

Structural Biology in JupyterLab and Colab

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Introduction

- Structural biology is vital for modern molecular biology and drug discovery.
- Biomolecular structure determination is done with crystallography, NMR, cryo-EM, SAXS, and other methods.
- Each method use several to many software packages.
- Doing some or all of the work in Jupyter notebooks would support reproducible research.
- It would also support literate programming for at least some steps.

Approach

1. Develop libraries of code templates for major software packages.
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. Deploy on <https://github.com/MooersLab>.

Conclusion

Jupyter notebooks can support reproducible research in structural biology.



Code templates ease running structural biology software locally in JupyterLab or in the cloud with Colab.

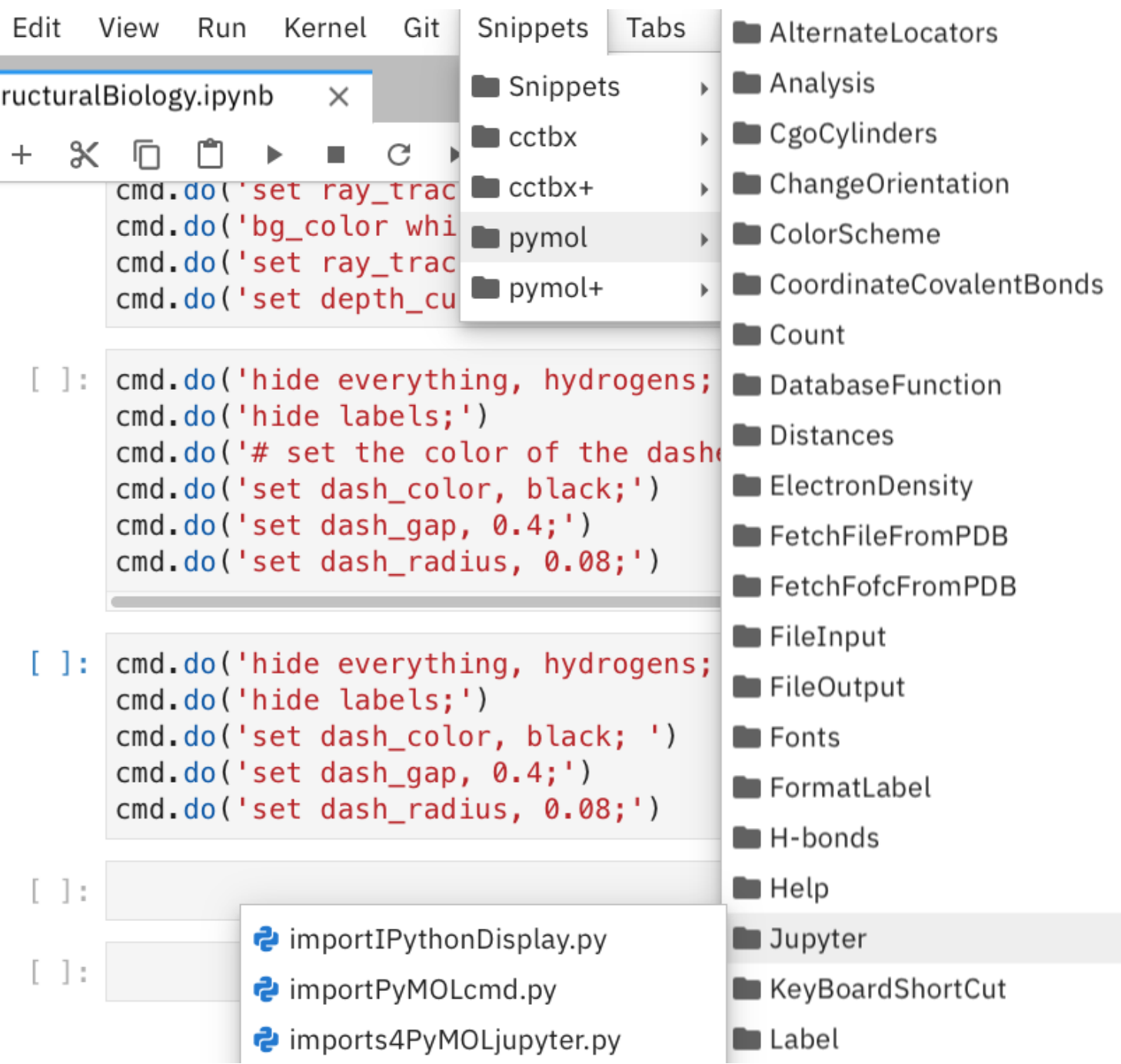


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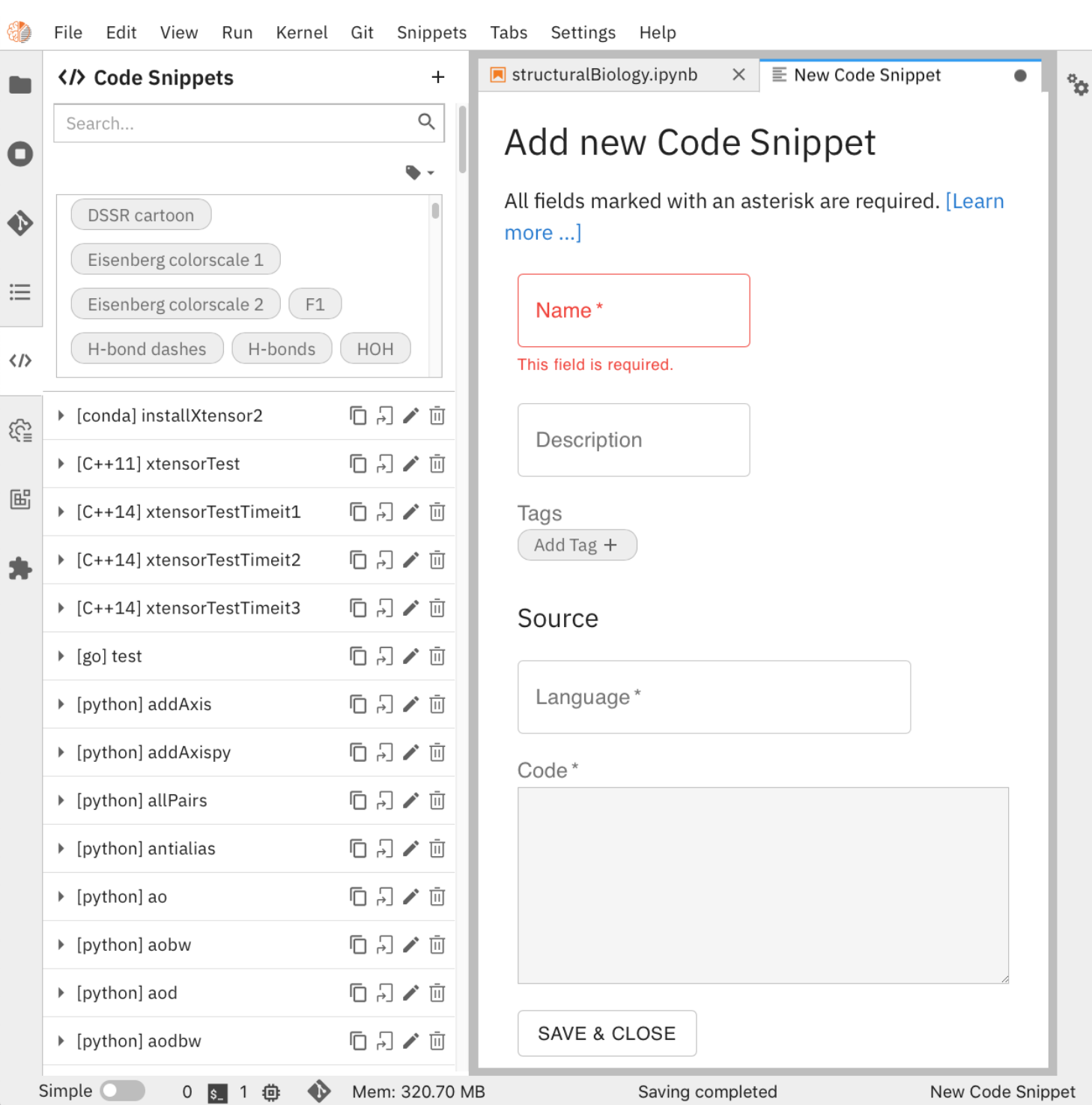
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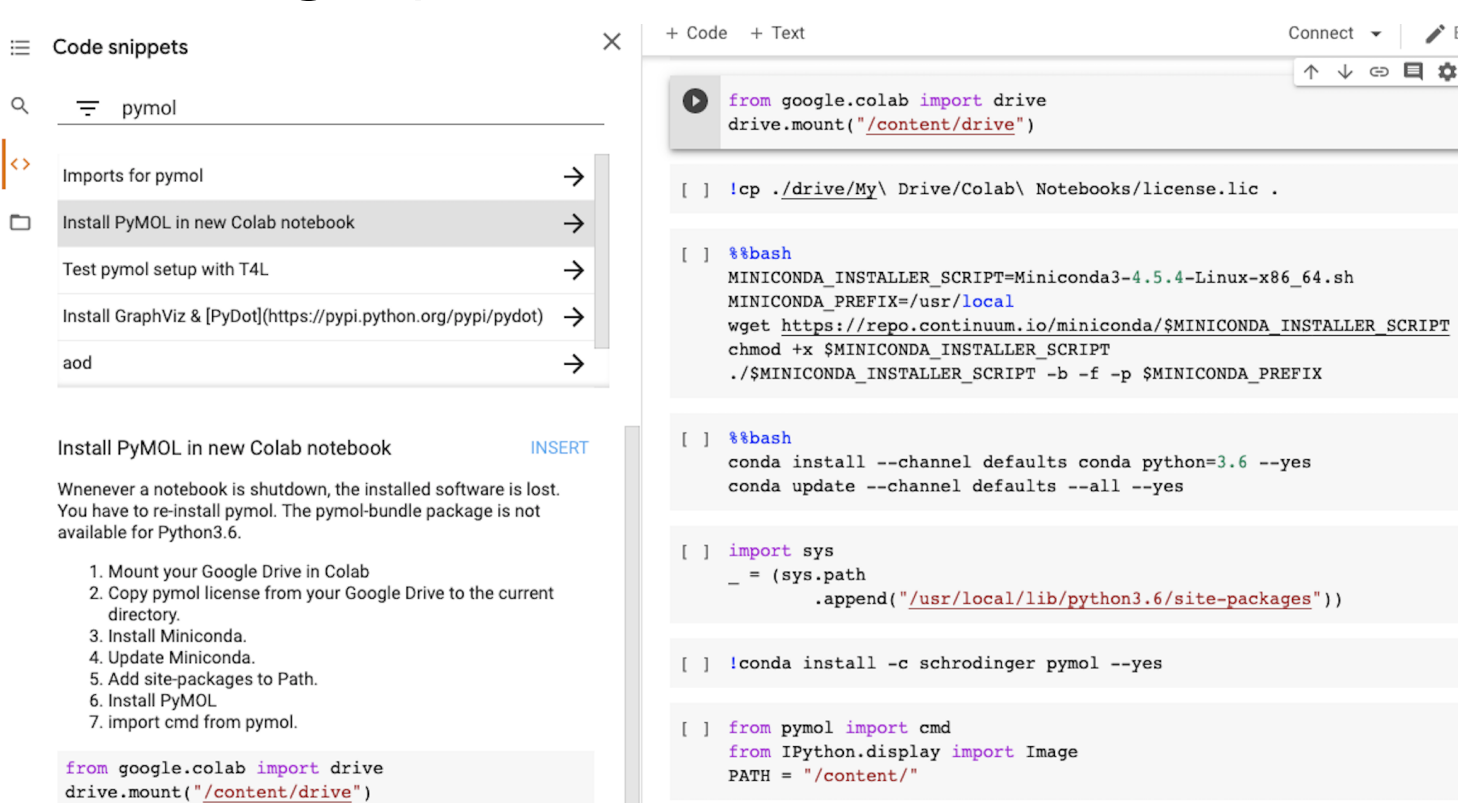
Snippet cascade in JupyterLab:



Elyra snippet manager in JupyterLab:



Installing PyMOL on Colab:



Code and molecular graphics on Colab:

