

# Common operations in Maestro 9.1

## Viewing Structures

**Rotate xy:** **Middle button**

**Rotate z:** **Ctrl+middle button**

**Fix rotation in x or y direction:**  
**Shift+middle button** and move mouse **up** or **down** for **x** and **left** or **right** for **y**.

**Translate xy:** **Right button**

**Translate z:** **Ctrl+right button**

**Fix translation in x or y direction:**  
**Shift+right button** and move mouse **up** or **down** for **x** and **left** or **right** for **y**.

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

**Spot Center:** **Right-click** an atom to center the view and rotation around it.

**Stereo view:** **Ctrl+S** to turn stereo view on and off.

**Save and restore views:** Click the **Save view icon** button in the **View Toolbar**, or by choose **View > Save**. To restore a view, click (**Numbered icons**) in the View Toolbar or choose **View > Manage Views**.

*The middle mouse button is often a scroll wheel, which can be pressed like a button.*



## Working with Projects

**Create a new project:** **Ctrl+N**

**Open an existing project:** **Ctrl+O** or click the  **toolbar** button

**Close a project:** **Ctrl+W**

**Save a project:** Choose **Project > Save as**. Subsequent work is saved automatically.

**Undo/Redo:** **Ctrl+Z** or use the  /  **toolbar** buttons.

**Display shortcut menus:** **Right-click** in a blank portion of the **Workspace**, on an **Atom** or **Bond**, in the **Sequence Viewer**, or on **Project Table** rows or column headers.

## Using the Project Table

**Open the Project Table:** **Ctrl+T** or click the  **toolbar** button.

**Include and exclude structures:** To include (place in the Workspace) only a single entry (row) from the Project Table, **click** the box next to that entry's name in the Project Table. **Shift-click** to include a range of entries in the Workspace; **Ctrl-click** to add or remove (exclude) an individual entry to or from the Workspace.

**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 only the next or previous selected entry in the Workspace:** **Right arrow** or **left arrow**, respectively.


**Display entry information in the Workspace:** Press the **S** key to display single-entry feedback. To change which properties are displayed, right-click on a column header and choose a **Workspace Feedback** option from the menu that appears.


**Fix selected entry in the Workspace:** **Right-click** an entry and select the menu option to fix that entry in the Workspace.



**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. This will not delete any entries from the Project Table.

## Working with Multiple Structures

**Import single or multiple structures:** **Ctrl+I** or click the  **toolbar** button.



**Clear the workspace:** Click the  **toolbar** button. This does not delete any rows (entries) in the Project Table; it only excludes them from the Workspace.

**Move one molecule while keeping others fixed:** Press **Ctrl+G** or click the  **toolbar** button to select molecules for local transformation. Press **Ctrl+G** or click the  button again to leave local transformation mode.

**Tile entries:** **Ctrl+T** or click the  **toolbar** button.

## Finding and selecting structures

**Find structures or entries:** **Ctrl+F** will find matches in the Workspace or Project Table. Use **Alt+N** and **Alt+P** to traverse matches.


**Select atoms in the Workspace:** Click the  **toolbar** button or press the **`** key to enter selection mode. **Drag** the mouse pointer over atoms in the Workspace to select them. Click and hold the  button to choose whether Workspace selections capture atoms, residues, molecules, chains, or entries.

## Working With Surfaces and Hypotheses in the Project Table


**Open the Manage Surfaces panel for a given entry:** Click **S** in the **Aux** column of the Project Table.


**Open the Manage Hypothesis panel for a given entry:** Click **H** in the **Aux** column of the Project Table.


## Building and Modifying Structures

**Building:** Click the  **toolbar** button to display the Build toolbar.

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


**Adjust torsions:** Click and hold the  **toolbar** button, select **QuickTorsion** from the menu that appears, and click on a bond to select it. **Click and drag left or right** to adjust the torsion.


**Create entry from Workspace:** Click the  **toolbar** button.


**Measurements:** Press and hold the  **toolbar** button.


**Structure sculpting:** Choose **Tools > Structure sculpting...** from the menu.

## Using the Workspace Style Toolbar

**Workspace Style:** Click and hold the  button to define visual styles. Click the button once to apply the currently defined style to the entire Workspace.

**Automatically apply style:** Click the  button to automatically reapply the workspace style when the contents of the workspace change.

**View interactions:** Click the  button to display H-bonds and contacts.

**Create surfaces:** Click the  button to create ligand or binding-site surfaces. Click and hold the button to show or hide existing surfaces.

# Keyboard and toolbar shortcuts in Maestro 9.1

## Working with projects and the Project Table

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**

Undo: **Ctrl+Z**

Open command script editor: **Ctrl+E**

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

Mark target entry: **X**

Display single-entry feedback in Workspace: **S**

Quit Maestro: **Ctrl+Q**

Open help page for active window: **F1**

Open online help: **Ctrl+H**

## Modifying structures

Toggle between local and global transformation: **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.

## Workspace operations

Full screen Workspace mode: **Ctrl+=**

Apply Workspace style: **Ctrl+Y**

Tile workspace: **Ctrl+L**

Transform all tiles: **Ctrl+Shift+L**

Fit to selected atoms: **Z**

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**

Enhance depth view: **D**

Stereo view: **Ctrl+S**

Go to previous/next scene: **Ctrl+<** or **Ctrl+>**

## Finding and selecting atoms

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

**Activate atom selection tool:** **`**

Select clicked atoms: **A**

Select clicked bonds: **B**

Select clicked residues: **R**

Select clicked chains: **C**

Select clicked molecules: **M**

Select clicked entries: **E**

Select all: **Ctrl+A**

## Using atom sets

**Save selected atoms as Atom Set 1:** Press **Ctrl+1**. **Ctrl+0** through **Ctrl+9** work similarly.

**Select atoms from Atom Set 1:** Press **1**. Keys **0** through **9** work similarly.

## The Scene Toolbar



- Exit scene
- Go to the first scene
- Step through saved scenes
- Go to the last scene

## The View Toolbar



- Save View
- Step through saved views
- Go directly to saved view 1, 2, 3, etc.
- Manage views

## The Builder Toolbar



- Draw structures
- Set element
- Increment/decrement bond order
- Increment/decrement formal charge
- Move
- Invert chirality or flip ring substituents
- Clean up geometry

## The Workspace Assistant



- Apply Workspace Style
- Automatically reapply style when Workspace contents change
- Display H-bonds and steric contacts
- Create binding site surfaces

## The Maestro Toolbar

*Described from left to right and top down.*

- Atom selection
- Undo
- Open project
- Import structures
- Show Project Table
- Save project as
- Create entry from from Workspace contents
- Delete atoms
- Show Builder toolbar
- Add Hydrogen atoms
- Local/Global transformation
- Adjust torsions, angles, etc.

- Fit to screen
- Clear Workspace
- Turn fog on/off
- Enhance 3D effects
- Rotate 90° around x axis
- Rotate 90° around y axis
- Tile entries
- Reset view

- Display only selected atoms
- Display only
- Also display
- Undisplay
- Display additional atoms within N angstroms
- Ribbons
- Render as wireframe
- Render as space-filling
- Render as ball-and-stick
- Render as tube
- Color schemes
- Color residue

- Atom labeling schemes
- Label picked atoms
- Show/hide H-bonds
- Measurements

