The Addition of Functionality to the Jmol/JSmol Application

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What's J mol/J smol?

- J mol/J smol is a molecular structure visualization tool
- J mol - In Java, Standalone
- J smol - In JavaScript, Web application
SASSIE WEB

- SASSIE Web is a program that uses atomistic models to predict and interpret scattering data (i.e. Neutrons, X-Rays)
- It’s my goal to add functionalities to J mol/J smol for SASSIE Web.
The Project as a Whole

- GenApp – program that converts standalone applications to other formats:
  - Web Application
  - Qt 3, 4, and pending 5
  - Android and soon iOS
- I have to make sure that Jmol is compatible with both SASSIE and GenApp
GenApp
Possibilities with Jmol/JSmol

- Load in multiple molecules at once
- Move structures independently
- Saving the universe of a molecule(s)
- View all sorts of structures, from proteins to DNA.
Addition of Jmol/JSmol Functionality

- Permanent/Fixed Command Console
- Persistent right click menu
- Second customized menu
- An Atom List
Permanent/Fixed Console
Persistent Right Click Menu
Second Customized Menu

- Work still in progress
- Will contain series of commands/options to help more easily manipulate structures
  - Center
  - Translate
  - Rotate
  - Align
  - Calculating Scattering
  - Calculating Properties
  - Dropping in Geometric Objects

Additional Menu - Prototype
Can select specific atoms for manipulation
Additional Menu With JSmol - Prototype

Atom List

<table>
<thead>
<tr>
<th>ID</th>
<th>File Name</th>
<th>T</th>
<th>A</th>
<th>D</th>
<th>F</th>
<th>Molecule</th>
<th>Atoms</th>
<th>Frames</th>
<th>Vol</th>
</tr>
</thead>
</table>

Open File Explorer

Messages will appear here. Enter commands in the box below. Click the console help menu item for online help, which will appear in a new browser window.

Run Load Clear input
Clear Output History State
Moving Forward

- GenApp will eventually begin testing with other applications other than SASSIE.
- Jmol/JSmol will eventually have all the functionalities and look and feel in full. Jmol/JSmol will also be fully implemented in SASSIE Web and its compatibility with GenApp will be ensured.
References

- Jmol: an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/
- SASSIE Program: http://www.smallangles.net/sassie/SASSIE/SASSIE_HOME.html
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