Amalgamated Molecular Visualization on Colab

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Introduction

- Molecular vizualization plays a vital role in drug discovery.
- NGLview, py3dmol, rdkit, and PyMOL can be run the same Colab notebook.
- The installation of some of these packages is complex on Colab.
- Our snippets reduce the installaion to a single mouse click.
- This eases the use of molecular graphics in workshops and classrooms.

Approach

1. Develop libraries of code templates for major software
2. Make templates available for JupyterLab and Colab.
3. Include the code for installing software quickly on Colab.
4. Supply template workflows in Jupyter notebooks.
5. Share on https://github.com/MooersLab.

Conclusion

Jupyter notebooks can support reproducible research in structural biology.

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Code snippets ease running four molecular graphics packages in Colab notebooks in the lab, in workshops, and in classrooms.

Take a picture to visit the GitHub repo

or visit https://github.com/MooersLab/polyglotmolviz.
The poster is found at https://github.com/MooersLab/scipy22poster222.
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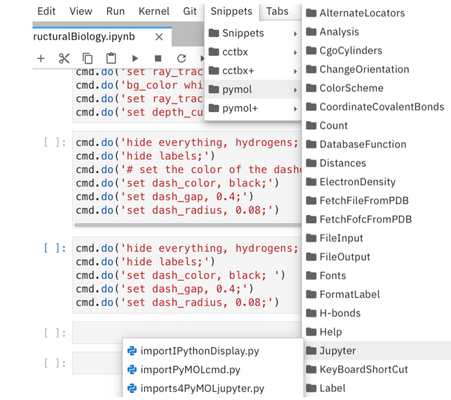
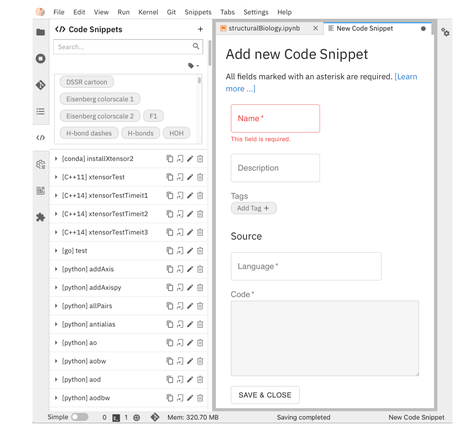
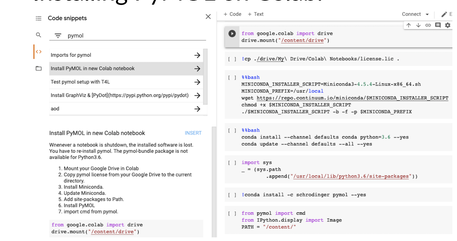
Snippet cascade in JupyterLab:



Elyra snippet manager in JupyterLab:



Installing PyMOL on Colab:



PyMOL commands in Python on Colab: