

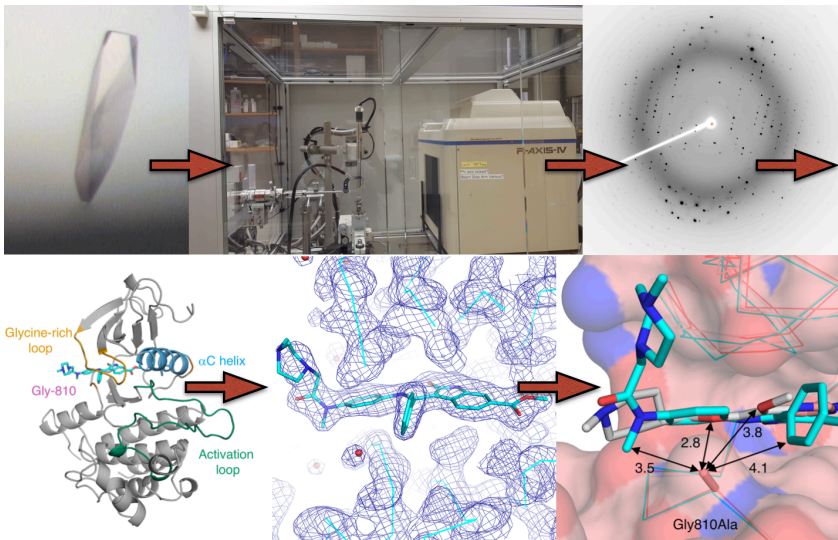
# Reproducible molecular graphics with Org-mode

**Blaine Mooers, PhD**  
**blaine-mooers@ouhsc.edu**  
**405-271-8300**

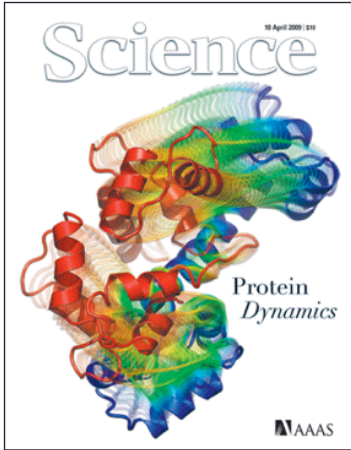
Department of Biochemistry & Molecular Biology  
University of Oklahoma Health Sciences Center, Oklahoma City

emacsconf 2021  
Virtual Meeting  
28 November 2021

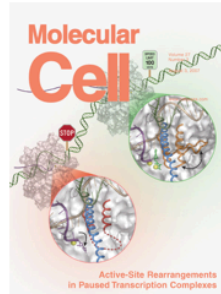
# Workflow in the Mooers Lab



# Cover images made with PyMOL



"Molecular visualization is a ... tool to simplify, clarify, model, analyze, illustrate, and communicate molecular structure, properties, and function."



PyMOL File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

PyMOL

cell dots labels nb\_spheres spheres wire

PyMOL>hide all, chain B

Error: unknown representation: 'all'. Choices:

angles	cgo	ellipsoids	licorice	nonbonded	sticks
callback	dashes	everything	lines	ribbon	surface
cartoon	dihedrals	extent	mesh	slice	volume
cell	dots	labels	nb_spheres	spheres	wire

PyMOL>hide everything, chain B

PyMOL>hide everything, chain C

PyMOL>hide everything, chain C

You clicked /6nec/A/A/PHE 937/CA

PyMOL>

all A S H L C

6nec

Action:

- zoom
- orient
- center
- origin
- drag matrix
- reset matrix
- drag coordinates
- clean

Preset:

- classified
- simple
- simple (no solvent)
- ball and stick
- b factor putty
- technical
- ligands
- ligand sites
- pretty
- pretty (with solvent)
- publication
- publication (with solvent)
- protein interface
- default

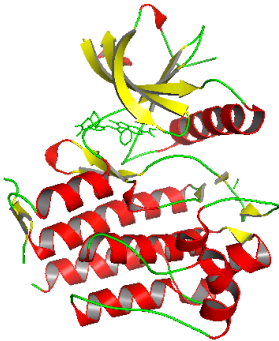
presets

- find
- align
- generate
- assign sec. struc.
- rename object
- copy to object
- group
- delete object
- hydrogens
- remove waters
- state
- masking
- sequence
- movement
- compute

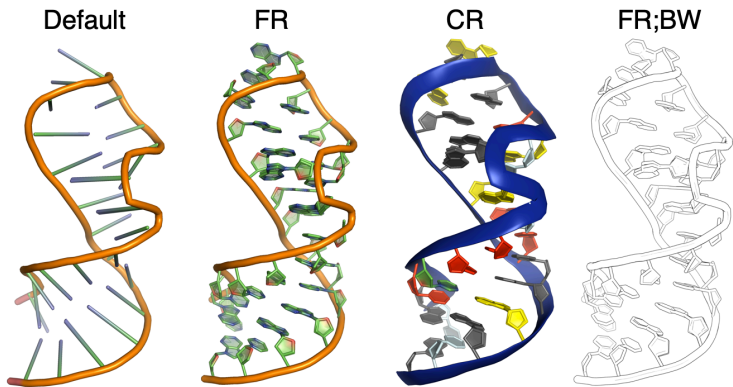
D61C1k

Selecting State

PyMOL>



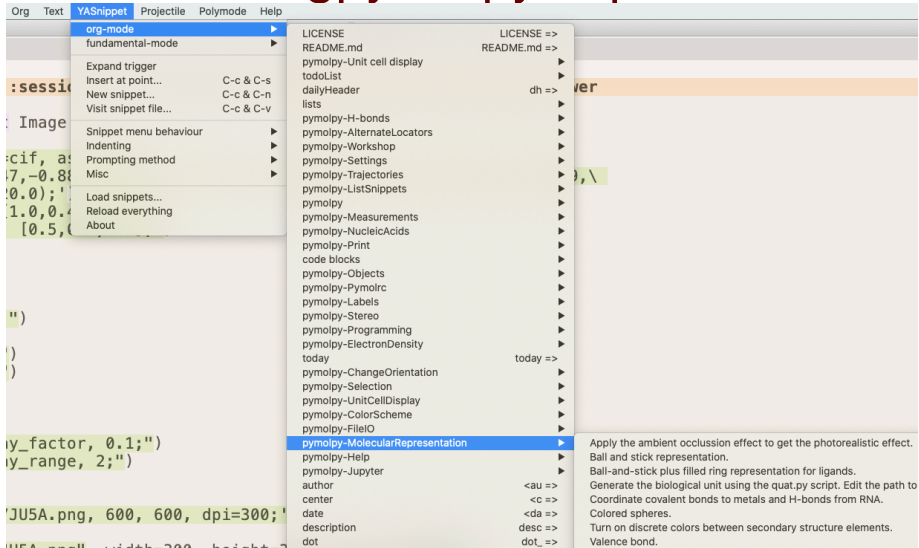
# Customized molecular representations



# Why develop a PyMOL snippet library for Org?

- Org supports literate programming via code blocks.
- Org can run PyMOL through PyMOL's Python API.
- Org file can serve as a gallery of draft images.
- Submit Org file as supplemental material.
- Can include in electronic diary.

# orgpymolpysnips



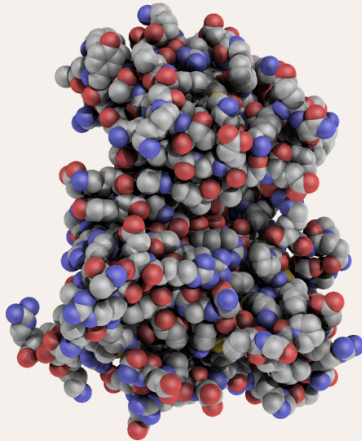
# Code block to make one image

```
#+BEGIN_SRC jupyter-python :session pymol :kernel cp38 :exports both :results raw drawer
from pymol import cmd
from IPython.display import Image

cmd.do('fetch 7JU5:A, type=cif, async=0;')
cmd.do('set_view (-0.11,0.47,-0.88,-0.56,0.7,0.44,0.82,0.54,0.19,0.0,0.0,-203.71,20.89,\
6.7,-25.54,174.56,232.88,-20.0);')
cmd.do("set_color oxygen, [1.0,0.4,0.4];")
cmd.do("set_color nitrogen, [0.5,0.5,1.0];")
cmd.do("remove solvent;")
cmd.do("as spheres;")
cmd.do("util.cbaw;")
cmd.do("bg white;")
cmd.do("set light_count,10;")
cmd.do("set spec_count,1;")
cmd.do("set shininess, 10;")
cmd.do("set specular,0.25;")
cmd.do("set ambient,0;")
cmd.do("set direct,0;")
cmd.do("set reflect,1.5;")
cmd.do("set ray_shadow_decay_factor, 0.1;")
cmd.do("set ray_shadow_decay_range, 2;")
cmd.do("set depth_cue, 0;")
cmd.do("ray;")
cmd.do('png /Users/blaine/7JU5A.png, 600, 600, dpi=300;')
PATH = "/Users/blaine/"
Image(filename=__PATH + "7JU5A.png", width=300, height=300, unconfined=True)
#+END_SRC
```



```
62 cmd.do("ray;")
63 cmd.do('png /Users/blaine/7JU5A.png, 600, 600, dpi=300;')
64 PATH = "/Users/blaine/"
65 Image(filename = PATH + "7JU5A.png", width=300, height=300, unconfined=True)
66 #+END_SRC
67
68 #+RESULTS:
69 :results:
70 # Out[1]:
```



71

# Features important for practical work

Features	Org Mode	Jupyter
Tab triggers	+++	-
Tab stops	+++	-
Snippet groups	+++	+
Parallel sessions in same document	+	-
Pass output data to another block	+	-
Rendering speed	-	++
Scrolling speed	-	++
Ease and speed to PDF	+++++	+

# Relevant part of .emacs file

```
551 ;; List jupyter last.
552 (org-babel-do-load-languages
553 'org-babel-load-languages
554 '((emacs-lisp . nil)
555   (C . t)
556   (js . t)
557   (ditaa . t)
558   (ipython . t)
559   (python . t)
560   (gnuplot . t)
561   (R . t)
562   (latex . t)
563   (plantuml . t)
564   (shell . t)
565   (jupyter . t) ) )
566
567 ;; enable use of python instead of python-jupyter
568 (org-babel-jupyter-override-src-block "python")
569
570 ;; Turn off security confirmation for langs in list.
571 ;; source: https://emacs.stackexchange.com/questions/21124/execute-org-mode-source-blocks-without-security-confirmation
572 (defun my-org-confirm-babel-evaluate (lang body)
573   (not (member lang '("C" "clojure" "sh" "jupyter-python" "jupyter-julia"))))
574 (setq org-confirm-babel-evaluate 'my-org-confirm-babel-evaluate)
```

<https://github.com/MooersLab/orgPyMOLpySnips>

# Acknowledgements

- Nathan Shock Data Science Workshop

## Funding:

- Warren Delano Memorial Open-Source PyMOL Fellowship
- NIH: R01 CA242845, R01 AI088011
- NIH: P20 GM103640, P30 CA225520, P30 AG050911-07S1
- OCAST HR20-002;
- PHF Team Science Grant