How to relax the BMRB

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The program relax [1, 2] (http://nmr-relax.com) is designed for the analysis of molecular dynamics using experimental NMR data. Currently relax's primary purpose is to perform the Lipari-Szabo model-free analysis of relaxation data. Additionally relax can perform reduced spectral density mapping [3, 4], exponential curve-fitting for determining R1 and R2 relaxation rates from peak intensities, and calculation of the steady-state NOE. It provides a set of modular tools for performing highly accurate and high quality analyses including Monte Carlo simulations, the gold standard for error propagation and analysis, many high-precision optimisation algorithms, a selection of techniques from the advanced statistical field of mathematical model selection (using Frequentist rather than Baysian methods), and model elimination for the removal of failed models. relax can interface with other programs including Molmol, PyMOL, Grace, and OpenDX for data visualisation, and both Dasha and Art Palmer's Modelfree. For the later two, relax can create input files, execute in-line, and read the output results files, effectively allowing relax to use both Dasha and Modelfree as replacement optimisation engines. Its Python prompt and script interfaces allow for very powerful and automatic scripting, such as the provided 'full_analysis.py' script which performs the new model-free analysis protocol as descibed in [2]. More details about the full set of features can be found at [5].

Open source licensing and the flexible, modular architecture allows others to extend relax to their needs. For instance a number of relax branches are under current development by various NMR spectroscopists to allow relax to run on large clusters using the MPI protocol, to perform relaxation dispersion analyses, to handle ellipsoidal CS tensors for RNA and DNA analysis, to name a few.

Although hundreds of model-free analyses have been published to date, providing a wealth of information covering macromolecular motions over the pico- to nanosecond timescales, most of this data is not easily available, or even inaccessible to current researchers preventing downstream usage. The BioMagResBank (BMRB, http://www.bmrb.wisc.edu/) provides the resources to store all of this data, yet these facilities are rarely used. To improve the utility of NMR dynamics data, relax is being designed to produce full BMRB NMR-STAR v3.1 formatted files to facilitate data submission. Once a model-free analysis has been performed, the BMRB input file can be generated very easily and submitted prior to manuscript publication.

Figure 1. This is the relax logo. It has absolutely nothing to do with anything.

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[3] Farrow, N. A., Zhang, O., Forman-Kay, J. D., Kay, L. E. (1995). *Biochem.*, **34**(3), 868-878.
[4] Lefevre, J. F., Dayie, K. T., Peng, J. W., and Wagner, G. (1996). *Biochem.*, **35**(8), 2674-2686.
[5] d'Auvergne, E. J. (2006). Protein dynamics: a study of the model-free analysis of NMR relaxation data. Ph.D. thesis, Biochemistry and Molecular Biology, University of Melbourne. (*Available in paperback form from amazon.com*).