

TIMPGUI: A graphical user interface for the package **TIMP**

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The package **TIMP** is in use by biophysicists who seek to discover models for (photo)-physical processes in complex systems. The measurements under consideration most often represent some spectroscopic property resolved with respect to time, and the goal is typically to discover a nonlinear model for the kinetics. This problem is approached by postulating an initial model, in which the spectra associated with the system are obtained as conditionally linear parameters, then optimizing the nonlinear parameters and finally validating the resulting model for physical interpretability.

We have been motivated to use **Java** to develop an interface to **TIMP** for several reasons. One reason is that many of the scientists using **TIMP** prefer a graphical user interface (GUI) to a command line interface. Another reason is that **Java**, and the JFreeChart plotting library we are using, along with the JRI library (part of the **rJava** package), allows for more possibilities for interacting with plots than is currently possible in **R** alone. This facilitates interactive data exploration, which can greatly improve the rate at which models can be formulated and tested. A third reason to use **Java** is that it allows the GUI to be programmed with a GUI builder (we use the Netbeans Integrated Development Environment (IDE)) as opposed to manually specifying the parameters of widgets in **R** code. We feel this allows for a flexible modular design which is easily extended by other developers. Finally, we require a fully crossplatform interface, for which **Java** is well-suited.

Here we showcase the current capabilities of the interface and demonstrate its usability by demonstrating several case studies, fitting kinetic models to time-resolved fluorescence and absorption data.