Scripting Wizards for Chime™ and RasMoL

Robert M. Horton, Attotron Biosensor, Carson City, NV, USA (rmhorton@attotron.com)

The molecule viewing program RasMoL and the Web browser plug-in Chime™ (reviewed in References 1 and 2) share a common scripting language for specifying how structures should be displayed. A "Wizard" is a program that "walks you through" the steps of a task and lets you select options. Here I present a set of Scripting Wizards intended to help new users begin using these remarkable visualization tools. They also take advantage of some of the new features introduced in Version 2.0 of Chime. They are written in client-side JavaScript™ and can be found on-line (http://www.attotron.com/pub/cs).

A Web of Wizards

Figure 1 shows how the various Wizard components are related and which other wizards each calls and answers to. The Chime Scripter at the top is the starting point for embedding Chime scripts and molecules in Web pages. The Script Wizard in the center does the actual assembly of scripts. The Chime Scripter coordinates construction of the HyperText Markup Language (HTML) tags to "embed" molecules and control buttons on a Web page. It presents a window with Add Molecule and Add Button buttons. Once a molecule tag has been created, buttons can be added to trigger execution of additional scripts.

A script can be added to either a molecule tag (to specify the initial display) or to a button (to present a particular view in response to a user click), so both the Add Molecule and Add Button wizards have the ability to call the Script Wizard.

Wizards at Work

Figure 2 shows the Chime Scripter in action. The window in the background contains the tags and scripts constructed by the various Wizards, and the Preview window shows how the molecule looks and behaves on a page. Only the hemoglobin protein backbone was initially displayed; clicking the buttons displayed iron, heme and oxygen, and zoomed to higher magnification.

The various Wizards (not shown for lack of space) are collections of menus. The Scripting Wizard presents the major categories of scripting commands in a navigation frame; choosing a category loads a pull-down menu in the Current Command frame, where you select a specific command. Commands may take parameters; for example, the colour command changes the color of the currently selected...
atoms, so the Script Wizard presents a sub-window with a list of available colors. Other sub-windows collect options such as numeric values. Most of these sub-windows are fairly simple, and their code is built into the Scripting Wizard page.

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The layout of the Expression Wizard is similar to that of the Scripting Wizard; a navigation frame lets you to choose types of expressions or predefined subsets of atoms. This specification process is complex enough to warrant a separate Expression Wizard.

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The presence of many open windows can be confusing, so be sure to fill out sub-windows from top to bottom. Terms in your script or expression that are set off in exclamation points, such as 'colour!' or 'expression!', are placeholders that should have been replaced by the value returned from a sub-window. If you see an odd exclamatory remnant, it means all sub-windows did not complete correctly or in the proper order.

These Wizards act as both quick reference manual and command template. Once you become familiar with a particular command, you might find it more efficient to simply type it into the Script box. Thus, scripts and HTML code are made directly accessible in the various Wizards. As your abilities grow, you can gradually take over typing the commands you know, and just use Wizards to generate HTML tag templates or to look up less familiar commands. At any point, you can copy scripts or HTML tags from the various Wizards to paste into other files or Web pages (for example, the Chime Presentation Template; http://www.umass.edu/microbio/chime/prsswc/template.htm).

The menu-driven approach taken by these Wizards can be complementary to graphical scripting interfaces currently under development by other groups, which let you do things such as select residues by clicking on them instead of having to know their numbers (see the RasMol Home Page [http://www.umass.edu/microbio/rasmol]). Since a wizard can be called from another browser window, it would be fairly simple to integrate wizards like those described here as accessories to other browser-based tools.

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REFERENCES