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 description 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:** Maestro > Mouse Actions to view and modify 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 Select buttons

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.
Performing Common Tasks in Maestro

Building and Modifying Structures
Click \(\text{to open the 3D Builder palette.}\)

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

2D building: Click \(\text{Edit} \rightarrow \text{2D Sketcher to open the 2D Sketcher. (This option is disabled when a macromolecule is in the Workspace.) To create a new, blank entry click the button.}\)

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 \(\text{in the 3D Builder palette to add missing hydrogens to all selected structures in the Workspace.}\)

Adjust torsions: Select \(\text{Edit} \rightarrow \text{Rapid Torsion Scan... from the top menu, then click on a bond to scan orientations around that bond.}\)

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

Create new entries in Workspace: The 3D Builder palette contains several options for creating new entries. Click \(\text{to create a new blank entry, or to duplicate the currently included entry or entries.}\)

Measurements: Select Workspace \(\rightarrow \text{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 \(\text{in the Workspace Toggles bar to quickly hide/show measurements that have been previously created.}\)

Working with Multiple Structures
Import single or multiple structures: Ctrl+I or select File \(\rightarrow \text{Import Structures from the top menu.}\)

Clear the Workspace: Select Workspace \(\rightarrow \text{Clear Entries to clear all entries from the Workspace.}\)

Tile entries: When more than one entry is included in the Workspace, press Ctrl+I or click the \(\text{button in the Workspace Toggles bar and then click \(\text{Tile Workspace}\) in the panel that appears.}\)

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

Working with Styles
Click \(\text{to open the Style Toolbox.}\)

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

Selectively display atoms: Click \(\text{the \(\text{button in the Style Toolbox to only display currently selected atoms or click \(\text{the \(\text{button to display/undisplay currently selected atoms without affecting other atoms in the Workspace.}}}\)

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 \(\text{, thin tubes \(\text{, thick tubes \(\text{, ball- and-stick \(\text{, or CPK \(\text{.}\)}\)

Display ribbons: Click \(\text{on the Style Toolbox to display protein ribbons for selected atoms. Click the \(\text{button in the Workspace Toggles bar to hide/show existing protein ribbons.}\)

Apply a predefined style: Click \(\text{to choose from several predefined styles or to create your own.}\)

Create surfaces: Click \(\text{in the Style Toolbox to quickly create a molecular surface on selected atoms. For more advanced options, use the Workspace \(\rightarrow \text{Surface menu.}\)

Getting Help
Online Documentation: Click \(\text{in any panel, or go to Help \(\rightarrow \text{Help...}\)

Tutorials: Help \(\rightarrow \text{Tutorials...}\)

Training Videos: Visit www.schrodinger.com/videos

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

### 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

### 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+> to store current selection; Ctrl+0 through Ctrl+9 work similarly
- **Find saved selections:** Use saved Selection 1 to select atoms: Press 1; keys 0 through 9 work similarly

### 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)

### 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