User Guide: NMR PRE Data Analysis

Code 1: PRE code
Number of files: 3
Names of the files: PRE_1, PRE_2, PRE_3

Purpose

The purpose of this code is to analyze data collected from the PRE (Paramagnetic Relaxation Enhancement) experiment in Nuclear Magnetic Resonance (NMR). The PRE experiment is used to study interactions between paramagnetic centers and amino acid residues in a protein.
Brief introduction about PRE:
A residue of protein is labelled with a paramagnetic label, the residues close to this label will have a faster relaxation rate in the NMR timescale than the ones which are further away, this helps us know which residue is close to our labelled residue in a 3D structural arrangement in solution.
The faster the relaxation rate, the quicker the drop of intensity measured by the instrument and the drop of the intensity follows an exponential decay function.
Y=Y0* exp (X/K), K is a constant obtained after fitting the datapoints in the exponential decay equation. 1/K = R2
The data obtained from protein after spin labelling is called paramagnetic data(para) or Oxidized (Rox)
We also run a controlled NMR experiment without the spin labelling and process the data file as diamagnetic(dia) or reduced(red) data.
The R2 for both the data sets is calculated and gamma(2) is obtained from the following equation:

$$\Gamma_2 = R_2^{PRE} = R_2^{para} - R_2^{dia}$$

The gamma(2) is fitted to the following equation to obtain distance of each residue from the paramagnetic centre:

$$r = \sqrt[6]{\frac{K}{\Gamma_2}\left(4\tau_c + \frac{3\tau_c}{1+(\omega_I\tau_c)^2}\right)}$$

Code Overview

The code is divided into three files: `PRE_1`, `PRE_2`, and `PRE_3`. Each file performs a specific analysis task related to the NMR PRE data.

PRE_1

This file contains functions for fitting data and plotting the results. It reads data from a text file, analyzes the data for each residue, performs exponential fitting, along with calculating how good of a Fit is this and giving you R^2 values and plots the fitted curve for visualization. Every residue is plotted separately for the user to be able to visualise and judge how good of a fit is this amino acid residue intensities. It prints out, Yo, K and R^2 values which you copy and save as a .txt file.

PRE_2
This file compares two sets of data (Rox data and red data which are derived by using PRE_1 on two data sets.) and calculates the difference between two values for each residue. It prompts the user to enter the file names containing the data and prints the differences and prints out the differences which you save as a .txt file.

PRE_3
This file calculates a parameter `r` based on the provided parameters (`tau_c` and `w`) and the data from a specified file which you saved after using PRE_2 code. It prompts the user to enter the file name, `tau_c`, and `w` (frequency in MHz) values. The code reads the file, extracts residue and difference values, calculates `r`, and prints the results.
tau_c is usually around 0.00000001 and w (in MHz) is between 600-1000

Data Format
The data derived from the PRE experiment is expected to be in the format of a text file. The file should have the following structure:

- The first column contains the number of amino acid residues.
- The first row contains the relaxation delay times.
- The rest of the numbers represent the relative intensities of each residue.
You must start with two such files for both oxidised and reduced residues each.

How to Use the Code
Follow the instructions below to use the code:

1. **File Setup**: Make sure you have the three code files (`PRE_1.py`, `PRE_2.py`, and `PRE_3.py`) in your working directory. Additionally, ensure that you have the necessary dependencies (`numpy`, `matplotlib`, `scipy`) installed.

2. **PRE_1**: Run the `PRE_1.py` script to analyze the data, perform exponential fitting, and plot the results. The script will prompt you to enter the name of the data file in the specified format. The plots and fitting parameters for each residue will be displayed, and the fitted parameters will be printed on the console.

3. **PRE_2**: Run the `PRE_2.py` script to compare two sets of data. The script will prompt you to enter the file names for the Rox data and red data. The differences between the values for each residue will be printed on the console.

4. **PRE_3**: Run the `PRE_3.py` script to calculate the parameter `r`. The script will prompt you to enter the file name, `tau_c` value, and `w` (frequency in MHz) value. The code will calculate `r` for each residue based on the provided parameters and print the results.

Note: Make sure to provide the correct file names and values as required by each script.

That's it! You can use this user guide to understand the purpose of the code and how to use it effectively for analyzing NMR PRE data.User guide to my codes