Please find in this folder the necessary software to reproduce our simulations and model fitting and predictions. Running this requires R and a c compiler (gcc for example).

The main function that encodes the model explained in section 'Compartmental model of RBC dynamics' is the *forward_sim.c* script, written in c. This needs to be compiled using a c compiler. The simplest way to do this with R is to run the following in the command line:

R CMD SHLIB forward_sim.c

This line generates a compiled script ready to be called by the R functions which provide an interface to the model. For a windows machine the script to be called is *forward_sim.dll*, for a Mac machine it is *forward_sim.o*. The code in *setupmodel.R* needs to be edited to make sure the right line is included (see top of this function).

I have provided a short script called *SimpleCodeExamples.R* which illustrates how the model can be used. This shows the functionality of some of the more important parameters and settings of the model.

The R script *Analysis of G6PD deficients.R* loads the MCMC samples and compares the posterior model predictions with the data. The code which runs the MCMC simulations is also provided. The last section of this script shows how we calculate the optimal ascending dose regimen using a greedy algorithm. This extrapolates a dose-response curve from both the historical data (Figures 1&2) and data from Kheng (2015). The algorithm simply minimises the gradient of the daily haemolysis over the twenty day regimen. This is of course highly dependent on the model parametrisation but provides a starting point for a Phase I type trial in healthy volunteers.