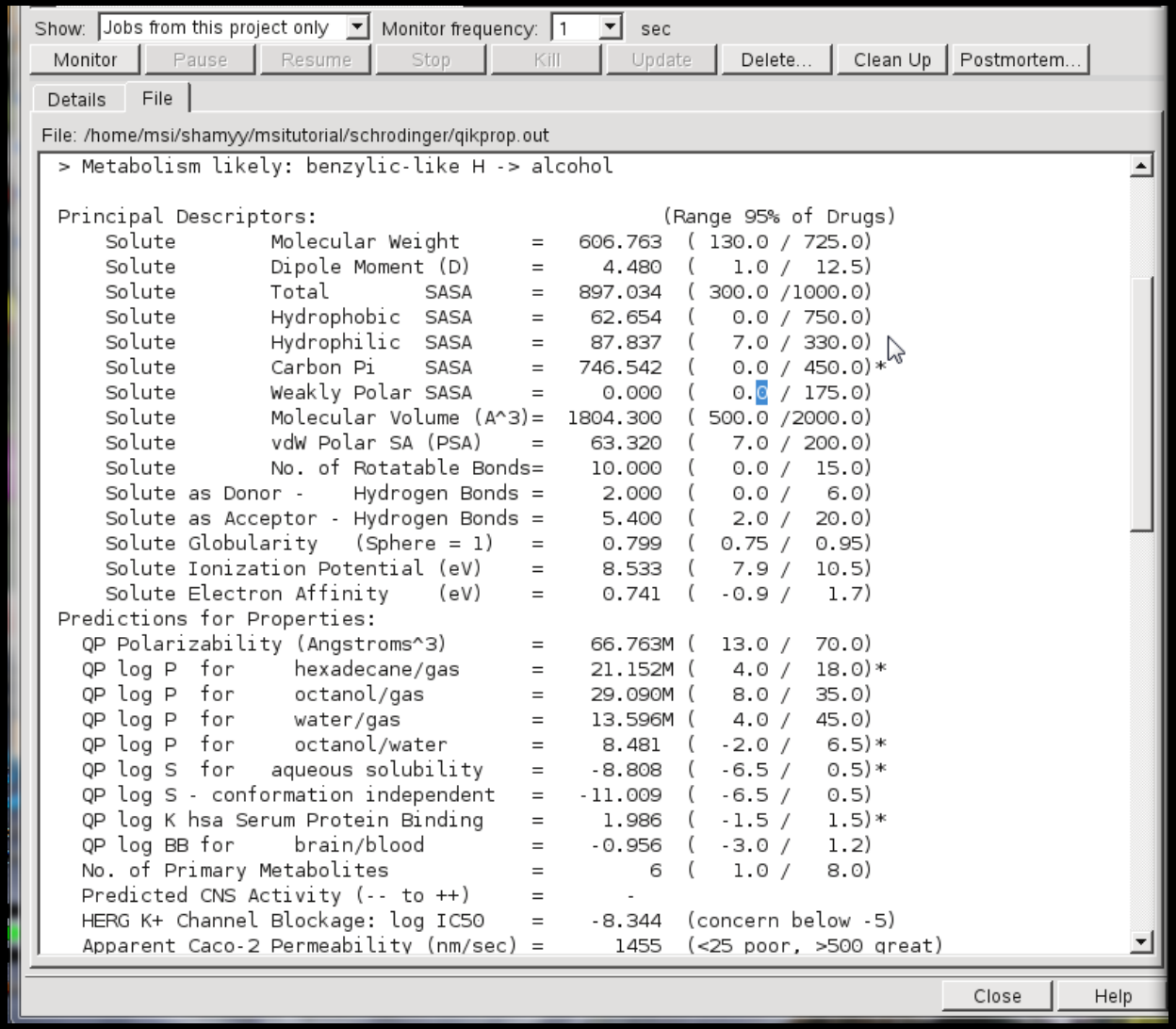
Tools / Measurements / Distance

QikProp



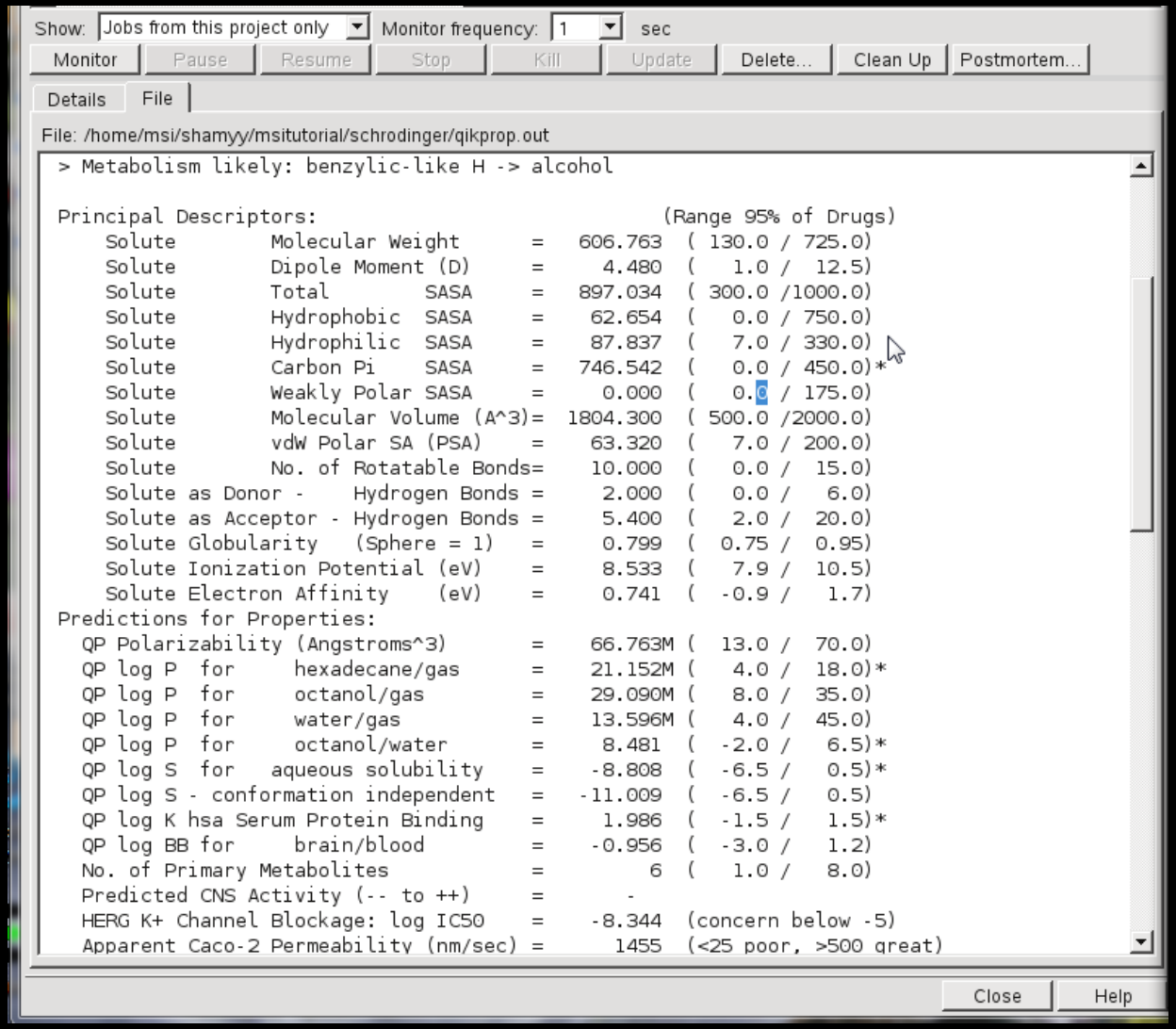
Applications / QikProp

QikProp



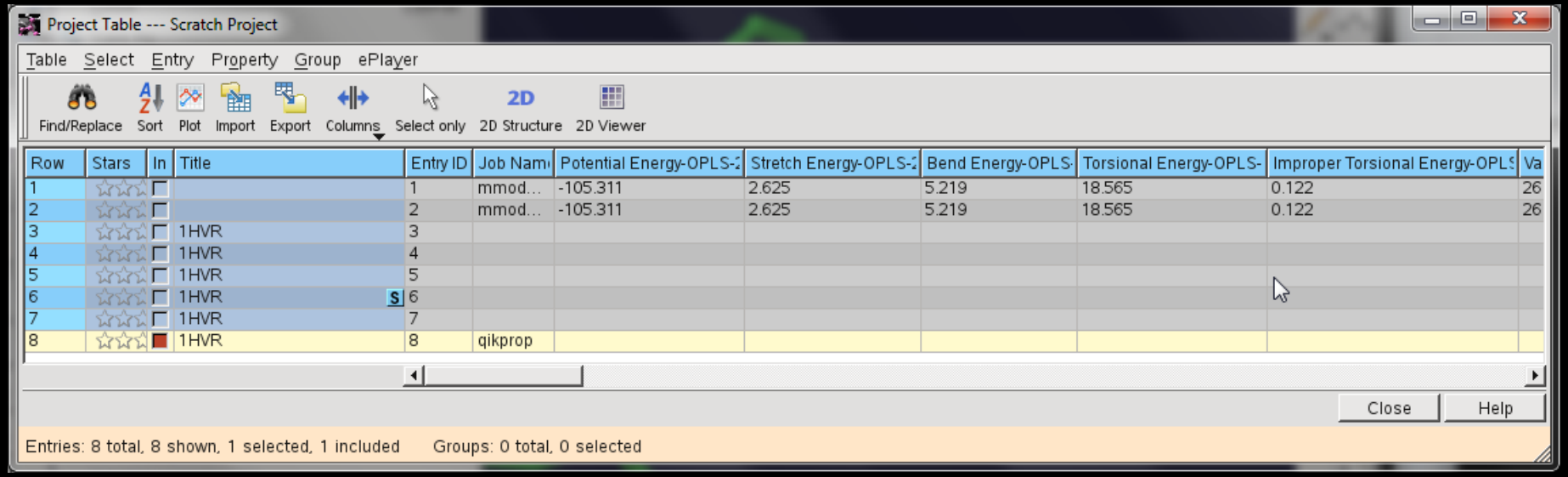
Applications / QikProp

QikProp



Applications / QikProp

Project Table



Project / Show Table

Questions?