# Leave-one-out-cross-validation

This code performs Leave-one-out-cross-validation and calculated the pre-specified performance measures. Through this model, one drug (with its probability distribution of torsade metric score) is left out and the remaining drugs (either 27 or 7) were used to train the ordinal logistic regression classifier, which was then subsequently used to predict the risk category probabilities of the left-out drug. This procedure was repeated until every drug has predicted probabilities in each of the three categories. These predicted probabilities were used to calculate the 8 performance measures.

## Data preparation

Model input is the metrics.rds calculated by AP\_simulation. The metrics.rds are used to performed the leave one out cross validation by mycompute\_TdP\_error.R and then calculate the performance measures by “plotTableLOOCV.R”.

## Running the code

Step1:

Rscript mycompute\_TdP\_error.R -u

This code uses the following R packages: optparse (version 1.4.4), ggplot2 (version 2.2.0), and rms (version 4.5-0).

The results are store in [results/uncertainty] folder and has a \*.csv format.

Step2:

Rscript plotTableLOOCV.R

This code use the Step1 results to calculate the performance measures.

The results are store in [Result\_PlotTableLOOCV] and has \*.txt format