Animation Kit for FirstGlance in Jmol

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Try the Animation Maker built into FirstGlance first.

FirstGlance can make a presentation-ready animation of any molecular view with just a few mouse clicks. Here is how to do that. Here are examples of such animations in Google Slides.

This Kit is provided in case the animation-maker built into FirstGlance does not do what you want. Sometimes the built-in mechanism fails to work. Also, if you want a full 360º spin (rather than rocking), the built-in mechanism is limited to a rather small size, which gets blurry when you put it in a slide and enlarge it. This Kit can make larger, sharper animations.

If FirstGlance's built-in animation maker gave you an error message, try it again. But **before you try it again, make a slight change** by rotating the molecule a tiny bit, or resizing the browser window a tiny bit. The built-in animation maker has two bugs. (1) If you submit exactly the same job a second time, it fails with an error message. So, make a slight change each time you try again. (2) if multiple people submit jobs at the same time, it crashes. So, if you make a slight change and then try a few minutes later, it may well work.

If FirstGlance's built-in animation maker doesn't give you what you need, follow the instructions below.

Animation Kit Instructions

1. Download the *Animation Kit* and unzip it. This will produce a folder (directory) named *animation_kit*. The animations you create will be made in this folder.

2. Install or update **Java**. You will need to run the stand-alone Jmol application (included in the kit), which requires Java. Go to java.com and follow instructions to download and install the current version. (Optionally, if you already have Java installed, you can verify the installed version – see instructions under Options below.)

> If you don't know where in FirstGlance to find something mentioned below, look it up in the How & Where Index.

3. In FirstGlance, get exactly the molecular view that you want to animate. Things to consider:
   A. Usually you will want to depress the **quality** button. It is near the top of the *Molecule Information Tab*, and in the *Button Box* in the Views or Tools tab.
   B. Give some thought to whether you prefer a **white or black background**, and set the background accordingly using the *Background* button (near the top of the *Molecule Information Tab*, and in the *Button Box* in the Views or Tools tab).

C. **Size** your browser window so that JSmol is the size you want for your animation. You can change the size later, but its simpler to start with the size and shape that you want. The animation can be rectangular if your molecule fits better in a rectangle. Large sizes will generate larger animation files. To avoid an unnecessarily large presentation file (.pptx), don't make the size larger than needed for a clear animation when projected. A square 500 pixels on a side is usually large enough.

D. **Zoom** your molecule to fill JSmol. If there is a lot of empty space around the molecule, that empty space will be in your animation, taking up wasted space in your slide.

4. Save a **pngj** file:
   A. Right click on or near the molecule in JSmol, and on the menu that appears, click on *Console*. It is near the bottom of the menu. If you can't see the bottom, click higher up in JSmol to give the menu more room.
   B. In the *lower* box of the yellow-framed Console, type *write filename.pngj* (where "filename" is an appropriate name for the molecular view). It is crucial that **.pngj** is at the end of the filename. Press Enter, and OK saving the file, being sure to save it into your animation kit folder.

5. Run Jmol: double click on the file **Jmol.jar** in your animation kit folder. A black window should appear. (Important: if you run Jmol.jar from a different folder, your animation file will be saved there, not in the animation kit folder.)

6. **Display** your molecular view in Jmol. Drag your pngj file and drop it into the black Jmol window. OK changing the window width and height to the size when you saved your molecular view. Your molecular view should appear.

   If the **slab** button is depressed in your molecular view, and for **Density Maps**, see Animating a Slabbed View (under *Options* below) for special instructions that supersede steps 7 and 8 below.

7. Set the **animation speed**: Drag the file *playback-slow.spt* and drop it onto your molecular view. (Later, if you repeat this step, you may choose a different speed.)

8. **Create** the animation file:
   A. Decide whether you want rocking or spinning. If rocking through 40, 60, or 90 degrees is sufficient, the animation file will be smaller. If you need to show all sides of the molecule, you can spin (360º), but the animation file will be larger.
   B. Decide whether to rock or spin around the X (horizontal) or Y (vertical) axis.
   C. Drag the appropriate file and drop it onto the molecule. For example, if you want to rock 60 degrees around the Y axis, drag and drop the file **rock-y-60.spt**. The molecule will begin to move. Wait until it stops moving. This may take several minutes.

9. **Rename** the animation file: The previous step will create a file whose name begins **rock** or **spin**, and ends in **.gif**, in your animation_kit folder. Rename it to something appropriate

(**keeping .gif as the end of the file name!**), because if you make another animation, it will overwrite this file.

10. Drag the .gif file and **drop it into a slide** in your presentation. Resize and position as desired. In Google Slides, it will animate automatically. In PowerPoint, it will animate only when you go into *Slideshow/Projection* mode. (Optional: you can preview the animation by dragging the .gif file and dropping it into a web browser window.)

Repeat steps 3-10 to make additional animations.

If you have any problems with the animation kit, we'd like to help, and to know how to improve it. Please contact   m0lviz@yahoo.com

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Options

Adjusting animation size, zoom (optional):

After you drop your pngj file into Jmol, and see your molecule, and *before* you set the playback speed and generate the .gif file, you may resize the Jmol window if you wish. The animation .gif file will be the same size as the window. You may also rotate the molecule to a different starting orientation, or zoom it (mouse wheel, or hold down Shift while dragging up/down).

Making other rocking angles or playback speeds (optional):

The files **playback....spt** contain Jmol commands that set the frame capture rate and playback speed. If you wish, you can try other values by duplicating one of these files and editing it with a plain text editor.

The files **rock....spt** contain Jmol commands that determine the rocking angle. If you wish, you can try other angles by duplicating one of these files and editing it with a plain text editor. Note that the value at the end of the command is *half* of the full sweep angle.

Animating a slabbed view including Density Maps

If the **Slab** button in FirstGlance was depressed when you saved your pngj file, or for **Density Map** views, the slabbed view will not be maintained in the animation, without the special methods below.

Note that the slab cut planes always remain parallel to the screen – they do not rotate in an animation. The molecule rotates, so the position of the slab cut on the molecule changes as different parts of the molecule pass through the fixed slab planes.

Aside from *Density Maps*, the most plausible reason for animating a slabbed view would be to show the inside of a hollow structure while it rotates. An example is provided of E. coli chaperonin GROEL/GROES: 1aon-rock-slabbed-y-40.gif
An example for the X-ray Density Map of an isopeptide bond is
6vzx-rock-slabbed-mid10-y-60.gif

Scripts, for example **slab-back50-rock-y-60.spt**, are provided that will animate the entire back half of the molecule. Use this for **Step 8** above. Step 7 is irrelevant as the script sets the playback speed (which you could edit). Also, the slab settings in the pngj file are irrelevant since the script applies slab settings to show the rear half of the structure.

Density Maps: Use **slab-back53-rock-y-60.spt**, or if you have changed the slab setting to, for example, mid 6%, use **slab-mid6-rock-y-60.spt**.

Verifying your Java version (optional):
You must be online to do this.

Windows:
A. In the *Type here to search* slot at the left in the Taskbar below your desktop, enter *control panel*.
B. If you are viewing by Category, select Programs. If you are viewing by icons, skip this step.
C. Click on Java.
D. In the *Java Control Panel* that opens, select the *Update* tab. Click the *Update Now* button at the lower right. It will tell you if you have the current version. If you don't, proceed to update.

macOS:
A. Open *System Preferences.app* (in your Applications folder).
B. Click on Java in the bottom row. (If Java is not there, you don't have Java installed. Go to java.com, download, and install.)
C. In the *Java Control Panel* that opens, select the Update tab. It will tell you if you have the current version. If you don't, there is a button to update.