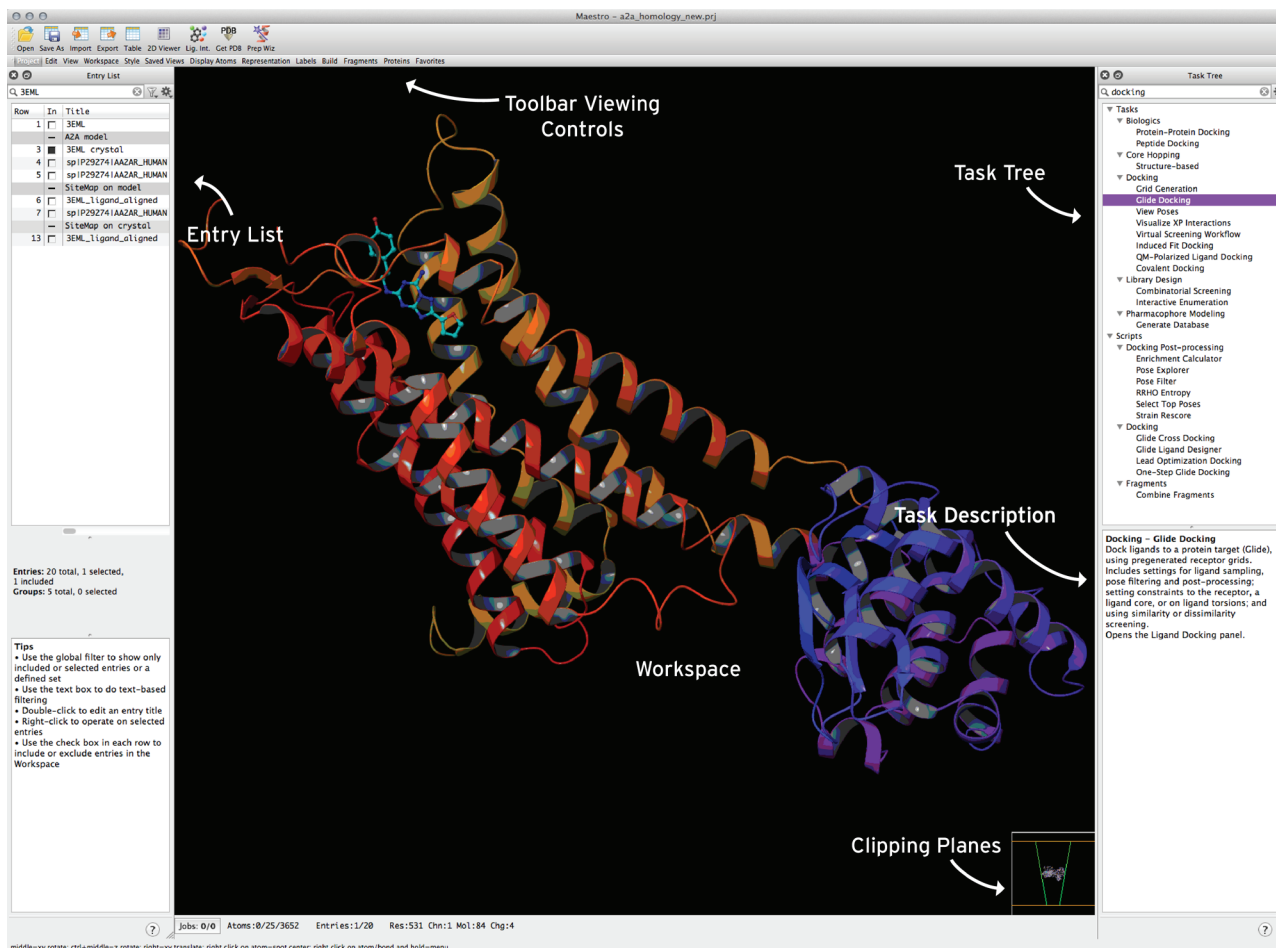# Getting Started in Maestro 2014

Viewing Structures

Mouse Controls

Zoom: Middle+right button or mouse scroll wheel.

Rotate xy: Hold down middle button and move mouse

Rotate z: Ctrl+ hold down middle button of mouse

Translate xy: Right button

More mouse controls: Maestro > Customize Mouse Actions to view and modify additional controls.

Stereo view: Ctrl+S to turn stereo view on and off; View > 3D Options > Stereo for more options

View Clipping Planes: Window > Clipping Planes; click and drag horizontal orange lines in clipping planes box to adjust location of clipping planes

View Protein Sequence: Window > Sequence Viewer

Selecting Atoms

Select atoms in the Workspace: Click the ⬚A button in the Edit Toolbar or press the ` key (located at top left of keyboard) to enter atom selection mode. You can then click and drag the mouse pointer over atoms in the Workspace to select them.

To choose whether a Workspace selection captures atoms, residues, molecules, chains, or entries, click and hold the ⬚A button, select a structure type, and then select structures in the Workspace.

Working with Surfaces

Create a surface: Workspace > Surface

Manipulate surface appearances: Click **S** in the Entry List or Project Table, or Workspace > Surface > Manage Surfaces

Importing Structures

Import your own files: Click 🗐 in the Project Toolbar.

Import a PDB file: Click PDB⬇ in the Project Toolbar.

Entry List

All structures in the project file are listed in the Entry List.

Select entries: Click on entry name. Selected rows are highlighted in yellow.

Include entries: Toggle the check box next to entry name. Shift+Click to include a range of entries in the Workspace. Ctrl+Click to add or remove an entry.

Add properties to Entry List: Click ⚙ > Show Property

Task Tree

Begin typing a task keyword into the search field at the top of the Task Tree. Search results are dynamically updated.

Click on an item in the Task Tree to see a description of the task in the bottom half of the Task Tree panel.

Setting up a New Project

Create a new Project: Ctrl+N

All job results are associated with the project file, and are saved automatically in the default directory as you work.

Change default directory location: Project > Change Directory

Performing Common Tasks in Maestro 2014

Building and Modifying Structures

2D building: In the Edit Toolbar, click the ⚒ button to open the 2D Sketcher. The 2D Sketcher is disabled when a macromolecule is in the Workspace. Clear the Workspace by clicking the 🧹 button in the Workspace Toolbar and the 2D Sketcher will be enabled.

3D building: Show the Build and Fragments Toolbars. Click and hold ✏, select an element, and then click on an empty portion of the Workspace to start drawing. Double clicking will end the drawing session. Select a fragment from the Fragments Toolbar and click in the Workspace to add it.

Add hydrogens: Double-click the +H button in the Edit Toolbar to add missing hydrogens to all structures in the Workspace.

Adjust torsions: Click the ✗ button in the Edit Toolbar, and then click on a bond to select it. Click and drag left or right to adjust the torsion.

Minimize structures in Workspace: Press Ctrl+M to perform a quick minimization.

Create entry from Workspace: Click the 🖼 button in the Workspace Toolbar to create a new entry in the Entry List and Project Table.

Measurements: Press and hold the 📏 button in the Labels Toolbar. Select an option from the drop-down menu, then select atoms or bonds in the Workspace as appropriate.

Structure sculpting: Click the 🔧 sculpting button in the Build Toolbar, then click and drag on an atom in the Workspace.

Using a Set of Selected Atoms

You may wish to save a set of atoms – such as a set of binding site residues – in your project file so that you can return to perform actions on the set at any time.

Save a set of selected atoms: Navigate to Tools › Sets. Click the New button in the Sets panel, name the set, then select the atoms you wish to save in the set by checking the box adjacent to Pick. Then, make selections in the Workspace for that set.

Working with Multiple Structures

Import single or multiple structures: Ctrl+I or click the 🖼 button in the Project Toolbar.

Clear the Workspace: Click the 🧹 button in the Workspace Toolbar.

Move one molecule while keeping others fixed: Click and hold 📦 in the Edit Toolbar, select a structure type, then select the desired structures in the Workspace to transform, using the mouse. Click 📦 again to leave local transformation mode.

Tile entries: Use the Entry List or Project Table to include more than one entry in the Workspace. Then, press Ctrl+L or click the 🔲 button in the View Toolbar.

Working with Proteins

Generate a 2D diagram of a ligand in a binding pocket: With a protein-ligand complex in the Workspace, select 🔬 in the Project Toolbar. Here, select View › LID Legend for a diagram legend.

Analyze protein quality: Toggle on the Proteins Toolbar. Select 📋 in the Proteins Toolbar to view Protein Reports of potential problems with the structure in the Workspace.

Manually adjust torsions: Select ✗ in the Proteins Toolbar and then select a bond in the Workspace. Click and drag the left mouse button to manually adjust the torsional angle.

View Ramachandran plot: Select 🔳 in the Proteins Toolbar.

Selectively Displaying Atoms in the Workspace

The Display Atoms Toolbar provides you with precise control over which atoms to display in the Workspace.

Toggle on the Display Atoms Toolbar. With a protein-ligand complex in the Workspace, click the Display Only icon 👁, and select Ligands from the drop-down menu. The Workspace is updated to only display ligands contained in the complex.

Then, click 👁, and select +4 Å from the drop-down menu. Everything within 4 Å of the previously displayed ligands will now be displayed in the Workspace.

Display an additional structure: Click ➕

Hide a structure: Click ➖

Display only selected structures: Click and hold 🖱 then select a structure type from the drop-down menu. Select the desired structure(s) in the Workspace using the left mouse button.

Changing Molecular Appearance

Change molecular rendering: Toggle on the Representation Toolbar. Click and hold 🔶 in the Representation Toolbar to view a drop-down menu of structure choices. As an example, select Residues from the drop-down menu and then click on an atom in the Workspace. The entire residue containing the selected atom will be rendered in CPK.

Structures can similarly be rendered in wireframe ⬡, thin tubes ⬡, thick tubes ⬡, or ball-and-stick ⚛.

Display ribbons: Select and hold 🎀 for options.

Apply a predefined style: Click 💥 in the Style Toolbar.

Keyboard Shortcuts in Maestro 2014

Project Operations

Show/Hide Project Table: Ctrl+T

New project: Ctrl+N

Open project: Ctrl+O

Close project: Ctrl+W

Import structures: Ctrl+I

Cut: Ctrl+X

Copy: Ctrl+C

Paste: Ctrl+V

Paste by placing: Ctrl+Shift+V, then click in the Workspace to place

Open Command Script Editor: Ctrl+E

Create Project Table entry from contents of Workspace: Ctrl+Shift+N

Display single-entry feedback in Workspace: S

Quit Maestro: Ctrl+Q

Open help page for active panel: F1

Modifying Structures

Toggle between local and global transformation mode: Ctrl+G

Delete selected atoms: Del

Clean up geometry: Press U to perform a quick minimization with loose convergence criteria

Minimize structures in the Workspace: Press Ctrl+M to perform a more thorough minimization

Project Table Operations

Show/Hide Project Table: Ctrl+T

Mark target entry in Project Table: X

Scroll up/down: Up/down arrow keys

Scroll up/down one page: Page Up / Page Down

Jump to top/bottom of the Project Table: Home/End

Jump to previous/next included entry: Ctrl+Page Up/Down

Jump to previous/next selected entry: Shift+Page Up/Down

Include the next or previous selected entry in the Workspace: Right arrow or left arrow, respectively

Display entry information in the Workspace: Press S

Include only selected entries in Workspace: Ctrl+N while the mouse pointer is over the Project Table

Exclude selected entries from Workspace: Ctrl+X while the mouse pointer is over the Project Table

Finding and Selecting Atoms

Find substructures or entries: Ctrl+F; Alt+N and Alt+P select next and previous matches

Activate atom selection tool: ` (located at upper left of keyboard)

   Select clicked atoms: A

   Select clicked residues, chains, molecules, or entries: R, C, M, or E, respectively

   Select all: Ctrl+A

Workspace Operations

Full screen Workspace mode: Press Ctrl+=; press Esc or Ctrl+= to exit

Apply Workspace style: Ctrl+Y

Tile Workspace: Ctrl+L

Transform all tiles: Ctrl+Shift+L

Fit to selected atoms: Press Z; if no atoms are selected, all Workspace contents will be fit to screen

Fit ligand to Workspace: L

Zoom in: K

Zoom out: J

Move clipping planes back: -

Move clipping planes forward: +

Move clipping planes together: F

Move clipping planes apart: G

Toggle enhanced depth view on/off: D

Stereo view: Ctrl+S

Go to previous/next scene: Enter Scenes Mode and use Ctrl+Shift+, and Ctrl+Shift+

Using Atom Sets

Save selected atoms as Atom Set 1: Press Ctrl+1 to save a set; Ctrl+0 through Ctrl+9 work similarly

Select atoms from Atom Set 1: Press 1; keys 0 through 9 work similarly