

# The Addition of Functionality to the Jmol/JSmol Application

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## Abstract

SASSIE, a program used to analyze scattering data, was the first program to be converted into a web application by GenApp. GenApp is a developing program that can convert standalone programs into different forms of media, like a web application. Jmol/JSmol is an open source molecular viewing program that is embedded in SASSIE Web. I helped set the base for increased functionalities of Jmol/JSmol application. All work done in Jmol/JSmol must be compatible with SASSIE Web and GenApp. Some of these functionalities include a persistent right click menu, a permanent console, an atom list, and a second menu of commands.

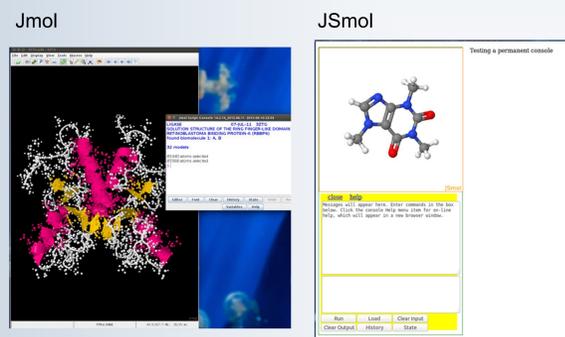
## What's Been Completed

SASSIE Web's JSmol applet should soon have a permanent console. The persistent right click menu is close to being finished. The second menu's base is being created as of now and the atom list is in its earliest stages of development.

## Background

### What's Jmol/JSmol?

- Jmol/JSmol is a molecular structure visualization tool used to look at chemical compounds, DNA, proteins, and more.
- Jmol is the Java only, standalone program. JSmol is the JavaScript version of the program and is intermeshed with the Java code. JSmol can be accessed online as a web application.
- Possibilities of Jmol/JSmol
  - Load multiple molecules at once
  - Move structures independently
  - Saving the universe of molecule(s)



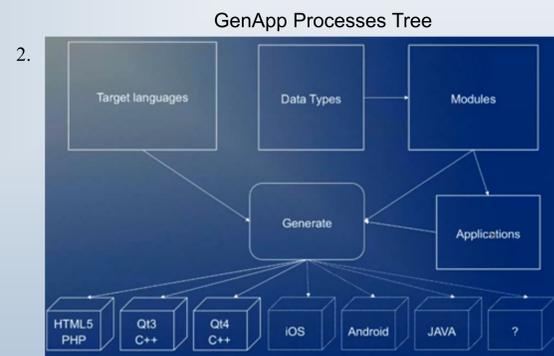
### What's SASSIE Web?

- SASSIE Web is a program that uses atomistic models to predict and interpret scattering data (such as Neutron or X-Ray Scattering).
- SASSIE Web contains JSmol for its molecular viewing purposes.
- SASSIE Web was originally a standalone program called SASSIE, but with the help of GenApp, SASSIE now has web capabilities.
- It's my goal to add functionalities to Jmol/JSmol for SASSIE Web.



### What's GenApp?

- GenApp is a program that converts standalone applications to other formats such as:
  - Web Application
  - Qt 3, 4, and pending 5 (Qt is a cross-platform application framework used for creating graphical user interfaces)
  - Android and soon iOS
- How it works:
  - GenApp takes in a JSON file (essentially a text file with structured data) that contains definitions to form the desired standalone program. GenApp uses the JSON and works as a compiler to develop the standalone program on different forms of media.



## Scope – Bringing it all Together

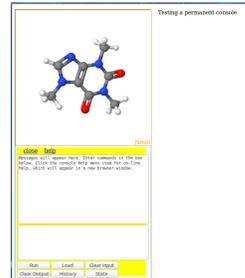
- All changes I make to Jmol/JSmol have to be compatible with SASSIE Web and GenApp.
- SASSIE is the first program to be turned into other forms of media using GenApp (it was the test program).

## Additions to Jmol/JSmol

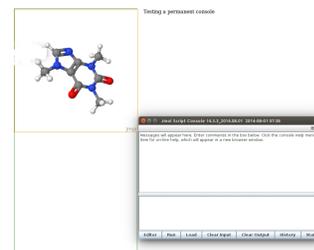
### Permanent Console:

Jmol/JSmol's console is a useful tool for manipulating molecules. There are hundreds of commands that can be used to get the molecule in the perfect position and record the molecule. In the original Jmol/JSmol program, the console is hidden and has to be opened from the right click menu. Now the console shows up upon launch of the program and cannot be closed. The console can also be fixed in place so that it's always in the same place when needed.

Fixed:

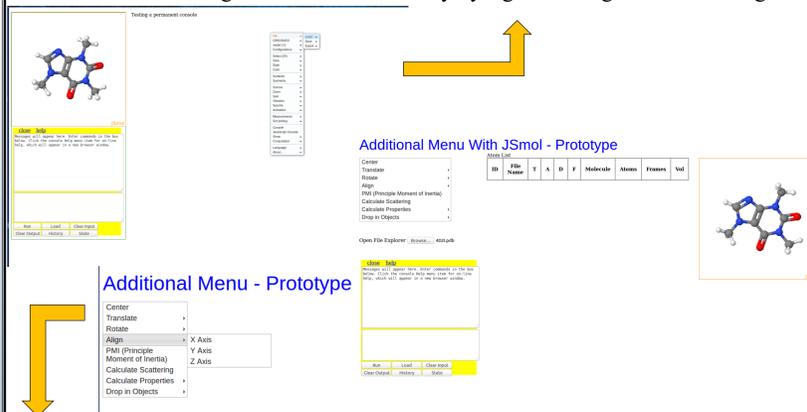


Not Fixed:



### Persistent Right Click Menu:

When a user right clicks on a molecule, a menu appears containing a slew of options such as saving a file, loading in a file, options to manipulate the universe and the molecule, getting the console, and getting help with the Jmol/JSmol application. Having the menu appear on the fly is useful, however as soon as a user mouses off the menu, even if by accident, the menu will disappear until right clicked again. What we have done is made it so after being opened the first time, the menu stays open for easy use. The Menu can be gotten rid of if necessary by right clicking the molecule again.



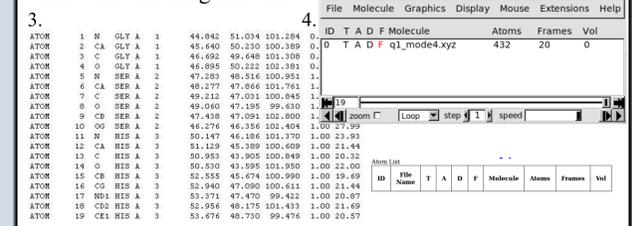
### Second Custom Menu:

A second menu is being implemented so that users do not have memorize all of the console commands and have access to a variety of new tools to manipulate their structures. These tools include: center (center the object in the universe), translate (move the structure), rotate (spin the structure), align (align the structure with another, or on a plane), calculating scattering (shape and dynamics of the molecule), and dropping in geometric objects (to compare to a molecule). This part of project is still in development.

### Atom List:

A new graphical user interface that has a list of all of the atoms in the universe. From here a client could select which atoms he/she would like to manipulate. We are aiming to have it be similar to the Visual Molecular Dynamics program's Atom List. We have yet to delve too deeply in this part of the project.

Will look something like this:



## Moving Forward

### Jmol/JSmol:

In the future, Jmol/JSmol will have all of these features completed (and possibly more) and fully operational on SASSIE Web and compatible with GenApp. Jmol/JSmol is program full of possibilities and is growing in usage among the scientific community. New tools are being implemented into the project everyday and the program will continue to grow.

### GenApp:

As for GenApp, SASSIE Web was just the first step in it's process of turning all sorts of programs into different formats. GenApp will continue to grow and become readily available.

## Acknowledgments/References

Huge help from:

- My Mentor, Dr. Joseph Curtis
- Dr. Emre Brookes
- Dr. Robert Hanson
- Steven Howell
- Julie Borchers, Yamali Hernandez
- SHIP, and SHIP Director
- All other Jmol/JSmol Developers

Links:

1. <http://pdroms.de/pandora/crippic-v0-32-0-1-pandora-java-application>
2. <https://wiki.apache.org/confluence/display/AIRAVATA/GSoC+2014+-+GenApp+Integration+with+Apache+Airavata>
3. <http://cns.org/content/5c318e-7807-4c76-95f8-65749251f6b6/6.3.2/Geometric+Methods+in+Structure>
4. <http://exciting-code.org/beryllium-animated-phonons>
5. [http://wiki.jmol.org/index.php/Recycling\\_Corner](http://wiki.jmol.org/index.php/Recycling_Corner)
6. <http://chemapps.stolaf.edu/jmol/docs/>
7. <http://jmol.sourceforge.net/>