The Addition of Functionality to the Jmol/JSmol Application

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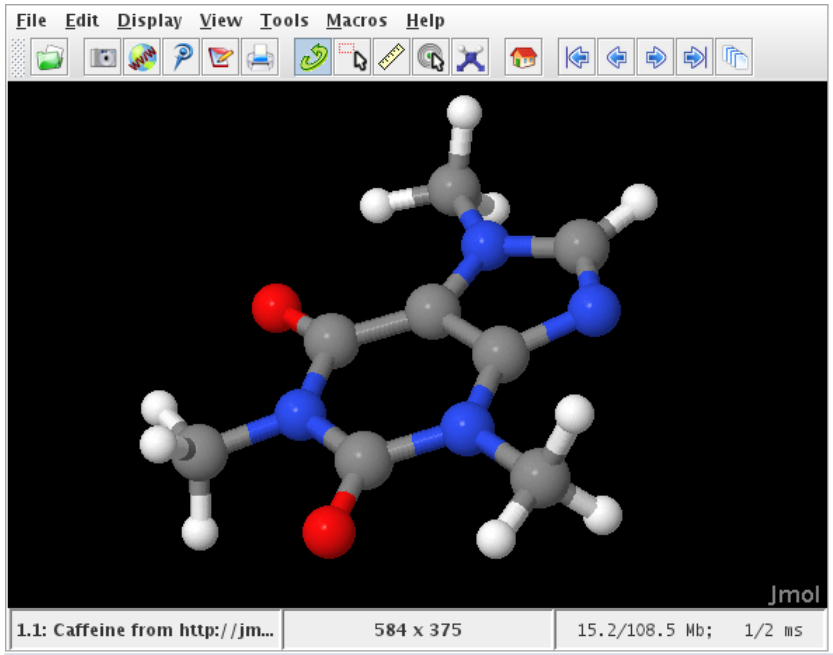
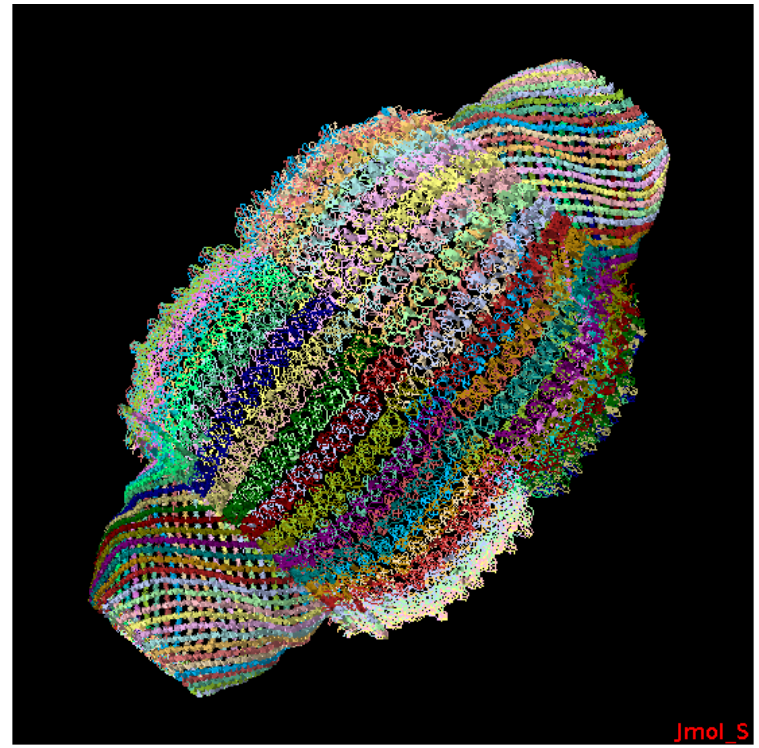
What's Jmol/Jsmol?

- Jmol/Jsmol is a molecular structure visualization tool
- Jmol – In Java, Standalone
- Jsmol – In JavaScript, Web application

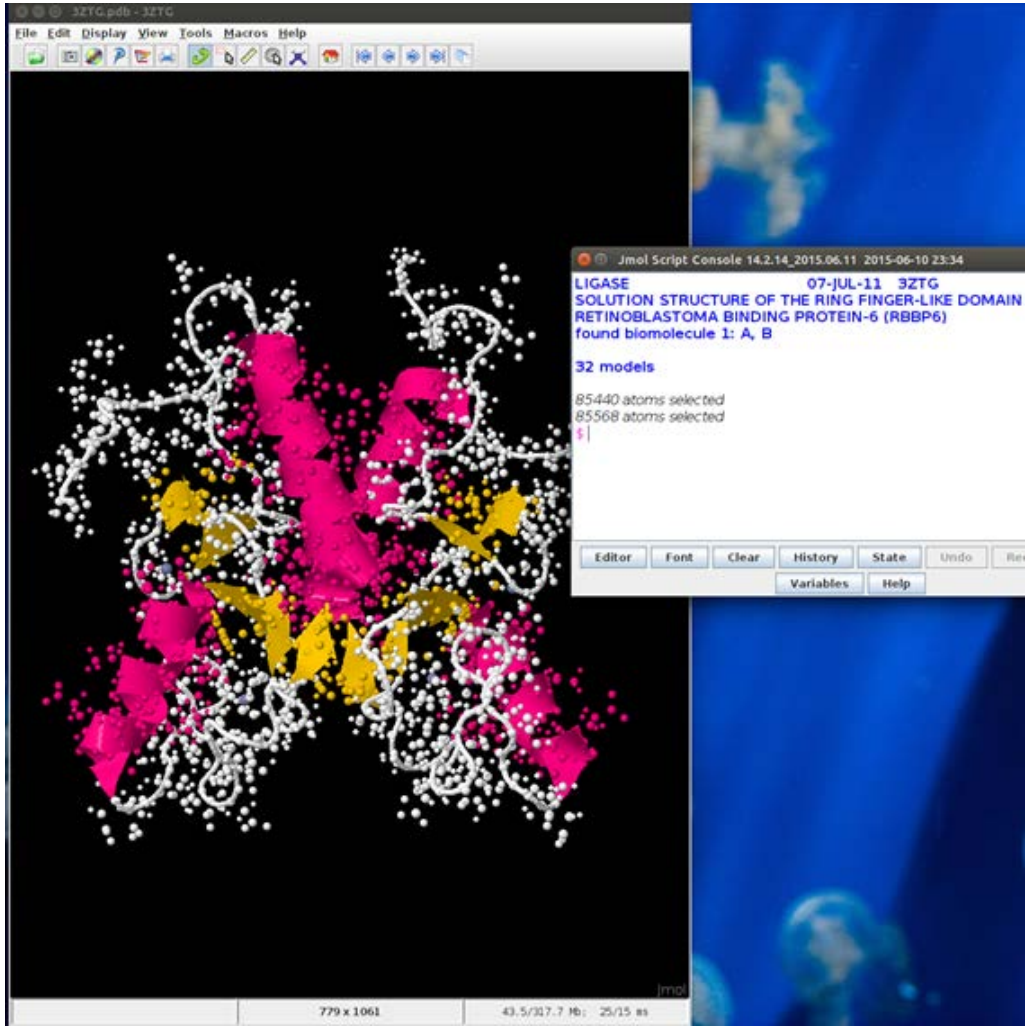


http://pdroms.de/pandora/cryppic-v0-32-0-1-pandora-java-application

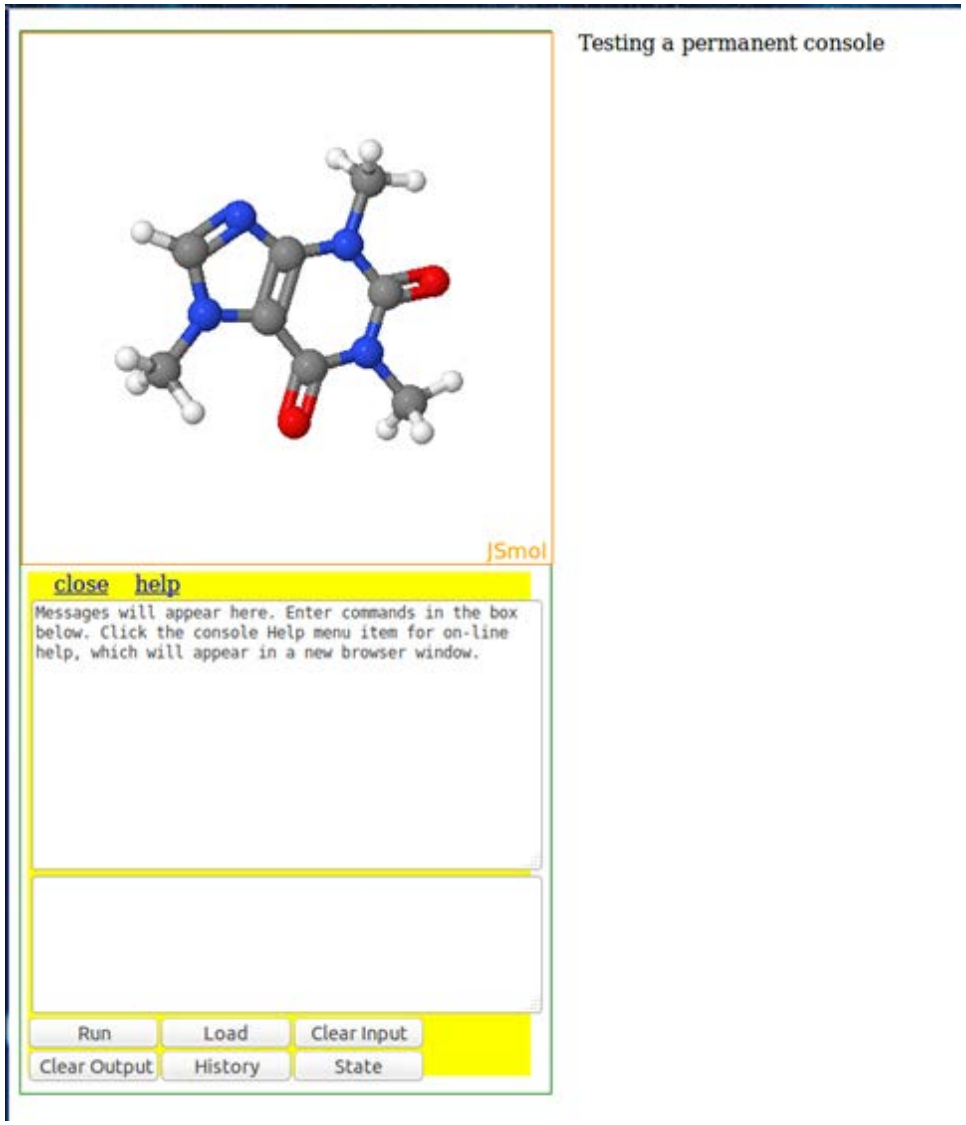


http://www.rcsb.org/pdb/static.do?p=general_information/whats_new.jsp?b=0911

Jmol

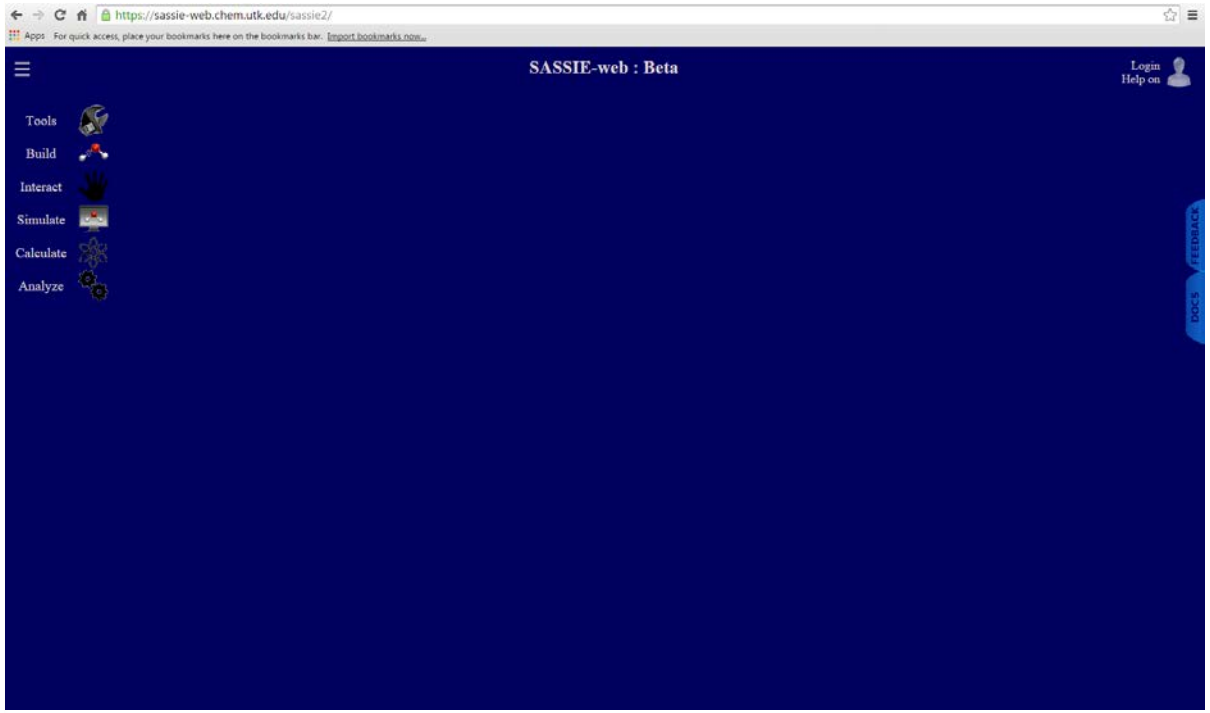

File Edit Display View Tools Macros Help
Jmol Script Console 14.2.14_2015.06.11 2015-06-10 23:34
LIGASE 07-JUL-11 3ZTG
SOLUTION STRUCTURE OF THE RING FINGER-LIKE DOMAIN
RETINOBLASTOMA BINDING PROTEIN-6 (RBBP6)
found biomolecule 1: A, B
32 models
85440 atoms selected
85568 atoms selected
Editor
Font
Clear
History
State
Undo
Variables
Help
779 x 1061

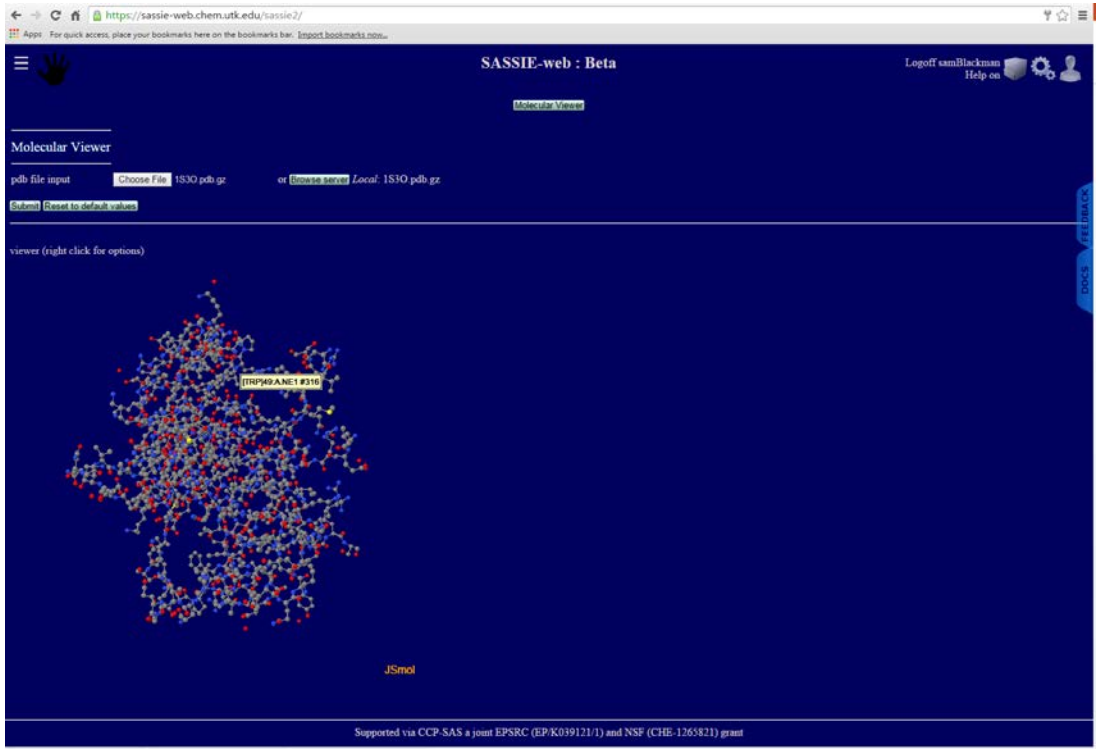
JSmol


Testing a permanent console
JSmol
close
help
Messages will appear here. Enter commands in the box below. Click the console Help menu item for on-line help, which will appear in a new browser window.
Run
Load
Clear Input
Clear Output
History
State

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 Jmol/Jsmol for SASSIE Web.

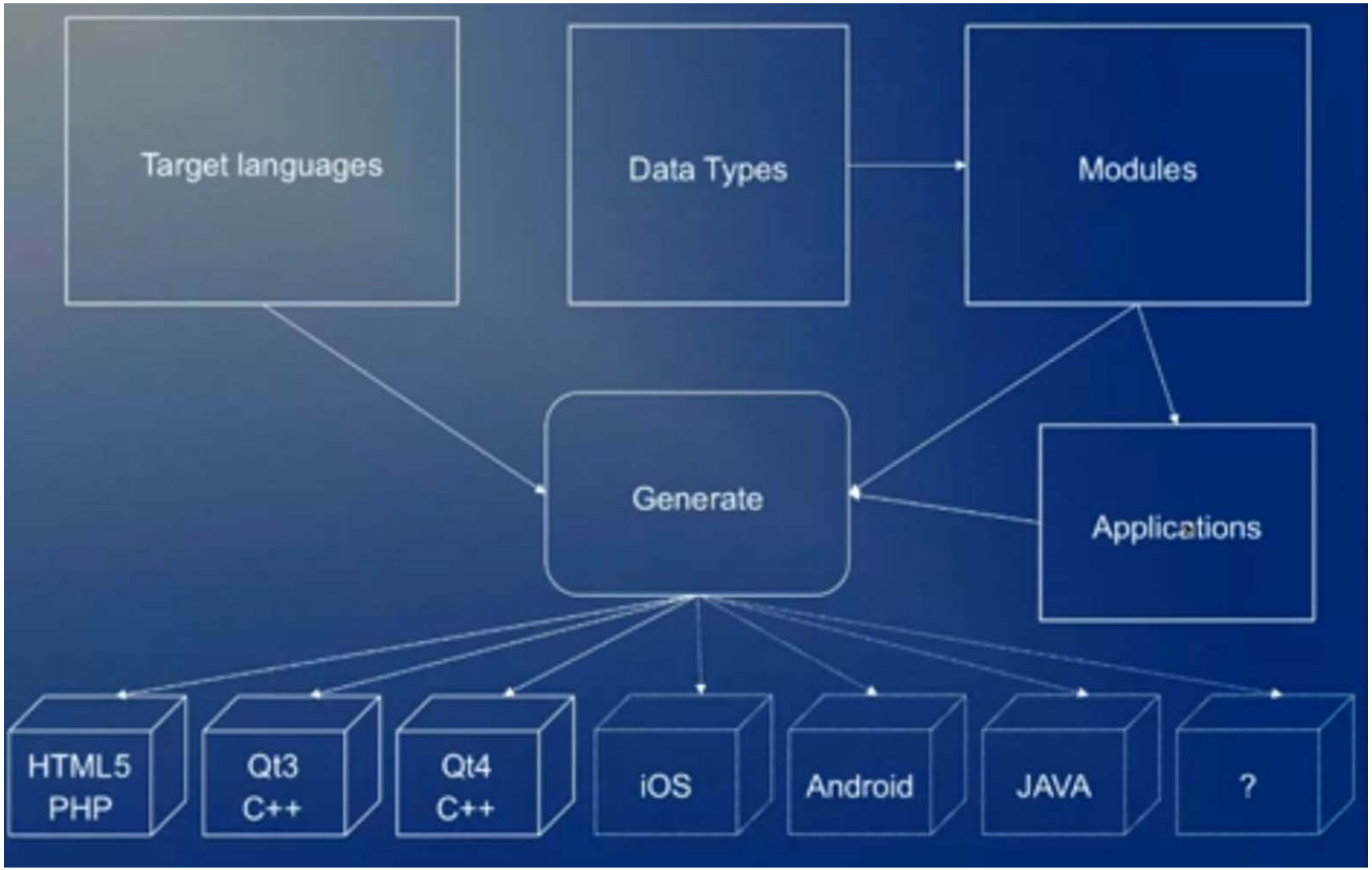




The Project as a Whole

- 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


Target languages
Data Types
Modules
Generate
Applications
HTML5
PHP
Qt3
C++
Qt4
C++
iOS
Android
JAVA
?

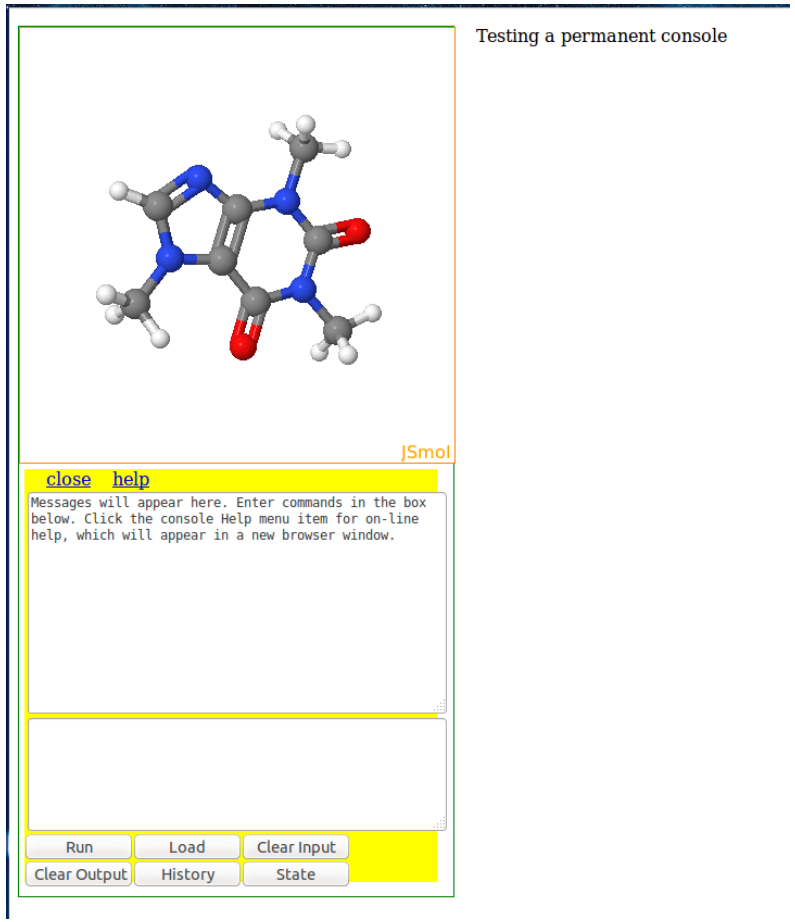
Possibilities with Jmol/JSmol

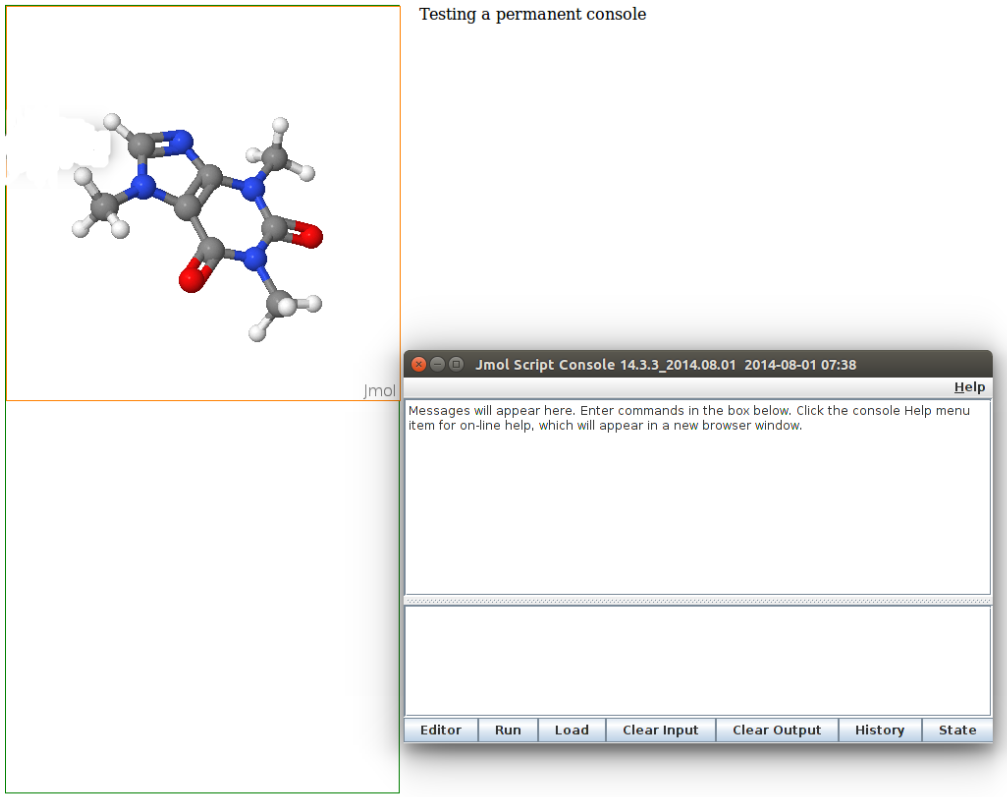
- Load in multiple molecules at once
- Move structures independently
- Saving the universe of a molecule(s)
- View all sorts of structures, from proteins to DNA.

Addition of Jmol/JSmol Functionality

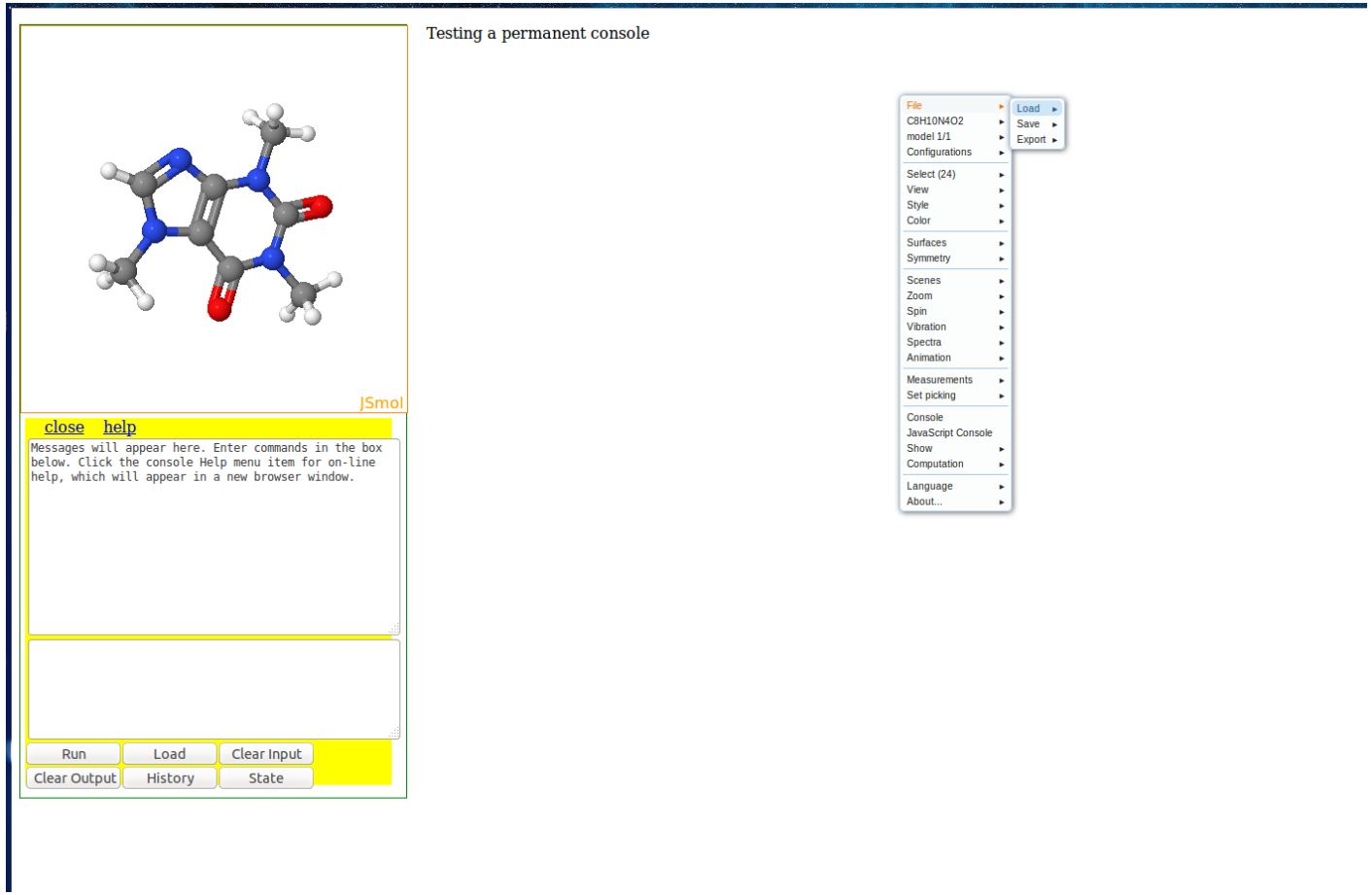
- Permanent/Fixed Command Console
- Persistent right click menu
- Second customized menu
- An Atom List

Permanent/Fixed Console



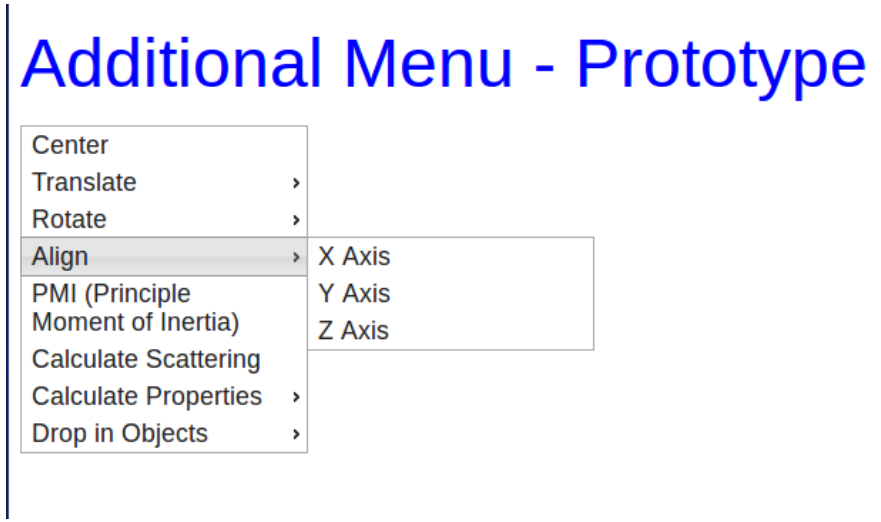


Persistent Right Click Menu



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



Atom List

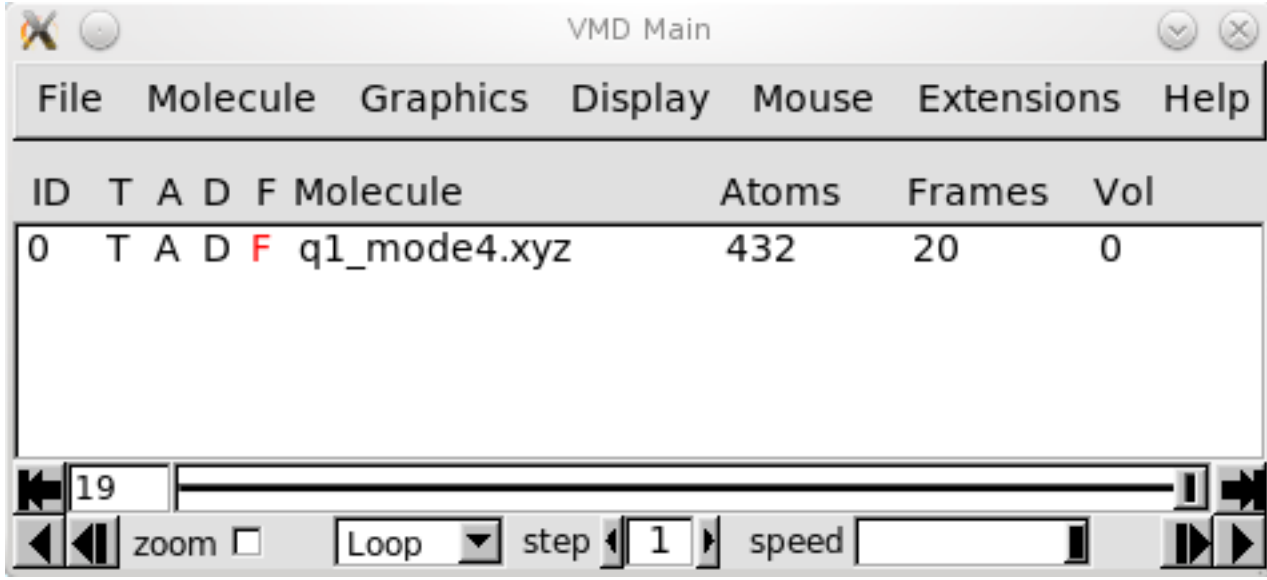
Atom List

ID	File Name	T	A	D	F	Molecule	Atoms	Frames	Vol

- Can select specific atoms for manipulation

```
ATOM      1  N   GLY A   1      44.842  51.034 101.284  0.01 27.20
ATOM      2  CA  GLY A   1      45.640  50.230 100.389  0.01 26.99
ATOM      3  C   GLY A   1      46.692  49.648 101.308  0.01 26.80
ATOM      4  O   GLY A   1      46.895  50.222 102.381  0.01 26.91
ATOM      5  N   SER A   2      47.283  48.516 100.951  1.00 26.26
ATOM      6  CA  SER A   2      48.277  47.866 101.761  1.00 26.17
ATOM      7  C   SER A   2      49.212  47.031 100.845  1.00 24.21
ATOM      8  O   SER A   2      49.060  47.195  99.630  1.00 19.77
ATOM      9  CB  SER A   2      47.438  47.091 102.800  1.00 26.31
ATOM     10  OG  SER A   2      46.276  46.356 102.404  1.00 27.99
ATOM     11  N   HIS A   3      50.147  46.186 101.370  1.00 23.93
ATOM     12  CA  HIS A   3      51.129  45.389 100.609  1.00 21.44
ATOM     13  C   HIS A   3      50.953  43.905 100.849  1.00 20.32
ATOM     14  O   HIS A   3      50.530  43.595 101.950  1.00 22.00
ATOM     15  CB  HIS A   3      52.555  45.674 100.990  1.00 19.69
ATOM     16  CG  HIS A   3      52.940  47.090 100.611  1.00 21.44
ATOM     17  ND1 HIS A   3      53.371  47.470  99.422  1.00 20.87
ATOM     18  CD2 HIS A   3      52.956  48.175 101.433  1.00 21.69
ATOM     19  CE1 HIS A   3      53.676  48.730  99.476  1.00 20.57
```

http://cnx.org/contents/f5c31f8e-7807-4c76-95f8-657d9251fdfb@6.3:2/Geometric_Methods_in_Structura



http://exciting-code.org/beryllium-animate-phonons

Additional Menu With JSmol - Prototype

- Center
- Translate ›
- Rotate ›
- Align ›
- PMI (Principle Moment of Inertia)
- Calculate Scattering
- Calculate Properties ›
- Drop in Objects ›

Open File Explorer [Browse...] 4D2I.pdb

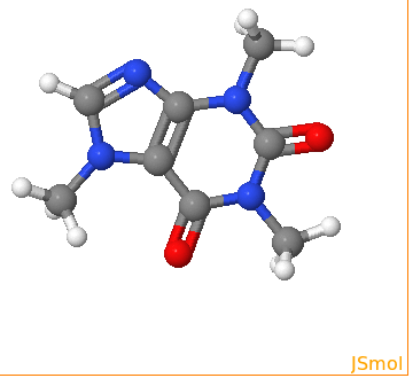
close help

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

Run | Load | Clear Input | Clear Output | History | State

Atom List

ID	File Name	T	A	D	F	Molecule	Atoms	Frames	Vol



JSmol

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 it's compatibility with GenApp will be ensured.

References

- *The GenApp framework integrated with Airavata for managed compute resource submissions* by Emre Bookes et al. http://dl.acm.org/citation.cfm?id=2690890
- 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

- Dr. Joseph Curtis
- Dr. Emre Brookes
- Dr. Robert Hanson

Acknowledgments

- Dr. Joseph Curtis
- Dr. Emre Brookes
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- Center for High Resolution Neutron Scattering