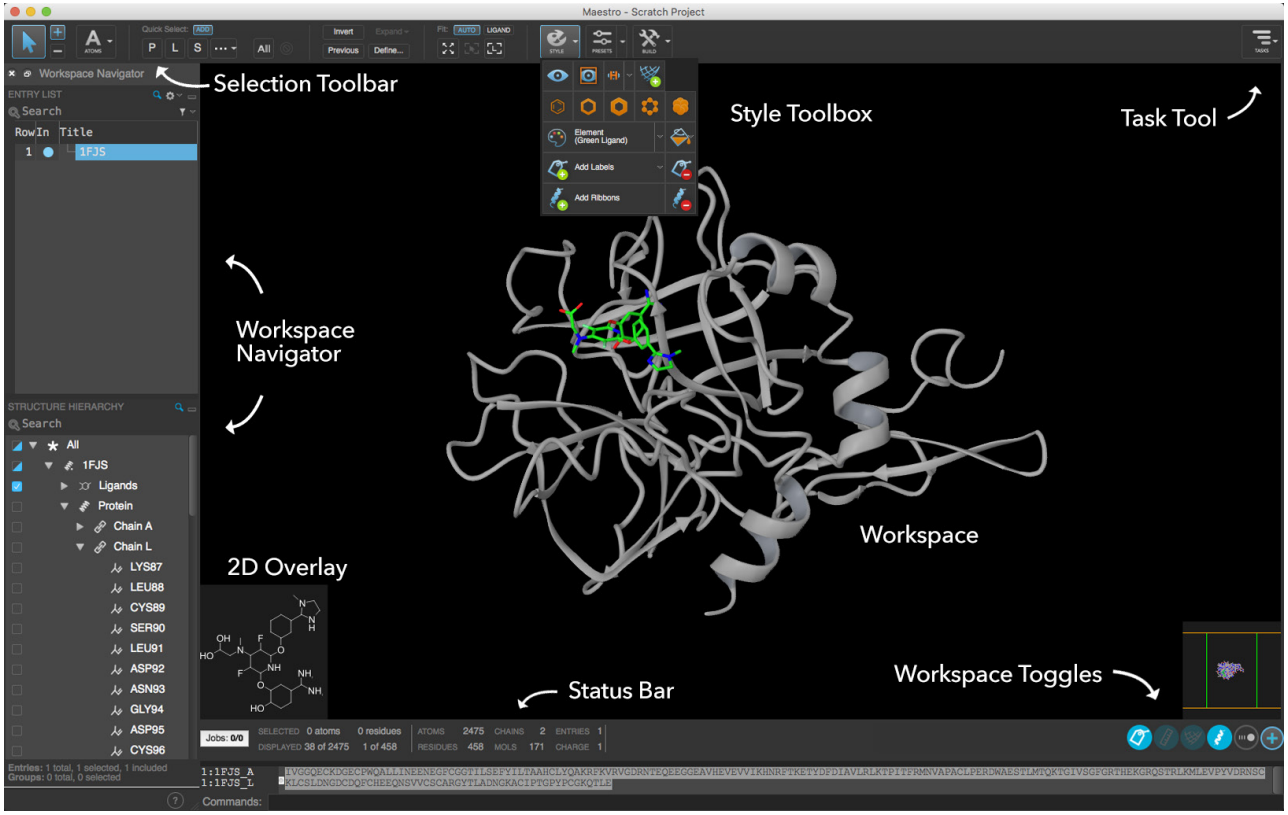
Getting Started in Maestro 11



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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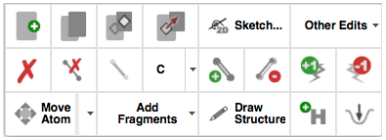
Performing Common Tasks in Maestro 11

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...

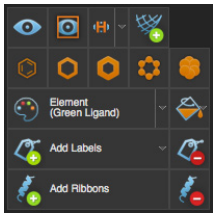
Training Videos: Visit www.schrodinger.com/videos

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.



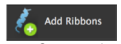
Selectively display atoms: Click the  button in the Style Toolbox to *only* display currently selected atoms or click the  button to display/undisplay currently selected atoms without affecting other atoms in the Workspace.

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 11

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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