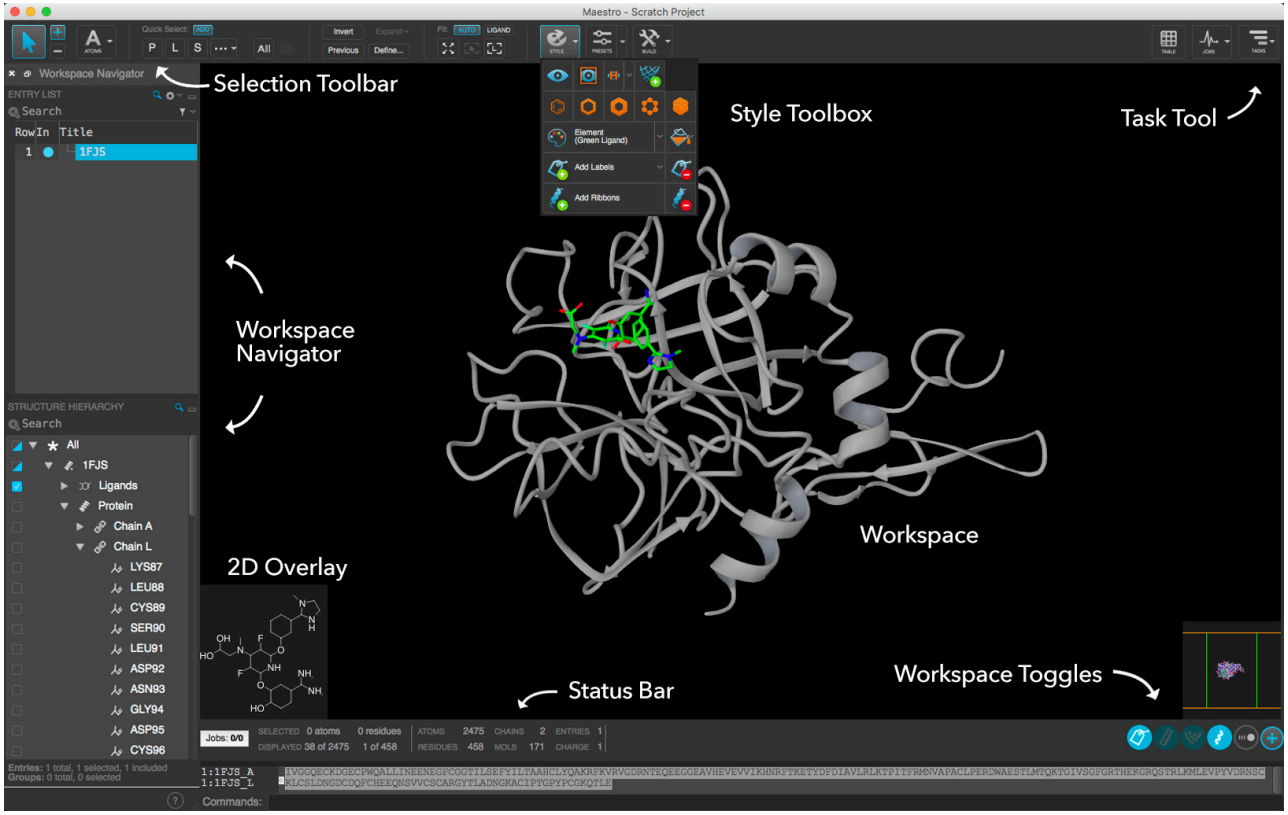
# Getting Started in Maestro




## Importing Structures

**Import your own files:** File > Import Structures; Ctrl+I

**Import a PDB file:** File > Get PDB

## Workspace Navigator

The Workspace Navigator includes the **Entry List** and the **Structure Hierarchy**. Each section can be resized or collapsed. Show or hide the whole panel using Ctrl+E or Window > Workspace Navigator.

**Select entries:** Click on the entry title in the Entry List. Selected rows are highlighted in blue.

**Include entries:** Toggle the circle next to the entry title. Shift+Click to include a range of entries in the Workspace. Ctrl+Click to add or remove an entry.

Use the **Structure Hierarchy** to locate and manipulate individual chemical components within each included entry. Click object names to select the corresponding atoms. Toggle visibility or hover and click to style.

## Task Tool

Click the button in the upper righthand corner to select from many common tasks. You can also begin typing a task keyword into the search field that appears (e.g., "docking"). Search results are dynamically updated.

Hover over an item in the Task Tool to display a desription or click to open the application panel.

## Workspace Toggles

The Workspace Toggles bar contains several buttons for showing and hiding visual components of the Workspace. Hover over any button to see a description of what it does.

Click to open a panel with additional Workspace configuration options.

## Viewing Structures

**Mouse Controls**

**Zoom:** Middle+right button or mouse scroll wheel

**Rotate xy:** Hold down middle button

**Rotate z:** Ctrl+ hold down middle button of mouse

**Translate xy:** Right button

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

**Select higher-level structure:** Double-click left button

**Stereo view:** Turn stereo view on and off using the panel opened from the Workspace Toggles bar, or type Ctrl+S.

**Clipping Planes:** Show or hide the gadget using the Workspace Toggles panel or the menu: Window > Clipping Planes. Click and drag the horizontal orange lines in the box to adjust the clipping planes' location.

**Protein Sequence:** Show or hide the gadget using the Workspace Toggles panel or the menu: Window > Sequence Viewer.

## Selection Toolbar

You can quickly select or deselect chemical objects in the Workspace using the Selection Toolbar.

Click or to build a selection or remove items from it.

Change the picking level by clicking

Several predefined features can be selected using the Quick Select buttons

## Style Toolbox

Use the Style Toolbox to modify the visual representation of selected atoms in the Workspace.

Click to modify the visual aspects of selected atoms.

Click for one-click styling of Workspace entries.

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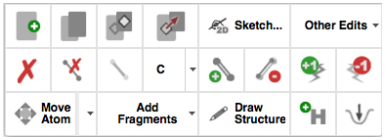
# Performing Common Tasks in Maestro

## Building and Modifying Structures

Click  to open the 3D Builder palette.

The 3D Builder palette can be used to edit existing entries or create new structures in the Workspace.




**2D building**: Click Sketch... in the 3D Builder palette or select Edit > 2D Sketcher to open the 2D Sketcher. (This option is disabled when a macromolecule is in the Workspace.) To create a new, blank entry click the  button.

**3D building:** The 3D Builder palette contains many useful tools for modifying structures in the Workspace. Hover over any button to see a description. Add structural fragments by clicking the **Add Fragments** button or choose from several advanced modifications in the **Other Edits** menu. (Note: Draw Structure is temporarily disabled.)

**Add hydrogens:** Click  in the 3D Builder palette to add missing hydrogens to all selected structures in the Workspace.

**Adjust torsions:** Select Edit > Adjust > Quick Torsion from the top menu, then click on a bond to select it. Click and drag left or right to adjust the torsion.

Minimize structures: Press Ctrl+M or click  to perform a quick minimization on selected structures in the Workspace. Press Shift+Ctrl+M to minimize only the ligand.

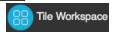
Create new entries in Workspace: The 3D Builder palette contains several options for creating new entries. Click  to ceate a new blank entry, or  to duplicate the currently included entry or entries.

Measurements: Select Workspace > Measure from the top menu. A banner will appear with a choice of measurement types (default is Distance). Select the appropriate atoms in the Workspace, and the value will appear. Click  in the Workspace Toggles bar to quickly hide/show measurements that have been previously created.

## Working with Multiple Structures

**Import single or multiple structures:** Ctrl+I or select File > Import Structures from the top menu.

**Clear the Workspace:** Select Workspace > Clear Entries to clear all entries from the Workspace.

**Tile entries:** : When more than one entry is included in the Workspace, press Ctrl+L or click the  button in the Workspace Toggles bar and then click  in the panel that appears.

**Move one entry while keeping others fixed:** Click the  button in the Workspace Toggle bar and then toggle the  button on/off to choose whether tiles are controlled separately or together.

## Working with Proteins

Click  to open the Task Tool, then select Browse > Biologics to select from many protein-specific tasks.

**Generate a 2D diagram of a ligand in a binding pocket:** With a complex in the Workspace, select Browse > Structure Building > Ligand Interaction Diagram from the Task Tool to open the 2D Workspace. Here, select View > LID Legend for a diagram legend.

**Analyze protein quality and view Ramachandran plot:** Select Browse > Biologics > Structure Quality from the Task Tool to view a Ramachandran plot and Protein Report of potential problems with the structure in the Workspace.

### Getting Help

**Online Documentation:** Click  in any panel, or go to Help > Help...

**Tutorials:** Help > Tutorials...

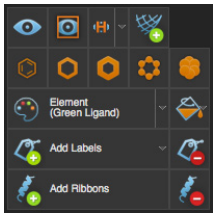
**Training Videos:** Visit www.schrodinger.com/videos

**Knowledge Base:** Visit www.schrodinger.com/kb

## Working with Styles

Click  to open the Style Toolbox.

The Style Toolbox provides you with precise control over how structures are displayed in the Workspace.



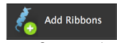

**Selectively display atoms:** Click the  button in the Style Toolbox to *only* display currently selected atoms or click the  button to display/undisplay currently selected atoms without affecting other atoms in the Workspace.

**Advanced selection options:** Several advanced selection modifiers are available to the right of the Quick Select buttons: 


Use these options to invert the current selection, expand it by a given distance, or other property, or create complex selection definitions.

**Change molecular rendering:** Select the structures to be modified and then choose from several representations available in the Style Toolbox. Structures can be rendered in:

Wireframe  , thin tubes  , thick tubes  , ball-and-stick  , or CPK 

**Display ribbons:** Click  on the Style Toolbox to display protein ribbons for selected atoms. Click the  button in the Workspace Toggles bar to hide/show existing protein ribbons.

**Apply a predefined style:** Click  to choose from several predefined styles or to create your own.

**Create surfaces:** Click  in the Style Toolbox to quickly create a molecular surface on selected atoms. For more advanced options, use the Workspace > Surface menu.

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# Keyboard Shortcuts in Maestro

## Project Operations

**Show 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+D

**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

**Delete selected atoms:** Del

**Minimize selected atoms in the Workspace:** Press Ctrl+M (minimizes currently selected atoms, or all atoms if none are selected)

**Minimize ligand:** Shift+Ctrl+M (minimizes all ligands currently included in the Workspace)

## Project Table Operations

**Show Project Table:** Ctrl+T

**Mark all included entries 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

**Select single atom or bond with click in Workspace:** A

**Select residue, chain, molecule, or entry with click in Workspace:** R, C, M, or E, respectively

**Select all:** Ctrl+A

**Clear selection:** Ctrl+U

**Find substructures or entries:** Ctrl+F

**Select higher-level structure:** Double-click left button on atom in Workspace

**Select chemical object:** Click left button on object in Structure Hierarchy

**Select and fit to chemical object:** Double-click left button on object in Structure Hierarchy

## Workspace Operations

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

**Apply Workspace style:** Ctrl+Y

**Tile Workspace:** Ctrl+L

**Fit Workspace to ligand:** L

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

**Zoom in:** K

**Zoom out:** J

**Move clipping planes back:** -

**Move clipping planes forward:** +

**Move clipping planes together:** F

**Move clipping planes apart:** G

**Stereo view:** Ctrl+S

**Go to previous/next scene:** Enter Scenes Mode and use Ctrl+< and Ctrl+>

## Using Saved Selections

**Save selected atoms as Selection 1:** Press Ctrl+1 to store current selection; Ctrl+0 through Ctrl+9 work similarly

**Use saved Selection 1 to select atoms:** Press 1; keys 0 through 9 work similarly

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