**First Time Use:**

Loading to start an analysis (Click Files Tab)

1. Set the Experiment Directory to match …\Frhodo\Example\Experiment
   1. You should see some data appear on the screen!
2. Set the mechanism directory to match …\Frhodo\Example\Mechanism
   1. You should see a blue line appear on the screen: this is some initial simulated data!
3. Set the Simulation Directory to be …\Frhodo\Example\Simulation
   1. Nothing will happen just yet, but when you try to do a parameter estimation, there will be data exported here!

Running an Analysis (Click Optimization Tab):

1. Click “Run Optimize”. The Log tab will blink, click on it.
   1. The Log Tab says that no reactions or coefficients were set to be optimized! This is an important lesson. Frhodo will keep all parameters as constant except those that it is given permission to optimize.
2. Click on the “Tables” tab. This contains the reactions and parameters. Next, click on R1, R2, R3.
   1. We see that R1 and R2 have rate constants “k” while R3 has a more complex display of kinetic parameters.
      1. *Currently, Frhodo only allows optimizing parameters that the rate constant depends on. If you wish to optimize a rate constant directly, you may use the trick of setting the pre-exponential to that value, setting n to 1, and setting the Ea to 0, which must be done at the level of editing the model which is contained in the ‘mechanism’ file.*
   2. The rate constants, k, are displayed *either* as the constants that are fed *or* what the value would be at 500K if there is a temperature dependence. (What about pressure? 1 atm for each reactant, including inerts?)
   3. The options are “F”, “%” “+/-“ , “+”, “-“. These are *bounds* for Frhodo to optimize inbetween. The F means *factor* and so for example, F=10 means bounds of value/10 to value\*10
      1. Let’s set R3 to have % 10 for each of the 4 settings.
      2. You can use your mouse and you can also use “tab” on your keyboard to cycle through the fields (note that the “%” field is selected last if you use “tab”)
3. Optimizing: Let’s go to the optimization tab again. Click “optimize”. This time you will see that the simulation “moves” around as different adjustments are attempted. Let’s now take a look at the flashing “Log” tab. The Log shows “success” for both the global and local optimization.
   1. Let’s click on the “Objective” tab. Here, we see some statistics related to the objective function. We see that there is a QQ-plot and on the right is a density plot of residuals. In the simplest cases, what you are looking for is \_\_\_\_\_.
4. Results:
   1. If you want to know what the final parameters were, click on the Tables tab. This is an example so you may not remember the original numbers: the numbers here have changed! Actually, they change in real time during optimizations.
5. Now click “Save” at the top of the Frhodo window. This will save the model you have just optimized. Without changing any settings, just click “Save” in the window which pops up.
   1. Check inside the simulations directory you specified earlier: now you will find that there is a new folder created with a futher directory called Sim1 with the optimized mechanism file inside (including the optimized rate constants).
      1. If you try running an optimization again, there will be an additional directory created called Sim2.
      2. These final mechanisms after each optimization are also stored in the Mechanism directory.