Reproducible molecular graphics with Org-mode

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

```python
# 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,-0.56,0.7,0.44,0.82,0.54,0.19,0.0,0.0,0,-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
```
cmd.do("ray;")

PATH = "/Users/blaine/

Image(filename = PATH + "7JU5A.png", width=300, height=300, unconfined=True)

# END_SRC

#+RESULTS:
:results:
# Out[1]:

```python

```
## Features important for practical work

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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
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