

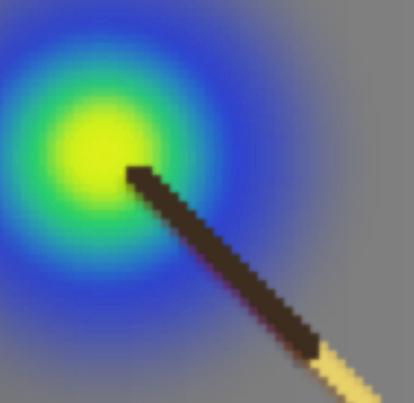
“One Stop Shop” for NMR-based Biomolecular Research

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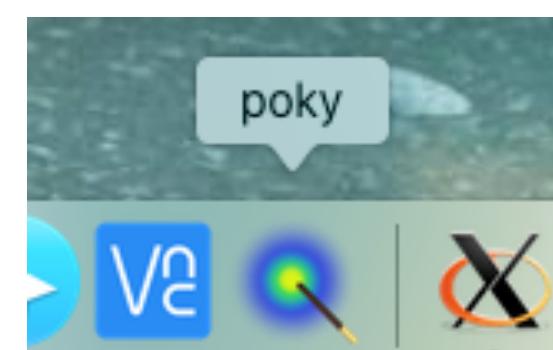


Background

While NMR spectroscopy is a versatile Swiss Army knife for biomolecular studies, different tools and methods are required for the analysis of different types of NMR data. To make such methods more widely accessible, our group is developing a “One Stop Shop” that aims for their integration, automation, innovation, and extensibility. Our latest software package called “POKY” combines NMRFAM-SPARKY and PONDEROSA-C/S into a seamless and interactive environment for bimolecular research. Users gain access with mouse clicks to tools for the assignment of protein solution and solid-state NMR data, 3D structure determination and refinement, and analysis of chemical shift perturbation data including deciphering of allosteric networks from perturbation data by artificial intelligence (AI). In addition, the package includes tools for integrative structural biology approaches that combine NMR data with results from small-angle X-ray scattering (SAXS), X-ray crystallography, or cryogenic electron microscopy (cryoEM).

Motivation

- Our software packages like NMRFAM-SPARKY, PONDEROSA-C/S, I-PINE, PACSY, etc are very popular indispensable tools
- However, the ‘technical debt’ has accumulated and it limits the future development.
- Therefore, we develop the new **POKY suite**.



Acknowledgements

- This work has been supported by National Science Foundation award numbers DBI-2051595 & DBI-1902076 (to Woonghee Lee), and the start up support from the University of Colorado Denver.
- The POKY suite will be available from <https://github.com/pokynmr> soon.

The POKY Suite

POKY Main

Enhanced Strip Plots

POKY Automation Guide (PAG)

I-PINE web server
ssPINE web server

POKY Structure Builder

Open Source PyMOL

POKY Structure Analyzer

Poky Notepad

Interactive Python Shell

Machine Learning in POKY

POKY includes machine learning and data science modules (TensorFlow, Keras, sklearn, etc) as well as NMRGlue for processing. This demonstration is fully automated in POKY.

Advertisement: We seek for researchers interested in joining our POKY group and living in the great Denver area. Contact: woonghee.lee@ucdenver.edu