Molecular modeling with InsightII

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How to run InsightII

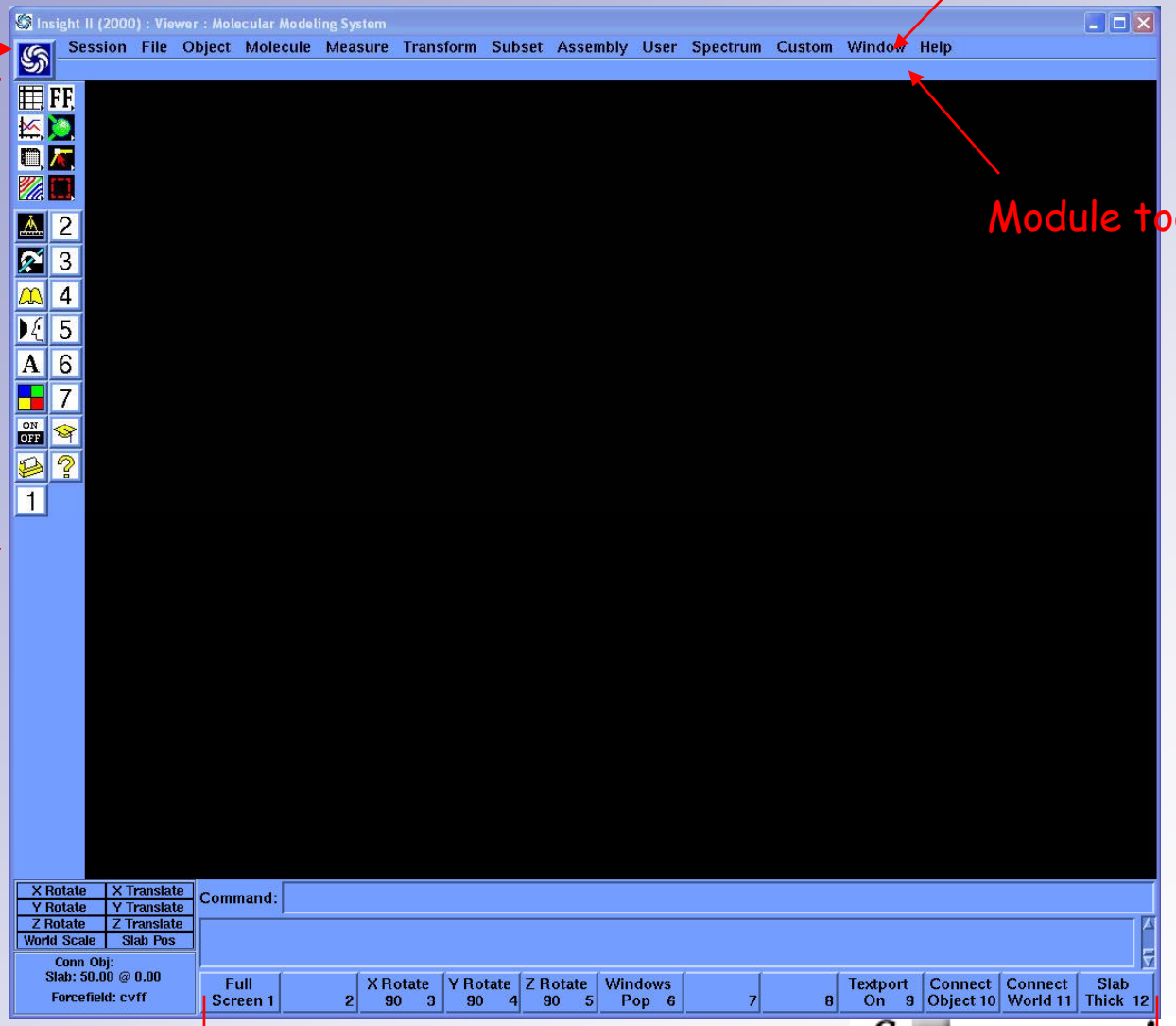
I. Log on a Silicon Graphics Workstation or a Linux Workstation in SDVL, BSCL, CGL or VWL

II. On the terminal window

source /usr/local/accelrys/accelrys.csh

insightII

InsightII the viewer



Accelrys logo

Viewer toolbar

Module toolbar

Frequently Used buttons

Frequently used buttons

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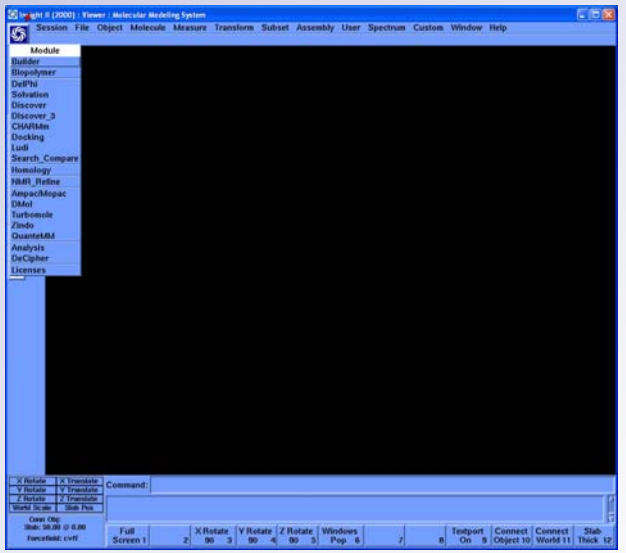
InsightII modules
(under Accelrys logo)

- Builder and Biopolymer (molecular building)
- Delphi (electrostatic calculation)
- Solvation (solvent effect)
- Search and Compare (conformation analysis)
- Homology (sequence comparison)
- Decipher and Analysis (numerical analysis and plotting tools)
- Ludi and Affinity (drug design)
- NMR refined (NMR noe studies)
- Discover, Discover3, Charmm (MD simulation)
- Ampac/Mopac,Dmol,Turomol,Zindo,QuanteMM (semi-empirical calculation)
- And more ….



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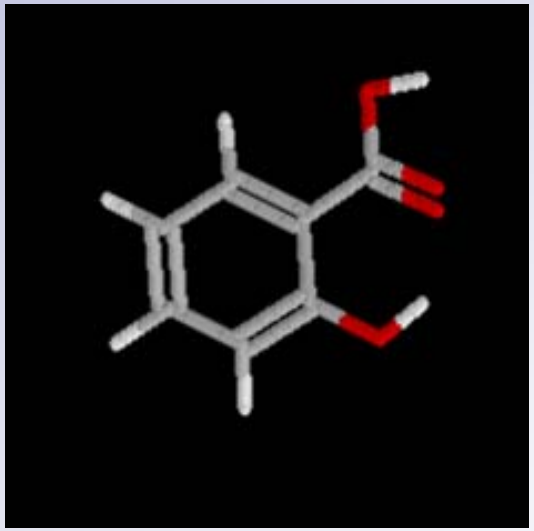
Some nice features of InsightII

- Import/export multiple file format
- Molecule editing and building
- Structure comparison
- Already has the I/O interface to many popular scientific software
- Easy definition and selection option
- High quality graphics
- Export command scripts
- Saving your environment

Building a molecule with Builder

- Salicylic acid (aspirin)
  - **Fragment/get** in the **biopolymer** toolbar, fragment window and get fragment panel will pop up
  - Click **Fragment library** to display desired fragments
  - Select fragment, execute
  - Connect fragment, execute
  - Repeat last two step until molecule is fully build



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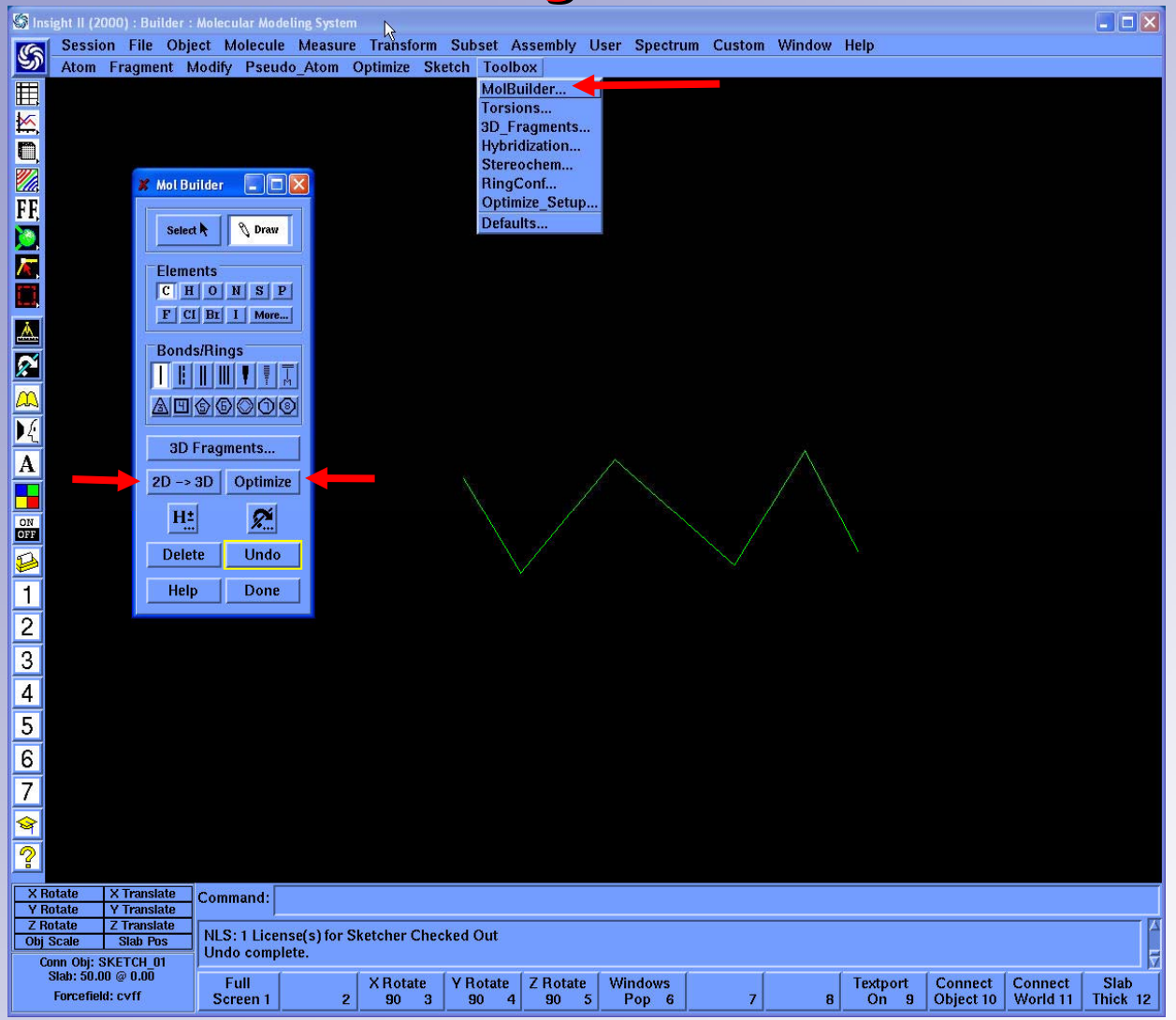
Building a molecule with Builder



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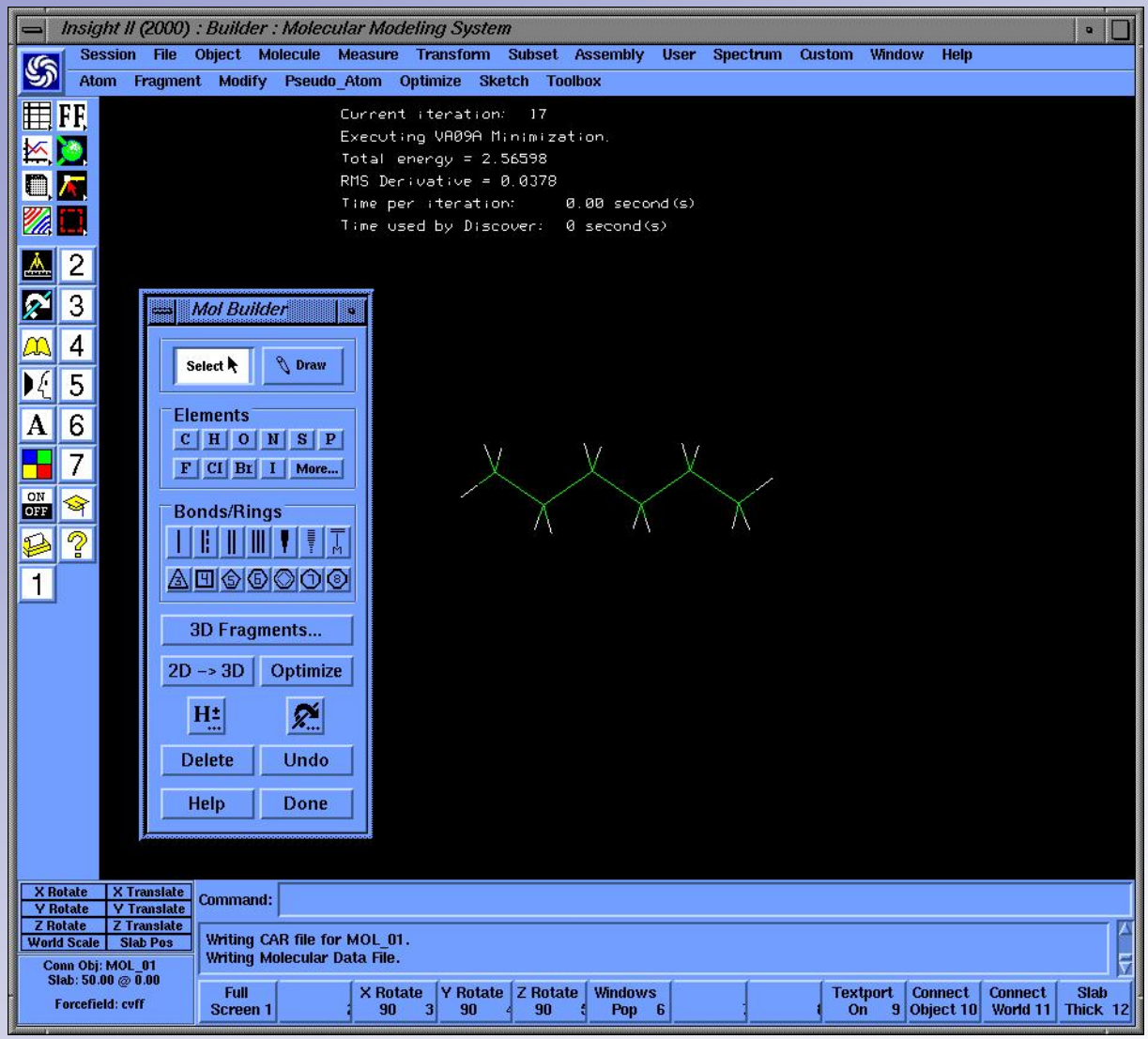
Building a molecule with Builder



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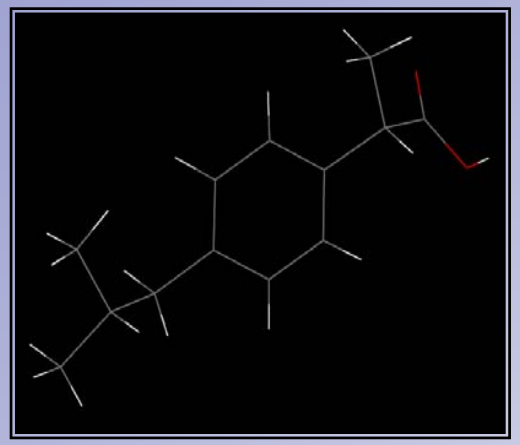
Looking at your molecule

- Rendering your molecule in different format
  - Molecule/render from the viewer toolbar, Render Molecule and Parameters panel will pop up
  - Under Render Style, select rendering format
  - Go to Molecule Spec, Select molecule from Parameters panel
  - Depending on your format selection, different parameters will appear for each rendering format. Change them to what you like
  - Execute

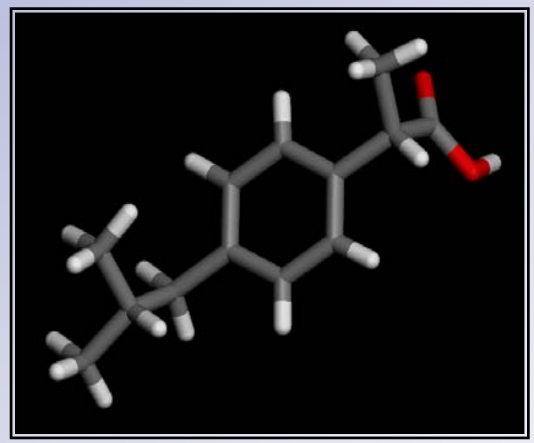
- Rendering the Secondary structure of a protein
  - Molecule/secondary render from the viewer toolbar, Secondary Render and Parameters panel will pop up
  - Go to Molecule Name box, Select molecule from Parameters panel
  - Under Render_Operation, select create
  - Under Classify_Source, Toggle on Kabsch_Sander or PDB_Classification
  - Toggle on Helices, Sheets, Turns and Random_Coil
  - Execute

(if running insightII without OpenGL, rendering in ribbon, secondary structure, sticks, CPK and ball and Stick format will not work)

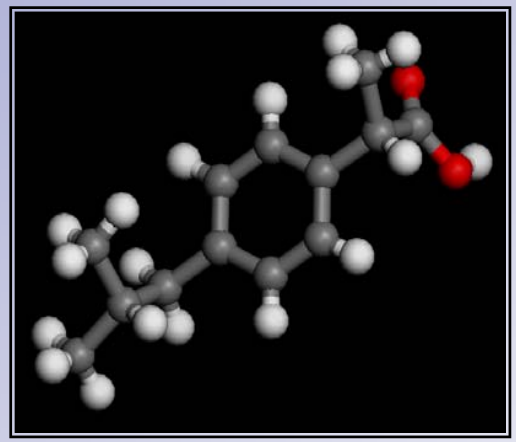
Rendering formats



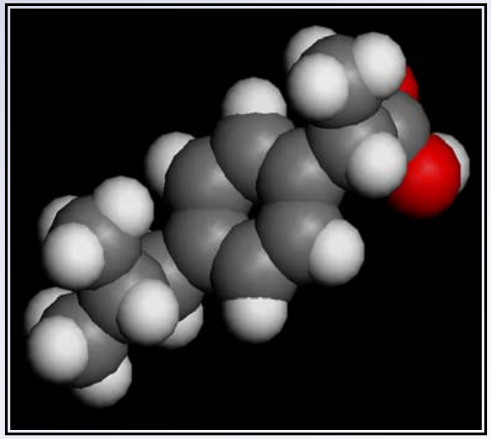
lines



sticks



ball and sticks



CPK

You and your mouse

- Right mouse click to rotate
- Middle mouse click to translate
- Left mouse click and drag to select
- Mouse point at atom or bond and left mouse click to select atom or bond
- Left and middle mouse click (together) to change the depth cue
- Middle and right mouse click (together) to zoom in and out

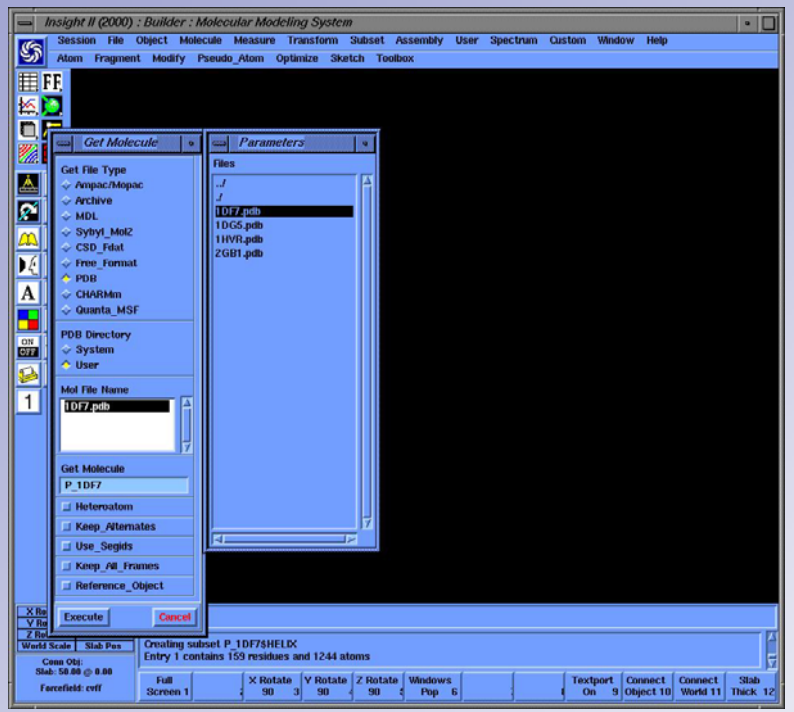
Distance, Angles, Dihedral

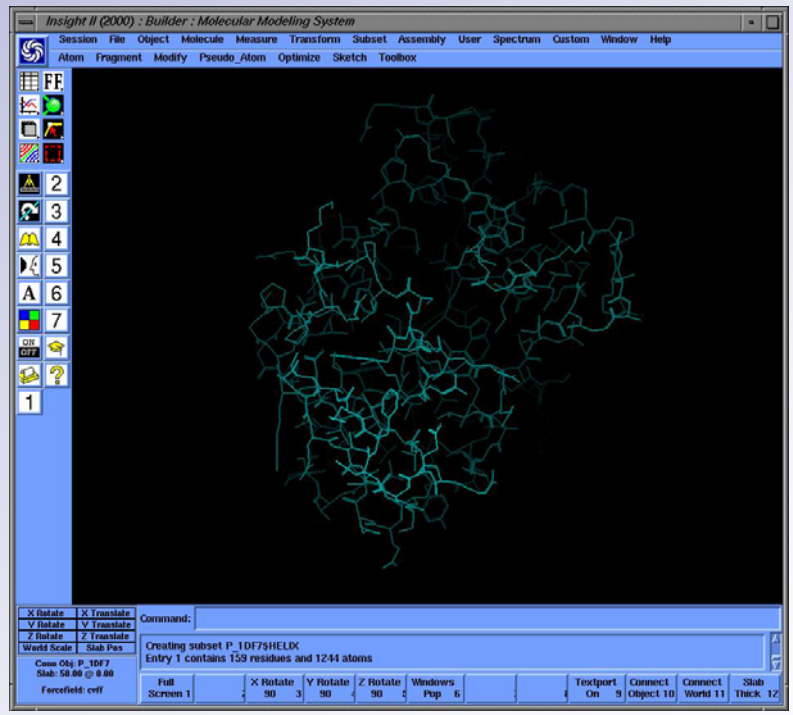
- Measuring distance between two atoms
  - Measure/Distance from the viewer toolbar, Distance panel will pop up
  - Toggle on Monitor
  - Under Monitor Mode, toggle on Add
  - Go to Atom 1 box, point and click first atom from viewer screen
  - Go to Atom 2 box, point and click second atom from viewer screen
- Measuring angle between three atoms
  - Measure/Distance from the viewer toolbar, Distance panel will pop up
  - Toggle on Monitor
  - Under Monitor Mode, toggle on Add
  - Go to Atom 1 box, point and click first atom from viewer screen
  - Go to Atom 2 box, point and click second atom from viewer screen
  - Go to Atom 3 box, point and click third atom from viewer screen
- Measuring dihedral angle between three atoms
  - Measure/Distance from the viewer toolbar, Distance panel will pop up
  - Toggle on Monitor
  - Under Monitor Mode, toggle on Add
  - Go to Atom 1 box, point and click first atom from viewer screen
  - Go to Atom 2 box, point and click second atom from viewer screen
  - Go to Atom 3 box, point and click third atom from viewer screen
  - Go to Atom 4 box, point and click fourth atom from viewer screen

Loading PDB file in insightII

- Viewing the biomolecule in pdb file format
  - Molecule/get from the viewer toolbar, Get Molecule and Parameters panel will pop up
  - Toggle on PDB in Get file type
  - Go to Mol File Name box, select the pdb file in parameter panel
  - Give a name in Get Molecule Box
  - Toggle on Heteroatom if you want heteroatoms (eg. Ligand, cofactors, water) to be loaded and display along with the protein
  - execute

Loading in a molecule





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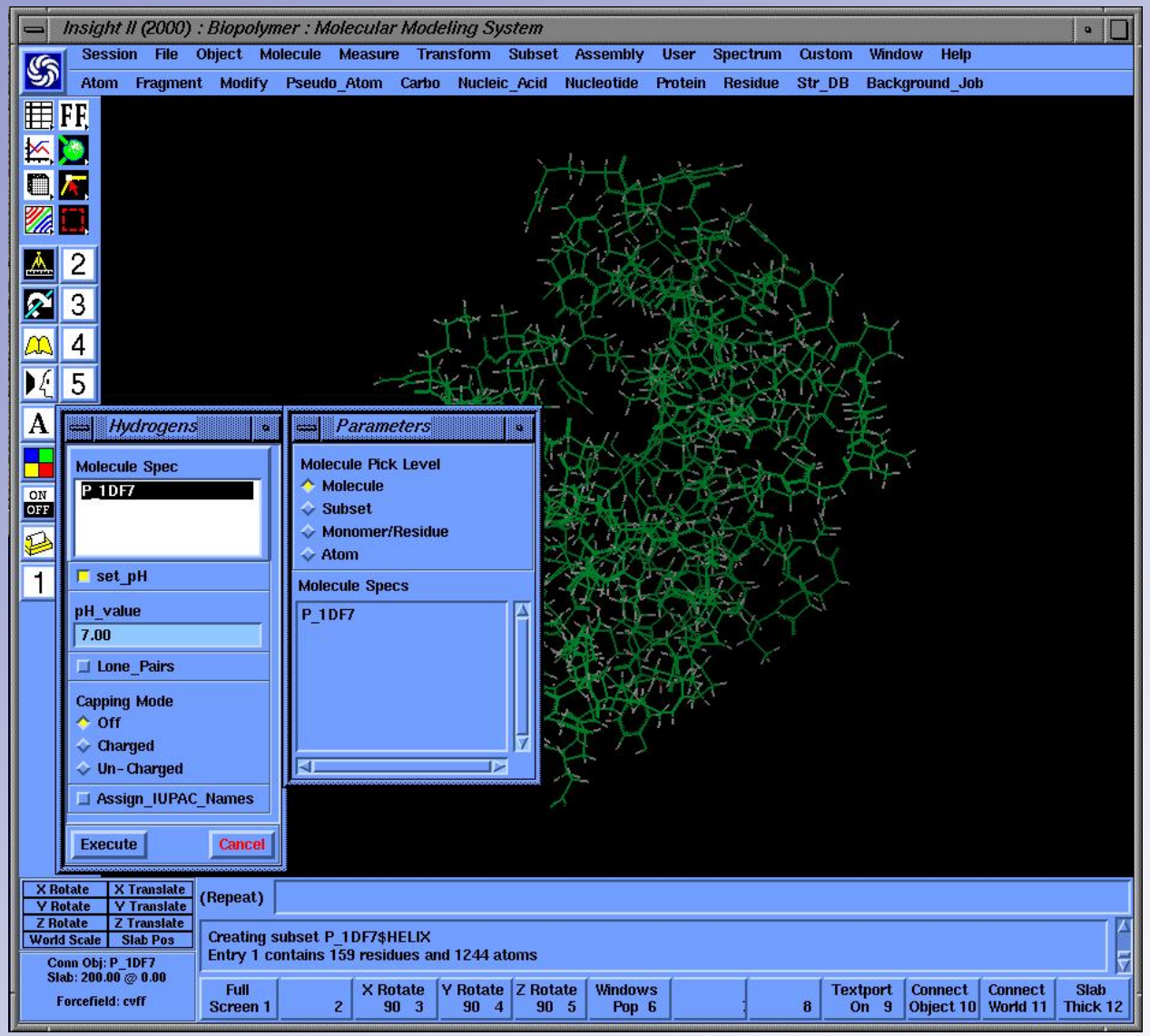
Patching up your protein molecule

- Patching missing residues
  - Residue/replace from the biopolymer toolbar, Residue Replace panel will pop up
  - In the Residue Replace box, define name of residue (general format is molecule name:residue id)
  - Go to Residue box, select residue type from Parameters panel
  - Define Chirality (L or R)
  - Execute
- Capping protein chain
  - Protein/cap from the biopolymer toolbar, Cap Protein and Parameters panel will pop up
  - Go to Molecule Name box, select objects in Parameters panel
  - Select C and N cap groups
  - Execute
- Adding missing hydrogens
  - Modify/hydrogens from the biopolymer toolbar, Hydrogen and Parameters panel will pop up
  - Go to Molecule Spec box, select molecule in Parameter panel
  - Toggle on set_PH, PH_value box will appear
  - Go to PH_value box, enter pH value (enter 7 for neutral environment).
  - Toggle on desired Capping mode
  - Execute

Add H's



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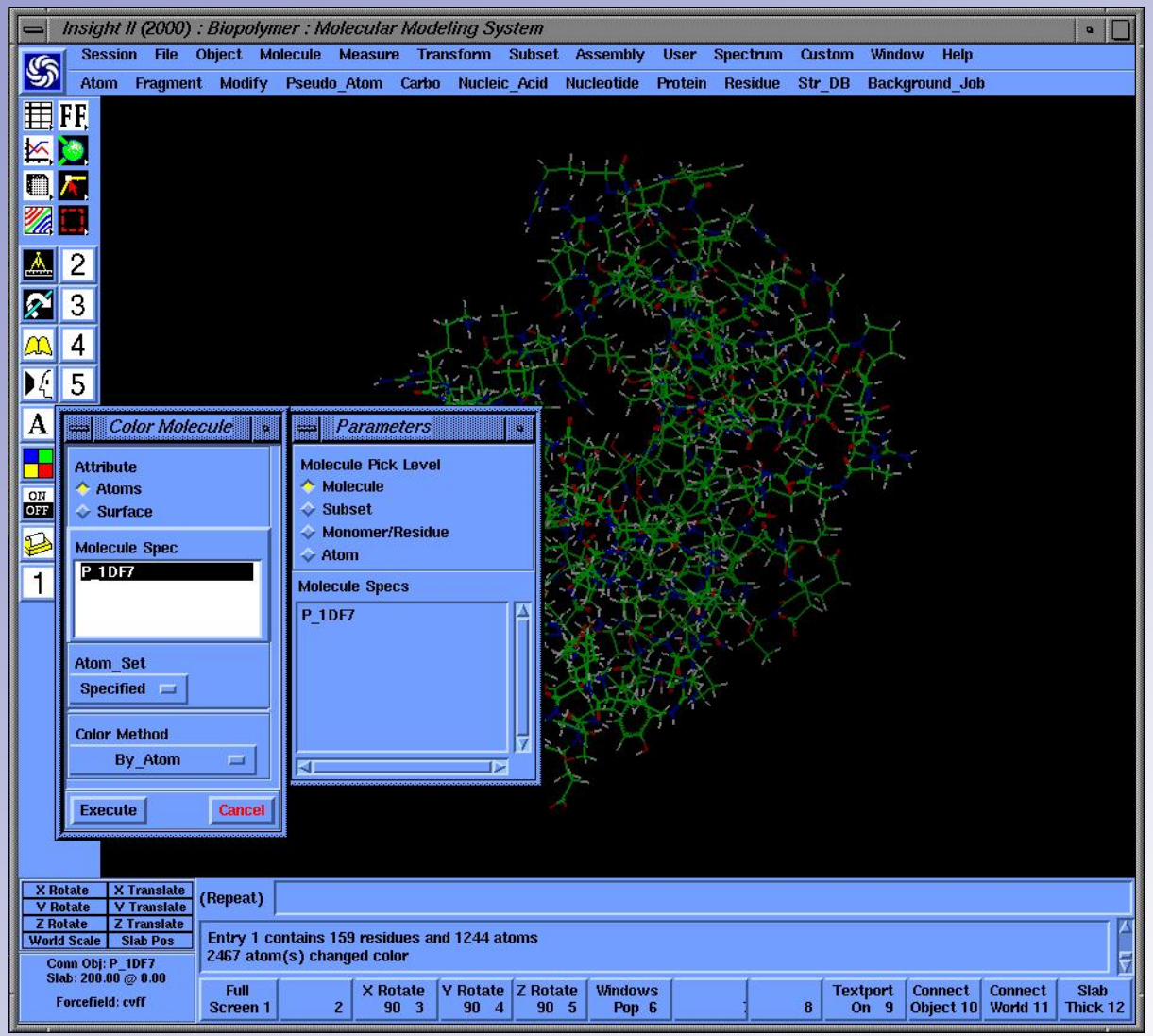
Coloring Atoms



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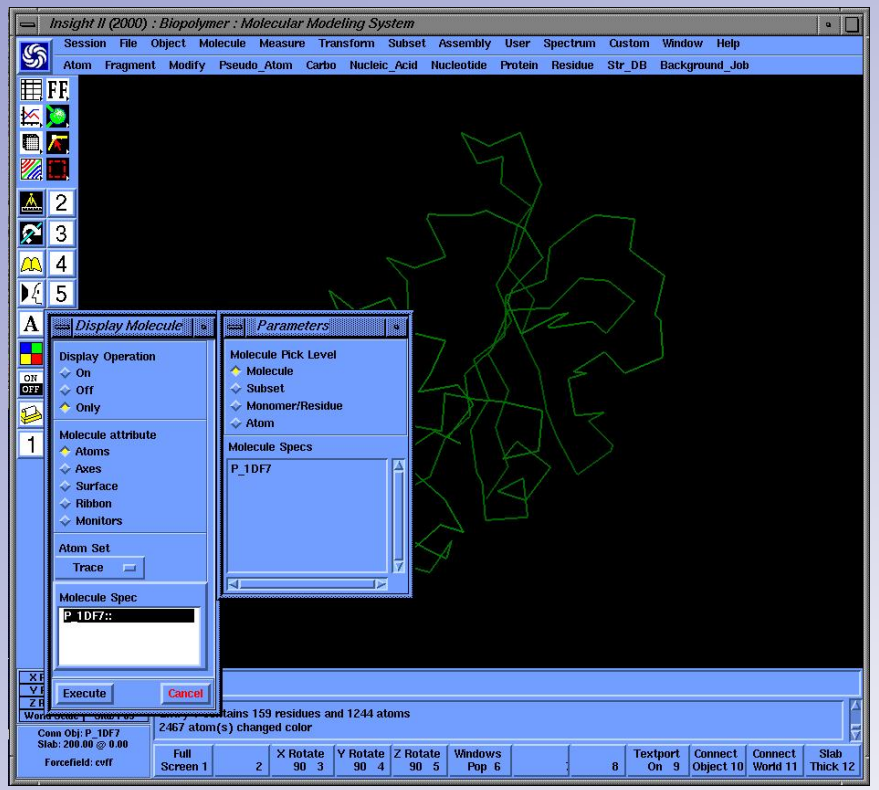
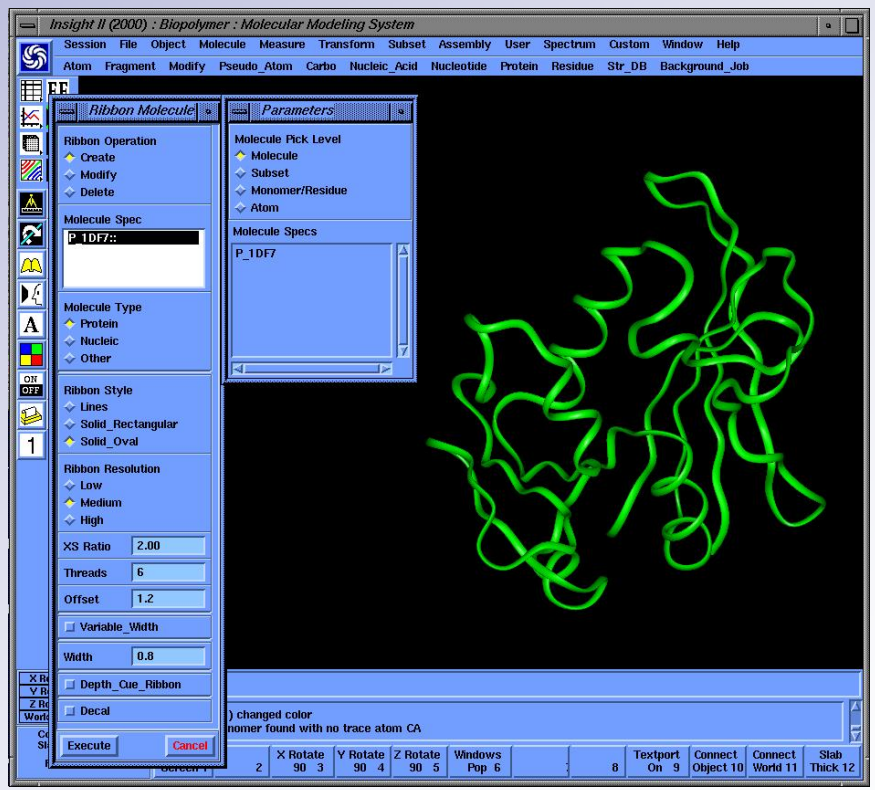
Looking at your molecule

- Displaying and turning off a specified atom set
  - Molecule/display from the viewer toolbar, Display Molecule and Parameters panel will pop up
  - Under Display Operation, select on or off option
  - Under Molecule attribute, select atoms
  - Click on Atom Set/Specified to find the list of predefined atom set. Select your set.
  - Go to Molecule Spec, Select molecule from Parameters panel
  - Execute
- Display your molecule as a Ribbon
  - Molecule/ribbon from the viewer toolbar, Ribbon Molecule and parameters panel will pop up
  - Under Ribbon operation, toggle on create
  - Go to Molecule Spec, Select molecule from Parameters panel
  - Under Molecule Type, toggle on Protein
  - Under Ribbon Type, toggle on the desired ribbon format
  - Define ribbon quality under Ribbon Resolution and change ribbon format parameters if necessary
  - Execute

Displaying and Rendering





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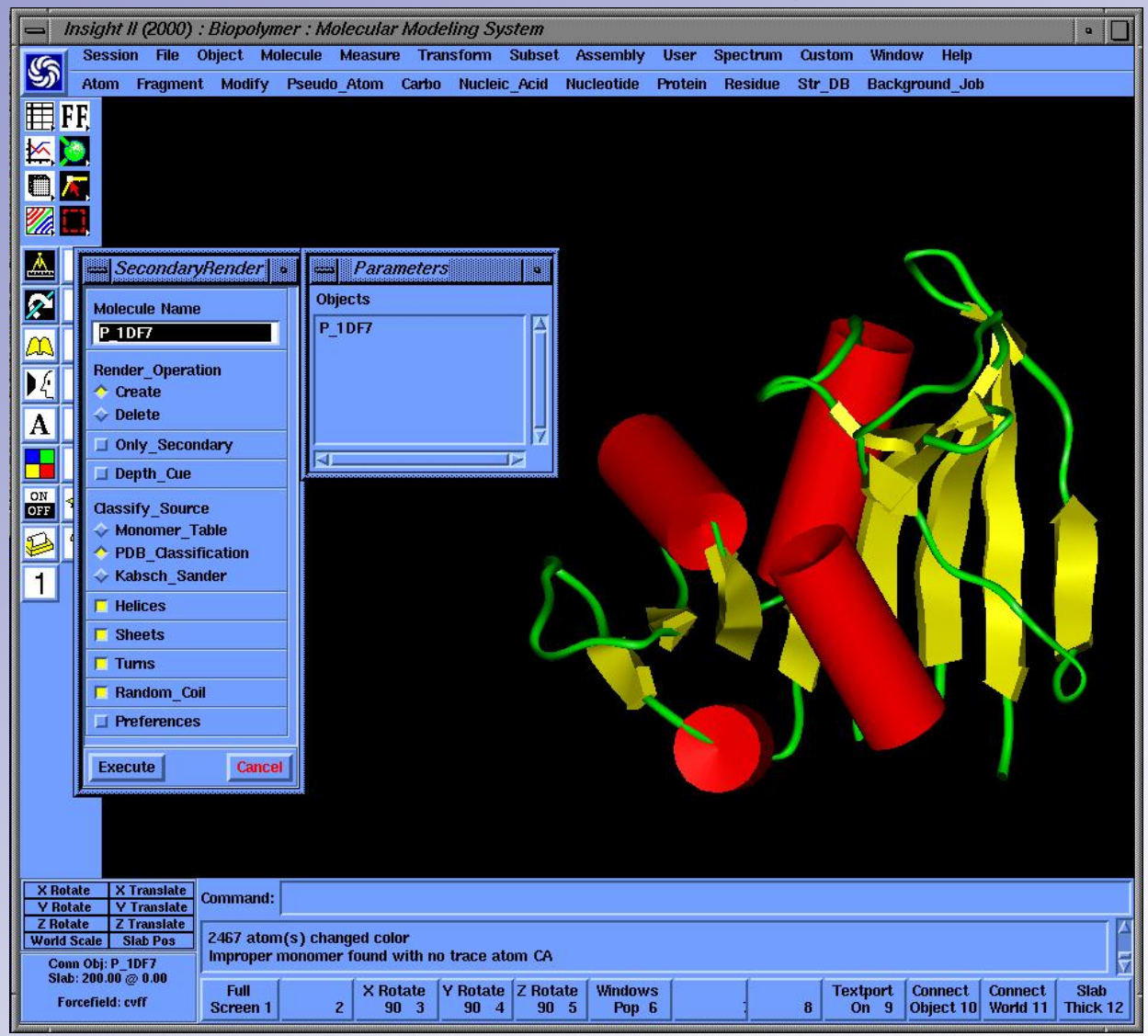
Displaying and Rendering



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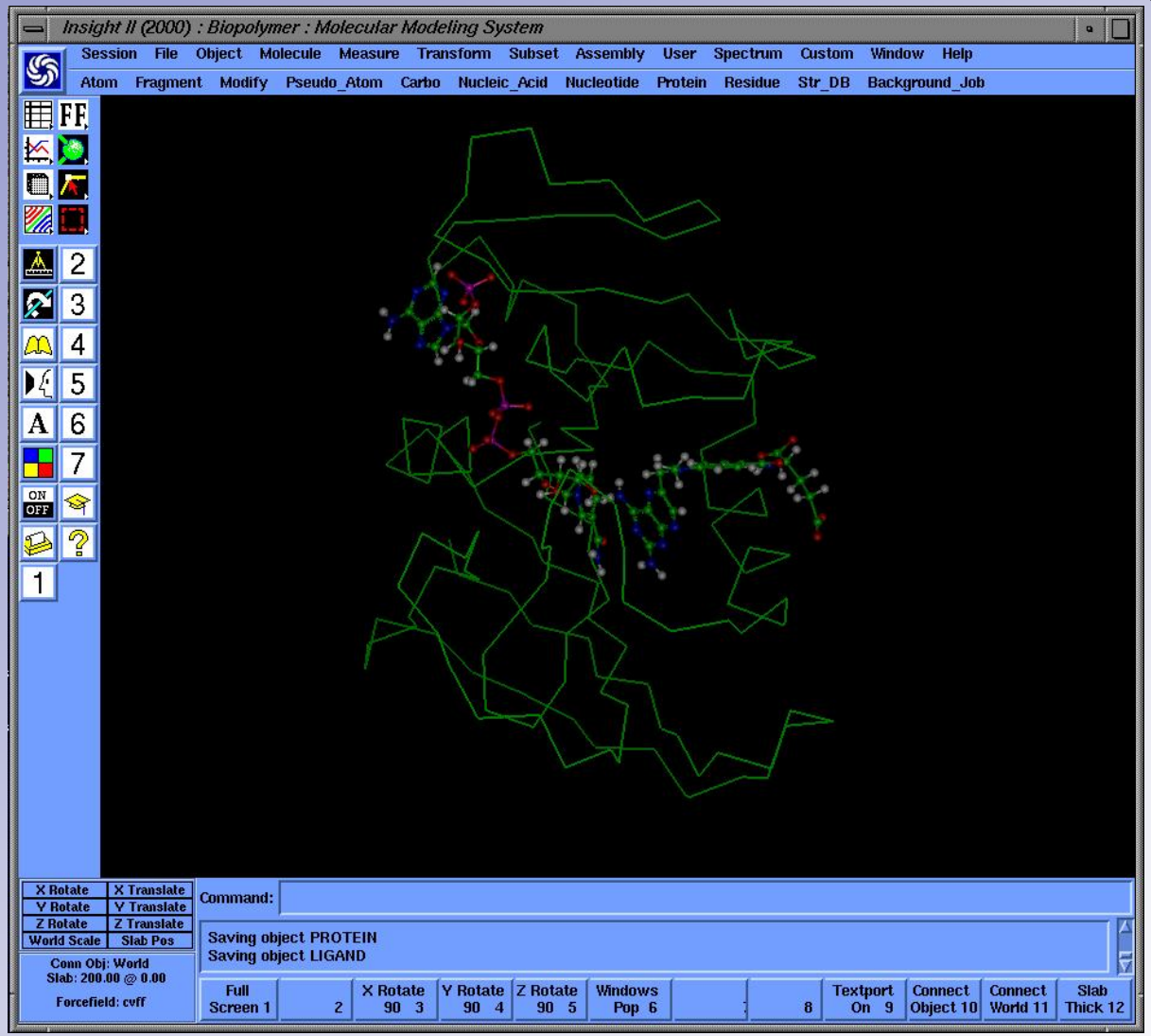
Protein Ligand Complex



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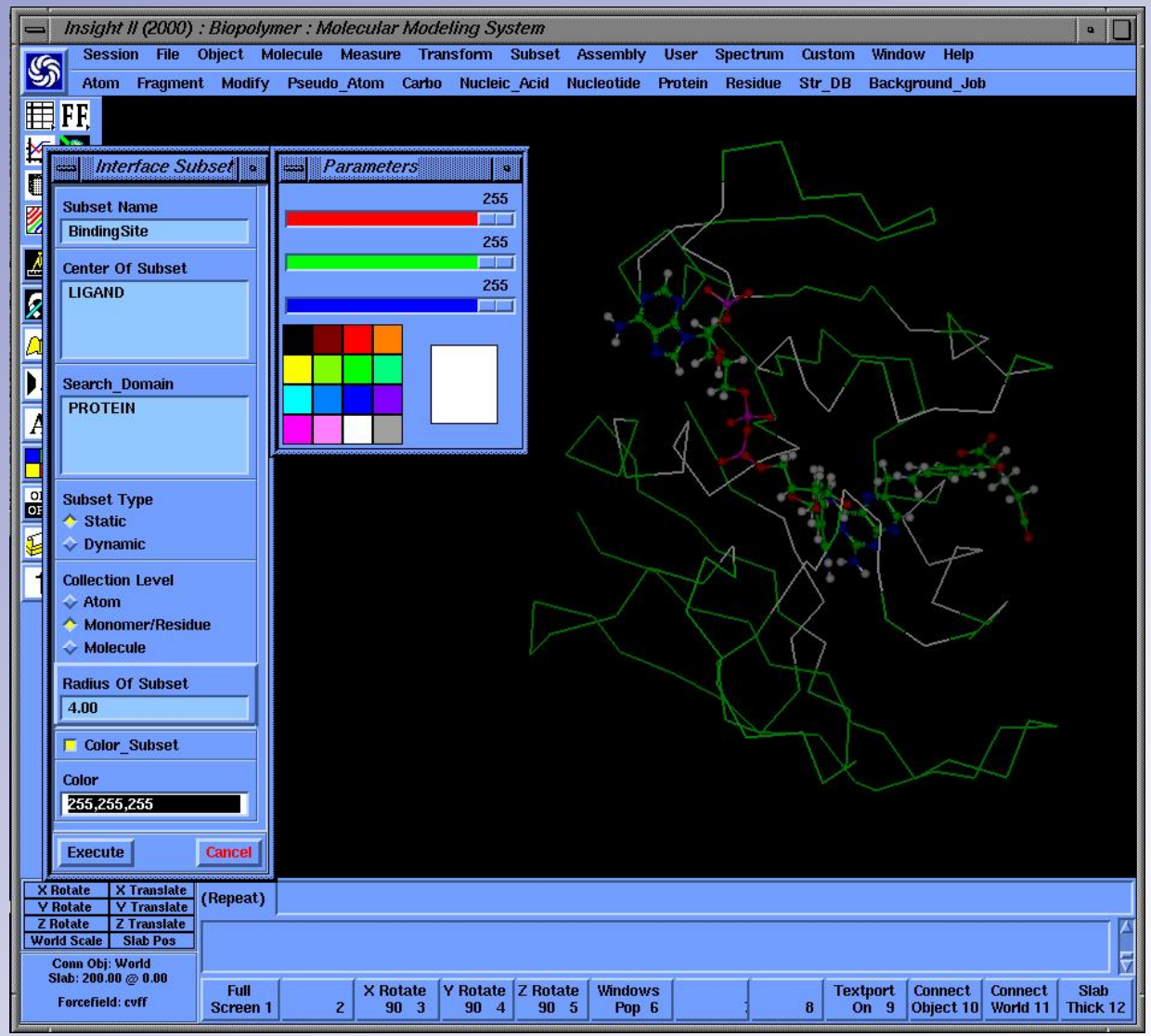
Protein Ligand Interface – Binding Site



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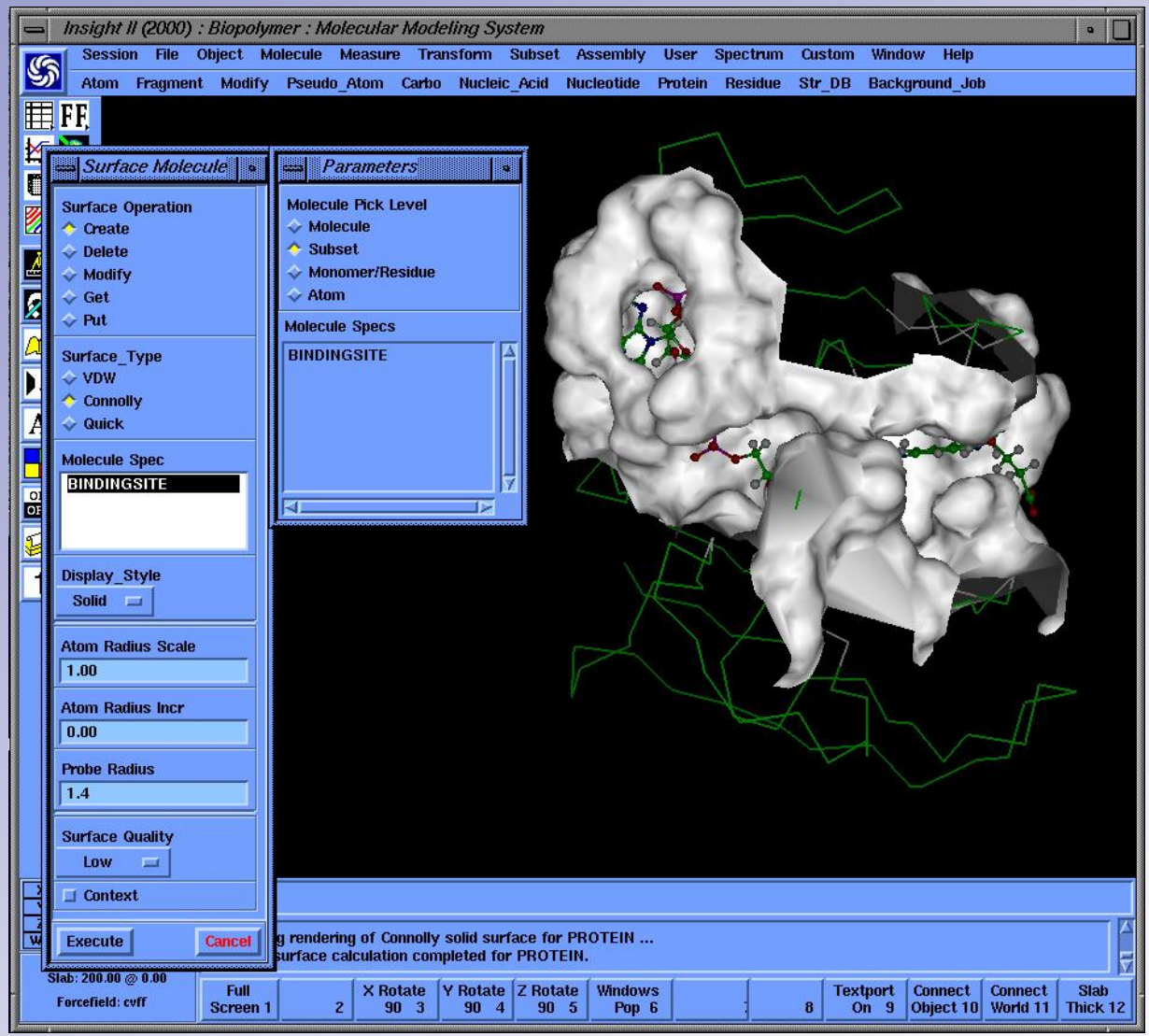
Creating a Connolly surface

- Creating a Connolly surface
  - Molecule/Surface from the viewer toolbar, Surface Molecule and Parameters panel will pop up
  - Under Surface Operation, toggle on create
  - Under Surface Type, toggle on Connolly
  - Go to Molecule Spec box, select subset from Parameters panel
  - Under Display_Style, select Solid
  - Change parameters for Atom Radius Scale, Atom Radius Incr, Surface Quality if necessary
  - Execute

Generating Binding Site Surface



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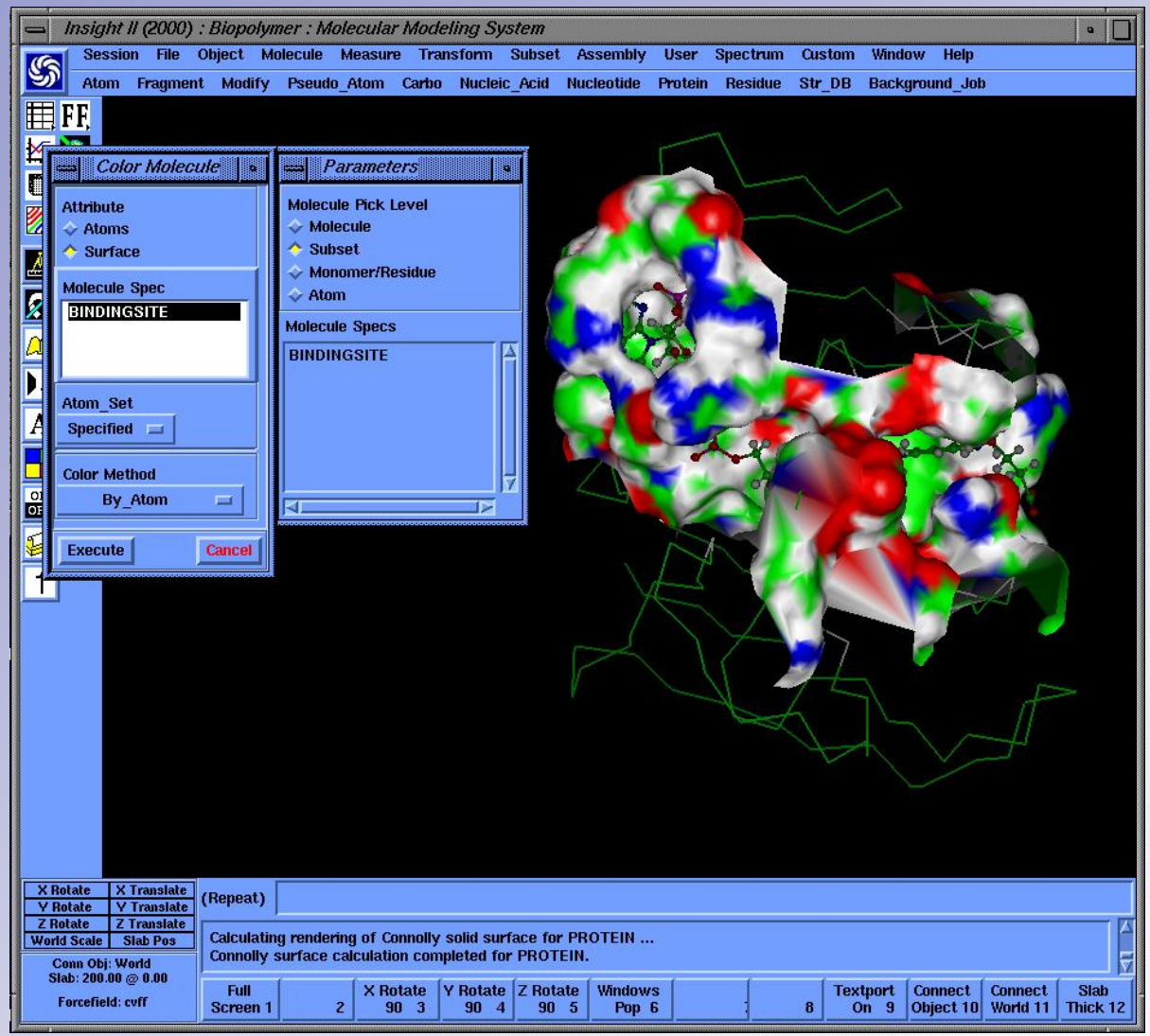
Generating Binding Site Surface



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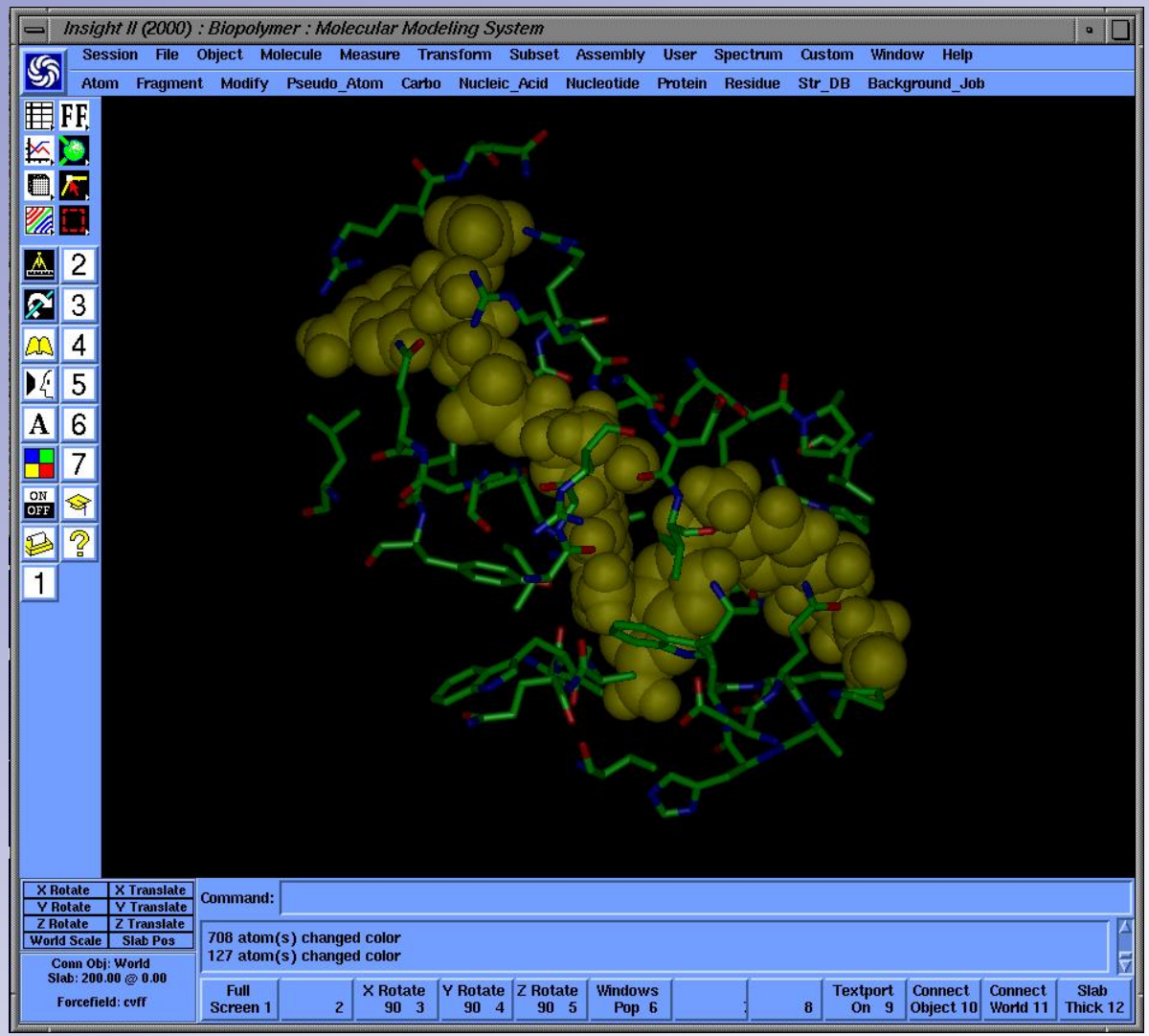
Display and Rendering Binding Site Residues



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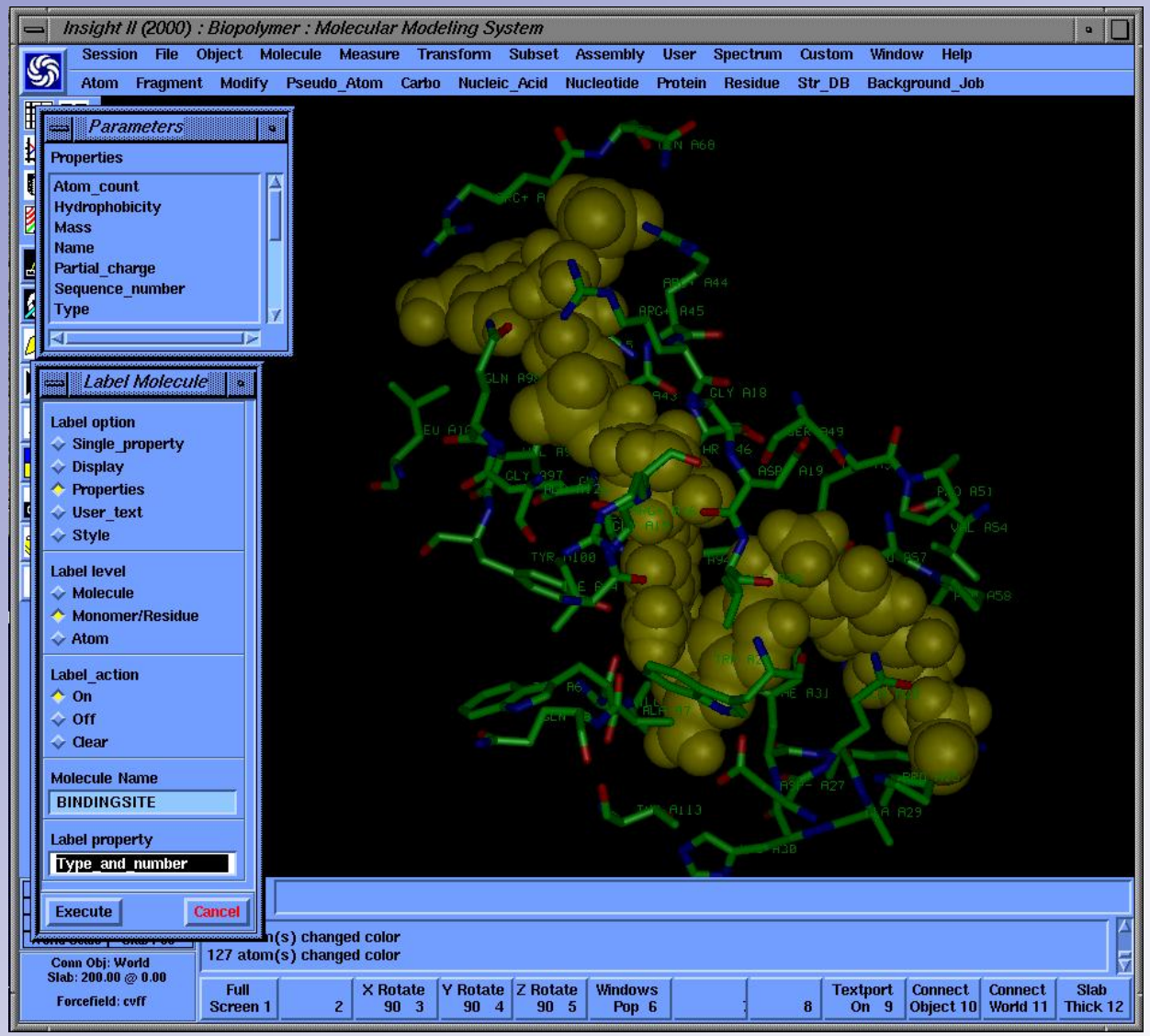
Labeling



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Saving your environment

- file/save_folder in the viewer toolbar, save folder and parameters panel will pop up
- In Save_Object box, type *
- Go to Folder_Name box, give a name for your folder
- Execute

Your whole environment is now saved in a file that ends with .psv

Learning more about InsightII and its modules on your own

- Pilot tutorials
- http://www.msi.umn.edu/tutorial/compBioGen/tutorial/InsightII_fall04.pdf

InsightII Documentation

- http://www.accelrys.com/doc/life/index.html

Username: msi

Passwd: msi-doc

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To get help

- By mail help@msi.umn.edu
- Web www.msi.umn.edu
- Phone 612 626 0802
- Appointment TBA

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