

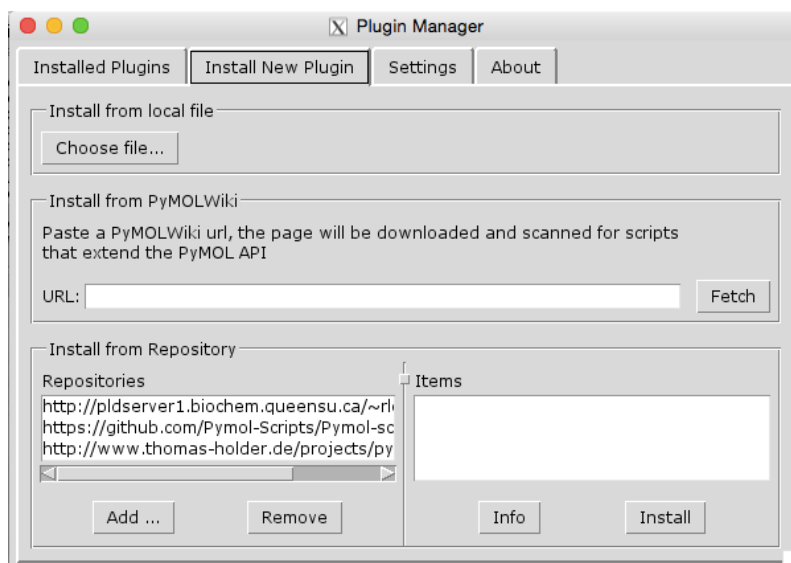
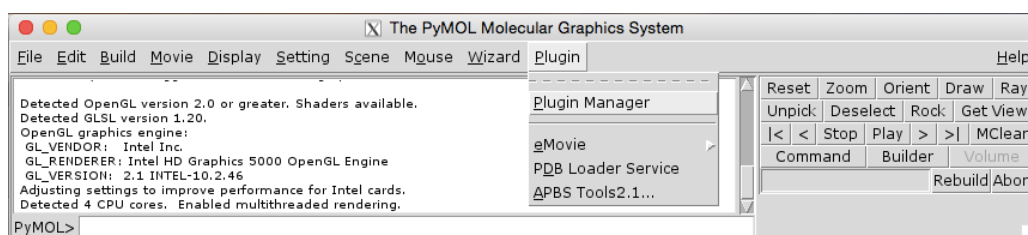
PyMOL mControl 1.0 Installation and User Guide

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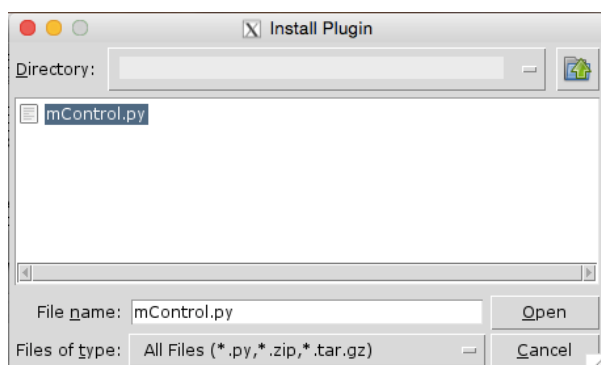


A. Installation of the mControl plugin

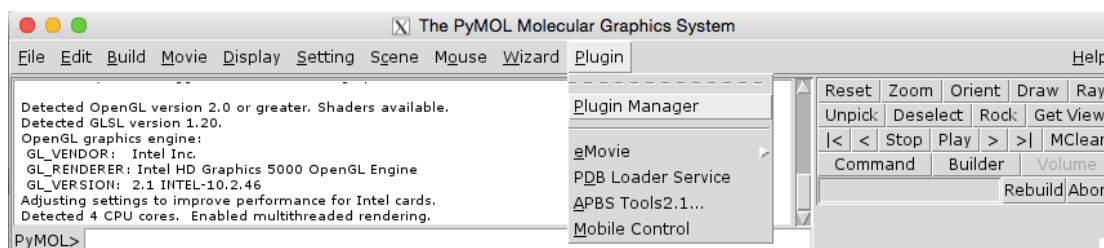
1. Open PyMOL
2. From the menu bar, select: *Plugin -> Plugin Manager -> Install New Plugin*



3. Select mControl.py

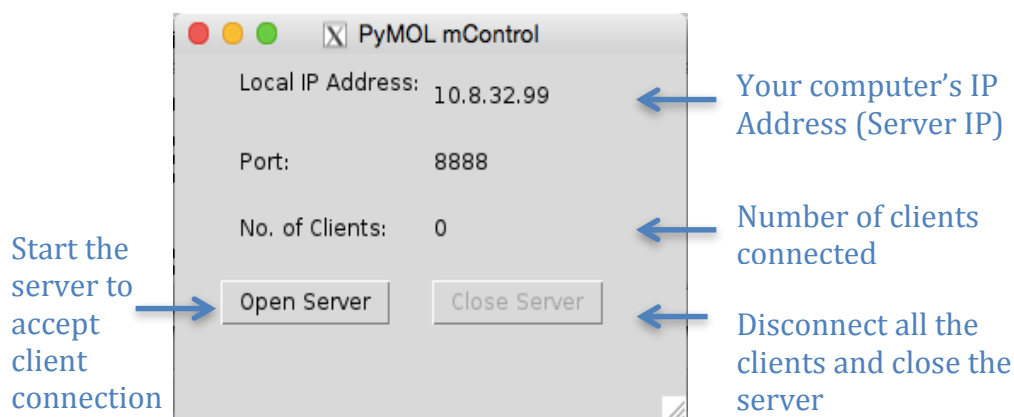


- If the installation is successful, the plugin will be available in the Plugin menu as Mobile Control (Some PyMOL versions may need to restart to begin using the new plugin).

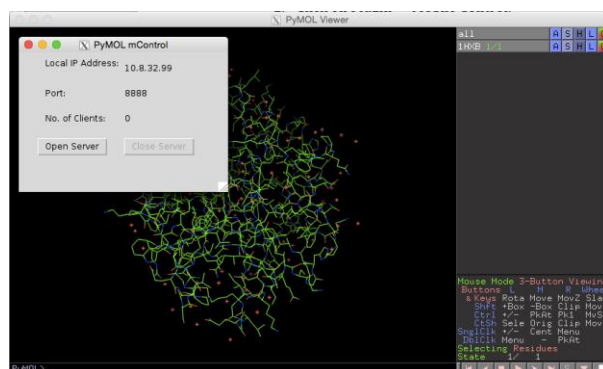


B. How to use PyMOL mControl plugin?

- Open PyMOL
- Load the molecule of your interest
- From the menu bar, select *Plugin -> Mobile Control*
Note that the IP address of the server will be automatically detected and displayed in the windows.



- Click on the *Open Server* button to start the server.



C. Installation of the mControl mobile app

The example below was using the iOS 8 platform in an iPhone 5.

1. Launch the web browser in your mobile device
2. Visit <http://cbbio.cis.umac.mo/software/mcontrol/webapp/>



3. Go to the *Output* tab, select *Add to Home Screen* option.



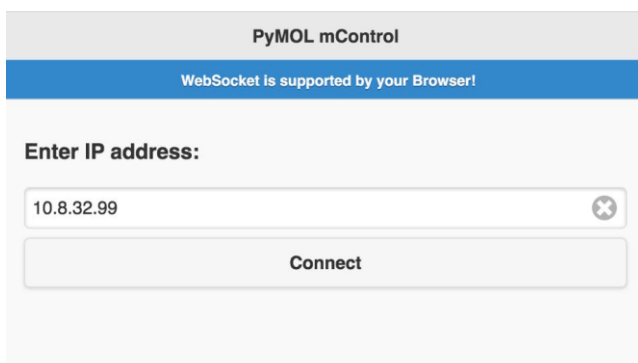
4. If the installation is successful, you will see the mControl mobile app logo in the home screen.



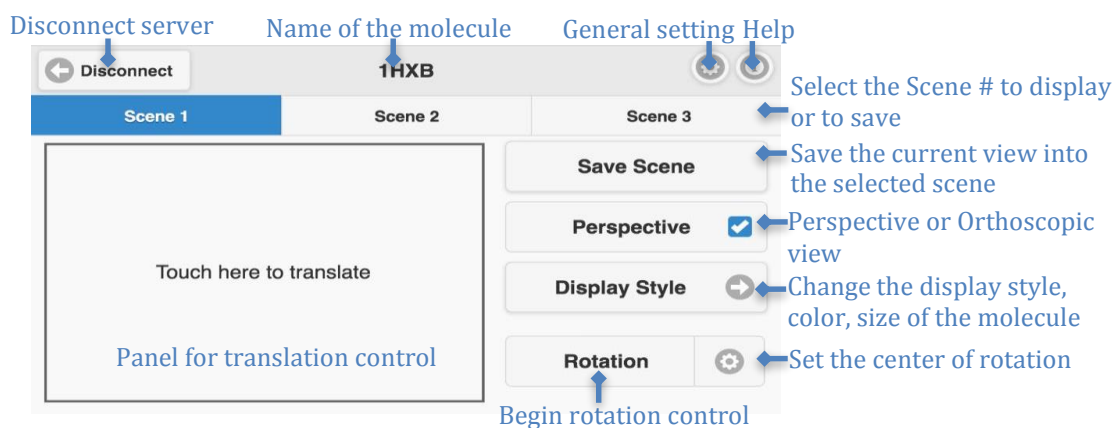
D. How to use PyMOL mControl?

1. In the main page of the mobile app, enter the IP Address that is displayed in the plugin windows (see Section B.3) and click *Connect*.

Note that your computer running PyMOL mControl plugin must be “network accessible” (both IP and port) from your mobile device, e.g. both devices are physically located in the same local area network.

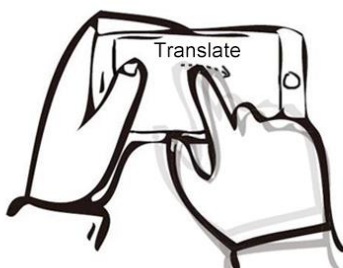


2. After connected, the main page will be displayed.



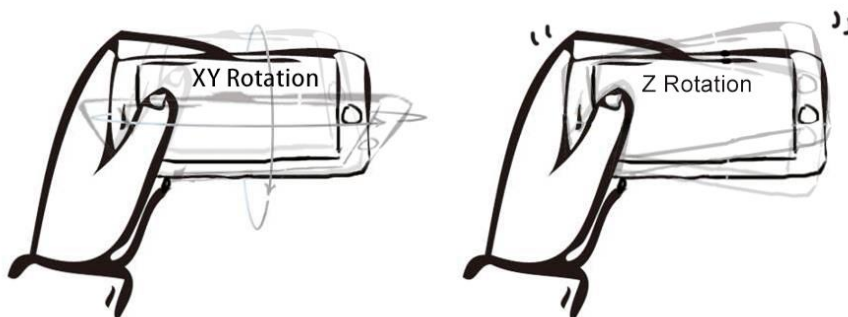
3. User can read usage instructions in the Help page to quickly learn how to perform viewing controls:

Translation: Slide your finger on the translation panel.

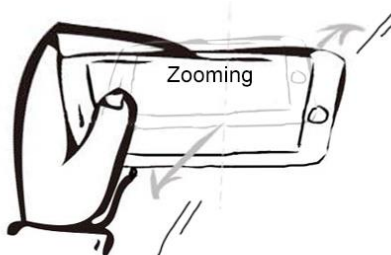


Rotation: Click the *Rotation* button and orient the mobile device as desired. A change in the orientation of the device from its initial orientation changes the orientation of the molecule in the display. Orient the mobile device along the X and Y axes results in XY-rotation of the molecule, along the Z-axis results in Z-rotation of the molecule.

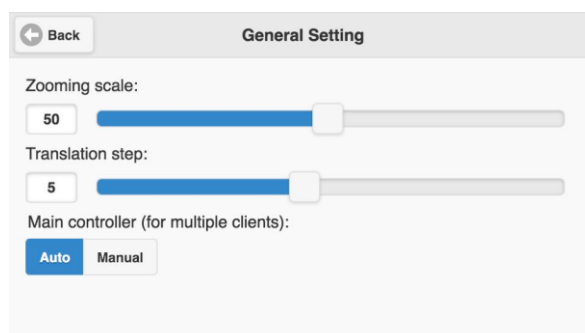
The center of rotation can be adjusted by clicking the *Setting* button next to the *Rotation* button.



Zooming: Tilt the mobile device slightly to your side and then wave it towards you to zoom in; tilt it away from you and then wave it against you to zoom out.

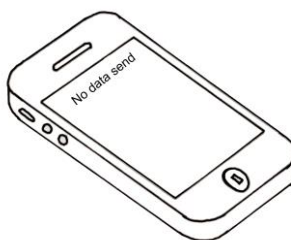


4. To adjust the step sizes for translation and zooming motions, the users can slide the appropriate bars in the *General Setting* page.



5. PyMOL mControl allows multiple clients to connect to the server concurrently, however, only one client will be the main controller at one time. There are two ways to switch between active and inactive modes in the *General Setting* page:

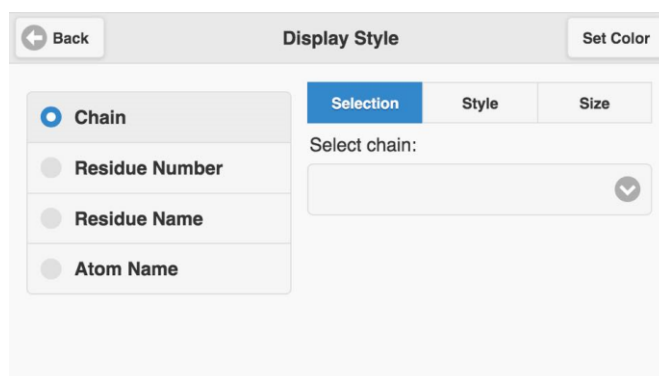
- Auto: When a mobile device is laid flat on a surface with the screen facing up, the mobile client is deactivated. When the device is hold on hand again by the user, the mobile client will be activated and take control automatically.



- Manual: The user has to activate its control manually. Users are supposed to agree among themselves who will be the main controller.
6. To perform selection for changing the display style or sizes of the drawing elements, click the *Display Style* button in the main page. Then, perform your desired operations. There are four operations: *Selection*, *Style*, *Size*, *Set Color*.

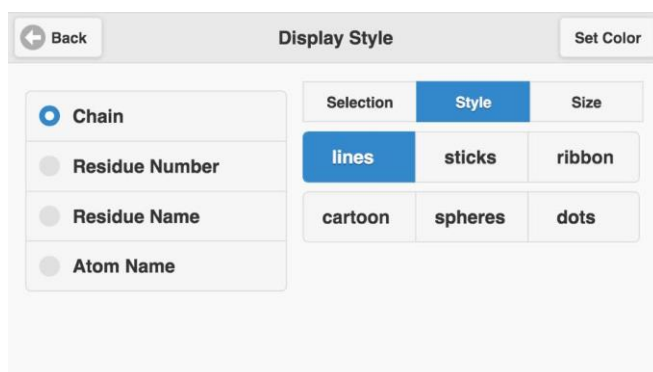
In the *Selection* page:

- Select the atoms/chains/residues/molecules at the left panel
- Select the suitable options provided in the right panel



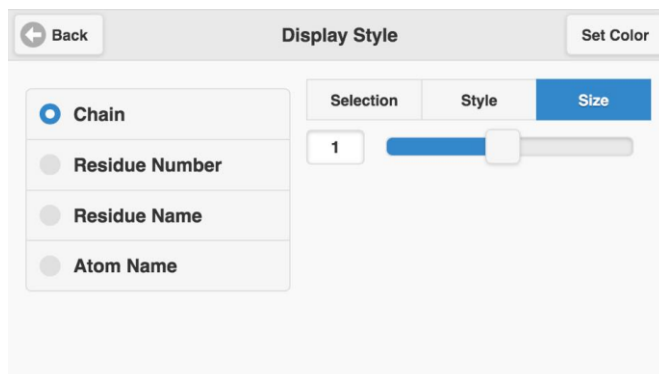
In the *Style* page:

- Select the suitable options provided in the right panel. Available display styles are lines, sticks, ribbon, cartoon, spheres, and dots.



In the Size page:

- To adjust the size of the display style of the selection.



In the Set Color page:

- Select the how coloring will be applied at the left panel: “Color by element” or “Color all”. For the former, one color can be assigned to one atom type.
- To change the color, select the desired color in the Color Palette on the right panel.
- Finally, click *Set* button to finish the selection.

