Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Material S1

This text is a supplement to:

Toward mobile 3D visualization for structural biologists

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1. *Biomolecular visualization software settings*

Table S1 - Hardware specifications

Model	**Toshiba® Qosmio F750-3D**
Method	autostereoscopic
Resolution	1920×1080 pixels
Screen size	15.6 inch
Battery	100 minutes
Weight	4 kg (with power adapter)
Cost	2,273 USD (glasses-free 3D laptop) 38 USD (gamepad)
Type of 3D screen	Full HD

Autostereoscopic laptop prerequisites

In order to enable the 3D molecular visualization software, the following tools need to be installed on Windows 7 operating systems.

1. Qosmio F750 (3D model) Win7 64bit: nVidia Display Driver update Version 8.17.12.9039
2. Qosmio F750 (3D model) Win7 64bit: Super-D IC Driver update version 1.0.1613.809
3. Qosmio F750 (3D model) Win7 64bit: Toshiba® Blu-ray Disc Player 1.0.0.871
4. Qosmio F750 (3D model) Win7 64bit: Toshiba® Blu-ray Disc Player update version 1.0.1.299_A
5. BIOS version 2.00 upgrade for Qosmio F750 (for PQF70*, PQF75*)

6. Super-D X-tune for Qosmio F750

Items 1 to 6 can be downloaded from Toshiba®'s supporting website .

7. 3D Screen Activator developed by Kevin Cox [2] is required to enable switching between different screens.

PyMOL settings:

Install PyMOL [3]. We have tested autostereoscopic capability on PyMOL 1.3 r1 (academic version). PyMOL allows the 3D interleaved stereo mode, which can be triggered through Zalman® stereo buttons included in the PyMOL version 1.3 packages. The Zalman® button needs to be activated outside the main program. After starting the program PyMOL and opening the associated file, go to the Menu bar and click on Display and then select Stereo. The picture is now available in interleaved format. Then, point the cursor to the right corner of the monitor, which has the '3D Screen Activator' icon, choose the tab which is related to the PyMOL graphical window and then click on the 3D-interleaved switch.

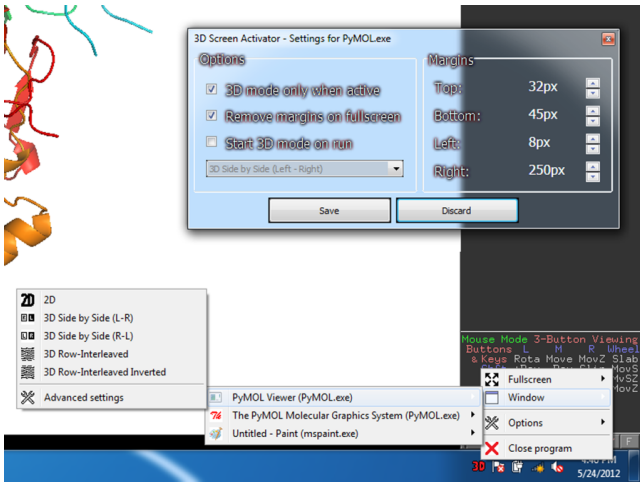

Figure S1 - Setting of the 3D screen activator to trigger the 3D interleaved mode in PyMOL

CCP4mg settings

Install CCP4mg-2.5.3 [4]. Start the CCP4mg program, select the Open menu item from the File menu and select a pdb file. Once the file is loaded, go to the menu bar, select the Zalman® Stereo menu item under the Display menu to activate the Zalman® stereo mode. Then click on the 3D icon from the 3D Screen Activator and select the 3D interleaved mode from the CCP4mg graphical windows to turn on the 3D display for the CCP4mg program.

Chimera Settings

Install Chimera-1.6.1 [5]. Start the program Chimera and open the file. After that, the Chimera stereo mode can be viewed from the Viewing Controls menu item under the Tools menu, Camera. A small window will appear. Choose the mode row stereo, right eye odd and then click save. After this stereo mode is activated, click on the 3D icon from the 3D Screen Activator. Select the Chimera Graphical windows and switch on the 3D interleaved mode.

Coot settings

Install WinCoot-0.6.2 [6]. Coot allows for working on the 3D interleaved stereo mode, which can be executed through the Zalman® stereo buttons. After WinCoot is started, go to the Open Coordinates menu item under the File menu, and then go to the Open Map menu item. Once the picture of the coordinates and the map are opened, go back to the Menu and then select the Stereo menu item under Draw menu. This will open the small window offering to display View Mode, and the radio button to activate Zalman® stereo. After the Zalman® stereo mode was activated, click on the 3D icon from the 3D Screen Activator. Select the WinCoot (coot_real.exe)

graphical windows and choose the 3D interleaved mode. The coordinates and the map should become 3D and you are settled for 3D exploration of your favorite model.

2. *Making movies with PyMOL*

We demonstrate how to obtain simple 3D movies of molecules by picturing at different molecular orientations. First of all, open the PyMOL Zalman® 3D program, and then open the .pdb file, or .pse file containing your molecule of interest. After that, change the style of representation and color as you wish from the right panel. Then select the Stereo menu item from the Display menu. The Scene selection buttons can be added by selecting the Button menu item from the Scene menu. At this point, you can add a scene by moving the molecule to the final orientation for the new scene, then select the Append menu item from Scene menu. PyMOL will automatically compute the transformation necessary to create a scene depicting the orientation change. Repeat the steps of appending scenes as desired. It should be noted that rendering a movie for 3 scenes could take up to an hour on a high-end workstation. When a molecule has moved into its final orientation of each scene, additional effects can be added. For example, a molecule can be shown swaying around the axis pointing towards the viewer for 4 seconds before starting the next scene. To add such an effect, select the Program menu item under the Movie menu and then select the Nutate option under the Scene Loop. The movie can be seen by clicking on the Play button. After this step, a movie with 3D capability can be created in different ways. In this paper, we will outline 2 methods, which are easy to execute.

The first method for creating a movie is by exporting a PyMOL movie into series of PNG images, i.e. selecting “Save movie as” from the PyMOL Zalman® 3D File menu. Then, these PNG images can be stitched together to create a MOV movie using the FFmpeg-0.10.3 program[7] through a command line interface. Below is an example of a command to create a movie file named model.mov from the files img_xxxx.png in the same directory. The movie in the Supplementary Data S2 is created by this method.

ffmpeg -sameq -r 60 -i img_%04d.png -y model.mov

Alternatively, a movie can also be recorded by a screen capturing program such as SnagIt. Both methods can preserve the 3D capability as long as the user activates the Zalman® 3D stereo option without turning on the face tracking system through 3D Screen Activator. While playing this movie file, turning on the Full Screen Mode will preserve the screen resolution for the 3D display. The movie can be viewed in 3D full screen mode on a Zalman® display or on Toshiba® Qosmio F75x with a 3D Screen Activator. For advanced movie creation methods, please consult PyMOL Wiki.

3. *Gaming input methods for Molecular Visualization*

Prerequisite: Logitech® Gaming Software-5.10 and ControlMK-0.232

We used a gamepad from Logitech®, Rumble Gamepad F510, for testing. We found that navigating with the gamepad is more efficient than with a keyboard and a mouse. However, it is less efficient with tasks like labeling and refining structures. For the settings, Coot, PyMOL and Jmol do not have a devoted functionality to support a gamepad. Instead, the user can map keyboard functionalities onto the gamepad controls using additional software. Proteopedia is implemented with Jmol and hence users can visualize biomolecules with a gamepad from their web browsers. Initially, the gamepad driver must be installed. Then, we used the program ControlMK[8] for the mapping task because it does not require any programming knowledge and it is compatible with the Windows operating system. After installing the ControlMK program, the program will show the detected gamepad in the Controllers Found pull down menu. Select the gamepad from the Active Controllers pull down menu and then click on the ">" button next to the Profiles pull down menu. Choose Add to create a new profile. The mapping table will appear under the Profiles pull down menu. Enter the setting options for ControlMK as provided in Table S2 into a profile. Then, click on the Save button to save the settings. It should be noted that the setting options provided in Table S2 are for controlling WinCoot, but most of the buttons in this profile can be applied to other molecular viewers as well. In the Joysticks Settings panel, the 'Max Value' option can be set to control the speed of the gamepad axis buttons. We recommend setting the value to within the range between 3 and 10. We found that the speed of 10 is suitable for navigating the model. However, if the user wants to select an atom or a button from the WinCoot panel, we found that the speed of 3 is more controllable.

Table S2 – Gamepad controller setting for the program ControlMK to control molecular viewers

Gamepad buttons	**Mapping on mouse action**	**WinCoot Function**	**PyMOL Function**	**Jmol Function**
X Axis -	Mouse Move X Negative*	left	left	left
X Axis +	Mouse Move X Positive*	right	right	right
Y Axis -	Mouse Move Y Negative*	down	down	down
Y Axis +	Mouse Move Y Positive*	up	up	up
Z Axis -	Mouse Wheel Forward	contour	slab	zoom
Z Axis +	Mouse Wheel Backward	contour	slab	zoom
Button 0	VK_Left Button + Ctrl, maximum speed	translate	-	-
Button 1	Mouse Left Click	rotate	rotate	rotate
Button 2	VK_Right Button + Ctrl, maximum speed	slab	-	translate
Button 3	Mouse Right Click	zoom	zoom	menu
Button 4	Mouse Left Click, 10 times per second	label	menu	label
Button 5	Mouse Middle Click	center	translate	zoom

*For use in combination with Button 0 to 3

Table S3 – Pricing information of 3D Technologies

Silicon Graphics	$50,000	IRIS 4D/60 by SGI
3D Graphics Card	$200	http://www.techspot.com/article/653-history-of-the-gpu-part-2/
Autostereoscopic Display	$1500	http://www.pcworld.com/article/117303/article.html
Glasses-free 3D laptop	$1479.99	http://us.toshiba.com/computers/laptops/qosmio/X870
Gesture Control	$79.99 – $99.00	https://www.leapmotion.com/press_releases/leap-motion-controllers-coming-soon-to-canadian-retail-stores http://www.microsoftstore.com/store/msusa/en_US/pdp/Kinect-for-Xbox-360/productID.253169000
3D Printer	$1000-$7000	

Please note that the prices were checked on the date of submission (August 2013), and may vary between different providers.

References:

1. ***Toshiba supports for Qosmio F750***, **http://www.mytoshiba.com.au/support/computers/qosmio/f750/pqf75a-067024/download?os=25.**
2. **K. Cox, *3D Screen Activator*, (2012), http://coxcoppes.nl/3DScreenActivator/.**
3. **SchrödingerLLC, *PyMOL-1.3*, (2012), http://pymol.org.**
4. ***CCP4mg-2.5.3*, http://www.ccp4.ac.uk/MG/.**
5. ***Chimera-1.6.1*, http://www.cgl.ucsf.edu/chimera/.**
6. **S. McNicholas, *WinCoot-0.6.2*, http://www.biop.ox.ac.uk/coot/.**
7. ***FFmpeg-0.10.3*, http://ffmpeg.org/.**
8. ***ControlMK-0.232*, http://www.redcl0ud.com/controlmk/.**