

Pirana

The flexible modeling environment for NONMEM



Quick Guide: Diagnostic graphics in Pirana using the integrated R-scripts library (without Xpose)

Version 1.1

Scope

This Pirana Quick Guide explains how to use Pirana to generate and modify diagnostic graphs using the integrated R scripts library.

Pirana has an integrated library of R scripts which can be used to generate diagnostic plots based on model output files. The library of R scripts can also be easily edited or extended with new scripts.

Creating diagnostic plots

- Select the model for which you want to create plots.
- In the right panel under Scripts, select the desired script.
- Via the context menu, select run script. clicking the right mouse button, and then selecting 'Run script', and subsequently selecting the plot you want to create (Figure 1).
- The plot will be created and opened automatically (Figure 2).

Troubleshooting problems with plot creation

- If an error occurs, the R output will be displayed, which can be used to diagnose the error (Figure 3).
- Most frequently this is due to a variable missing in the output table files (e.g. column IPRED not available in output table).
- The expected input variables for each script are depicted at the bottom of the right panel.

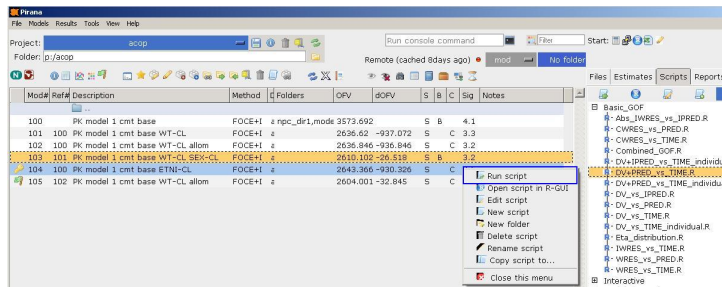


Figure 1: Running a script on a model run

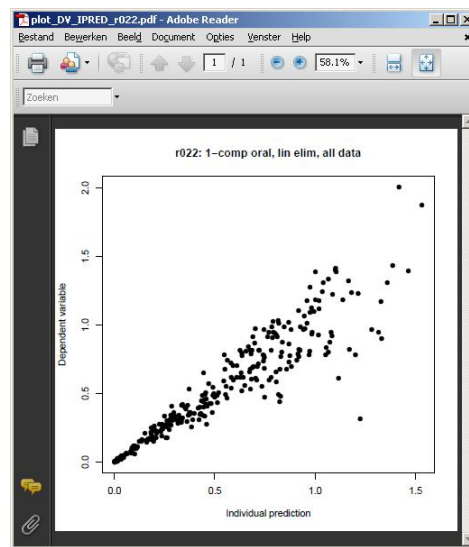


Figure 2: Diagnostic plot created

Customizing diagnostic plots

- Instead of running the script through Run Script (above), the script may also be outputted to the R GUI ("Output script to R GUI") (Figure 4). Now, you can easily tweak the plot, and save it in the format you like.
- After sending the script to R GUI, it will be opened there, where it may be further modified. Next, the script can be executed and the plot will be created within the R GUI (Figure 5).

Editing and creating scripts

- When one wishes to permanently make changes to the scripts library, this can be done using the option "Edit script" in the right panel context menu. (Figure 5).
- Any changes made to the script will be saved permanently. You can choose to make

```

> setwd('p:/Examples')
> model_names <- names(models)
> if (!file.exists("pirana_temp")) { dir.create("pirana_temp") }
> if (file.exists(paste("pirana_temp/plot_DV_IPRED_", names(models)[1], ".pdf", sep=""))) {
+   file.remove(paste("pirana_temp/plot_DV_IPRED_", names(models)[1], ".pdf", sep=""))
+ }
> pdf(file = paste("pirana_temp/plot_DV_IPRED_", names(models)[1], ".pdf", sep=""))
> for (i in 1:length(model_names)) {
+   mod <- models[model_names[i]]
+   tab_file <- mod$tables[1]
+   if (file.exists(tab_file)) {
+     tab <- read.table(tab_file, skip=1, header=T) # NONHEM table with ONEHEADER option
+     if ("MDV" %in% names(tab)) { tab <- tab[tab$MDV==0, ] }
+     if ("EVID" %in% names(tab)) { tab <- tab[tab$EVID==0, ] }
+     colnames(tab)[match("IPRED", names(tab))] <- "IPRED"
+     not_found <- req.fields[is.na(match(req.fields, colnames(tab)))]
+     if (length(not_found) > 0) {
+       cat(paste("The variable(s)", not_found, "were not found. Please check your output tables."))
+       quit()
+     }
+     plot(x=tab$IPRED, tab$DV, main = paste(model_names[i], ":", mod$description, sep=""),
+          pch=19, xlab="Individual prediction", ylab="Dependent variable")
+   }
+ }
> dev.off()
null device
1
>
> print(paste("#", "PIRANA_OUT ", "pirana_temp/plot_DV_IPRED_", names(models)[1], ".pdf", sep=""))
[1] "#PIRANA_OUT pirana_temp/plot_DV_IPRED_r022.pdf"
Pirana: Trying to load file pirana_temp/plot_DV_IPRED_r022.pdf
>
> quit()

```

Figure 3: Output of the script

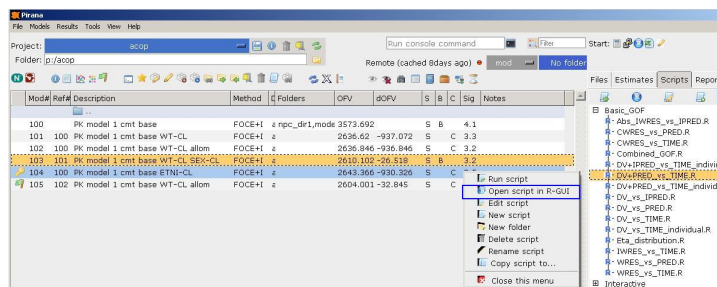


Figure 4: Output of a script to the R GUI for further customization

- changes in the script that are originally supplied with Pirana, or have them in your own user library.
- Script files are located either in the user folder (e.g. C:\Documents and Settings\Username\._pirana\scripts), or in the main Pirana folder (e.g. C:\Program Files\Pirana). The organization of scripts in sub-menus is according to the folder structure in these scripts folders (Figure 6), and can be adjusted accordingly.
 - Note that when you install a new version of Pirana over the old one, any R script you have in the Pirana folder will be overwritten with the one supplied by the new version of Pirana (if you haven't given the R-script another name).
 - Through the menu 'Scripts' → 'New scripts', it is also possible to define new scripts. Please note that at current, you will have to restart Pirana for the script to show up in the interface.

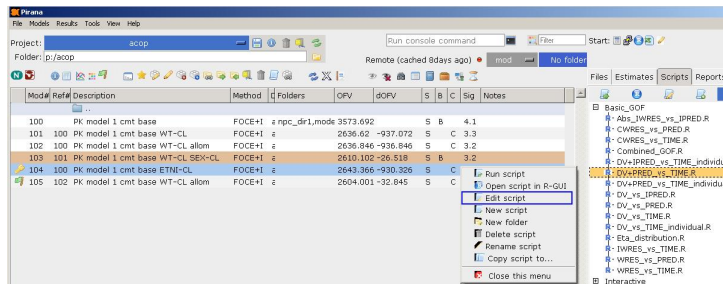


Figure 5: Editing templates for scripts

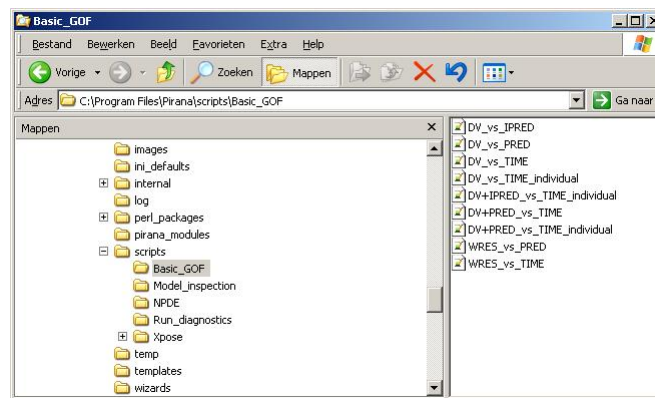


Figure 6: Script files present in the scripts sub-folder of Pirana