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CR: Functionality update to Pharmacometrics TFL Generator

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Assigned CR number:	

Definitions

Purpose

To validate Functionality update to Pharmacometrics TFL Generator requirement of the Pharmacometrics TFL Generator app.

Figure updates

Verification that ggplot2 udpates have been implemented successfully

The application includes numerous figures for exploratory analysis and model evaluation. All graphics are rendered using the current R:::ggplot2 package which has had a major version change since the original validation of the Pharmacometrics TFL Generator app. Because of this change, all figures will undergo exhaustive testing for response to inputs provided by the Pharmacometrics TFL Generator app. Screenshots are used to document evidence of this.

Additionally, three new plots have been added: a multipanel distribution plot, barcharts describing frequencies, and VPC plots to describe model fit. All three will be validated as proposed in the attached testing log, following the same validation approach as used in version 1.0.0 for the original set of figures.

Theme modification works as expected

This version of the application allows users to specify background color, text size, tick length, and other theme elements via the GUI interface. As part of the procedure for validating the fidelity of the figures under the new ggplot2 plotting package, new functionality around theme modification is tested as well.

Usability enhancements

The hard reset button returns the app to the initial state

As extensive use of objects in the global environment of a user's instance of the Pharmacometrics TFL Generator app occurs during use of the app, the ability to return to an initial state of the application (not retaining any prior inputs) is not trivial. A "hard reset" button has been added to the application to allow users to reset the session to the initial state and will be tested as outlined in the testing log.

Reporting

The app creates RTF output for all specified figures, tables, and listings

As a critical feature of the Pharmacometrics TFL Generator, the ability to create a report consisting of objects (TFL's) that have already undergone QC will be checked to validate completeness as well as responsiveness to user defined ordering of TFL's.

The app creates an R script that can reproduce the analysis outside of the app

In addition to a report ready document, the Pharmacometrics TFL Generator generates an R script that allows the user complete reproducibility of the analysis, including the R packages used to developed the TFL. This step compares the output from the R script to the doc file generated in the previous step to assure that this critical functionality remains intact.

Deployment

The app is under version control

The application was developed using git version control. The tagged release will exist on the master branch of git@gitlab.metrumrg.com:danp/TFLgenerator.git. The release commit ID will be logged as part of the validation, and will serve as proof that the app's development cycle has a valid commit history.

Installation package and instructions work to create new app on a new Envision workflow

The `deliv` directory of the git repository contains a README and installation package for instaling and configuring the application. Tests performed under this task will verify that the installation steps are adequate when using a Metworx Envision workflow, as is expected for all deployments of the Pharmacometrics TFL Generator app.

Testing procedures

Testing procedures are outlined in the attached testing document. Testing will be performed by Jonathan Sidi and Dan Polhamus.

Appendix

Testing log

Overview

Topic	RID	Requirement	Reference
Figures	1	Serum Concentration Versus Time-Individual	v1.2.0_protocol.pdf
	2	Serum Concentration Versus Time-Groups	v1.2.0_protocol.pdf
	3	Observed Versus Predicted	v1.2.0_protocol.pdf
	4	Parameter Distribution	v1.2.0_protocol.pdf
	5	Categorical Covariance	v1.2.0_protocol.pdf
	6	Continuous Covariance	v1.2.0_protocol.pdf
	7	Correlation Pairs	v1.2.0_protocol.pdf
	8	Quantile Plot	v1.2.0_protocol.pdf
	9	Goodness of Fit	v1.2.0_protocol.pdf
	10	Variable Distribtuion	v1.2.0_protocol.pdf
	11	Bar Charts	v1.2.0_protocol.pdf
	12	VPC	v1.2.0_protocol.pdf
Usability	13	Hard reset button gives an environment with no input retained from previous sessions	v1.2.0_protocol.pdf
Reporting	14	The app creates RTF output for all specified figure, table, and listings	v1.2.0_protocol.pdf
	15	The app creates an R script that can reproduce the analysis outside of the app	v1.2.0_protocol.pdf
Deployment	16	App is under version control	v1.2.0_protocol.pdf
	17	Installation package and instructions work to create new app on a new Envision workflow	v1.2.0_protocol.pdf

Functionality updates

RID	Topic	Test ID	Step Description	Expected Result	Qualification Note(s)	Pass/Fail
1	Serum Concentration Versus Time-Individual	1	Create plot panel: Analysis Selection -> PKInputFigures -> SErum Concentration Versus Time-Individual to 1	ConcvTime panel created in Figures		
		2	Figure renders and respects inputs for all "Plots Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		3	Figure renders and respects inputs for all "Change Defaults" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		4	Figure specific limits work: Enter the following into "Limit": EVID != 1&DV>100	Plot is updated, respecting inputs. Screencap as evidence		
		5	Figure renders and respects changes in Theme Size Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
		6	Figure renders and respects changes in Theme Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
2	Serum Concentration Versus Time-Groups	1	Create plot panel: Analysis Selection -> PKInputFigures -> Serum Concentration Versus Time-Groups to 1	ConcvTimeGroup panel created in Figures		
		2	Figure renders and respects inputs for "Group Plots" Marky by discrete	Plot is updated, respecting inputs. Screencap as evidence		
		3	Figure renders and respects inputs for "Group Plots" Marky by continuous	Plot is updated, respecting inputs. Screencap as evidence		
		4	Figure renders and respects inputs for "Group Plots" Add text inputs	Plot is updated, respecting inputs. Screencap as evidence		
		5	Figure renders and respects inputs for "Group Plots" Facet by inputs	Plot is updated, respecting inputs. Screencap as evidence		
		6	Figure renders and respects inputs for "Group Plots" Scales Free inputs	Plot is updated, respecting inputs. Screencap as evidence		
		7	Figure renders and respects inputs for "Group Plots" Scales Free_x inputs	Plot is updated, respecting inputs. Screencap as evidence		
		8	Figure renders and respects inputs for "Group Plots" Scales Free_y inputs	Plot is updated, respecting inputs. Screencap as evidence		
		9	Figure renders and respects inputs for all "Plots Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		10	Figure renders and respects inputs for all "Change Defaults" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		11	Figure renders and respects inputs for all "Summarize Data?" boxes (Mean Standard Deviation)	Plot is updated, respecting inputs. Screencap as evidence		
		12	Figure renders and respects inputs for all "Summarize Data?" boxes (Median 95% confidence interval)	Plot is updated, respecting inputs. Screencap as evidence		
		13	Figure renders and respects inputs for all "Limits and Transformations" Inputs: DOSE<=7	Plot is updated, respecting inputs. Screencap as evidence		
		14	Figure renders and respects changes in Theme Size Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
		15	Figure renders and respects changes in Theme Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
3	Observed Versus Predicted	1	Create plot panel: Analysis Selection -> Model figures -> Observed vs Predicted to 1	OBSvPRED panel created in Figures		
		2	Figure renders and respects inputs for all "Group Plots" inputs: Marky by Discrete	Plot is updated, respecting inputs. Screencap as evidence		
		3	Figure renders and respects inputs for all "Group Plots" inputs: Marky by Continuous	Plot is updated, respecting inputs. Screencap as evidence		
		4	Figure renders and respects inputs for "Group Plots" Facet by and add text inputs	Plot is updated, respecting inputs. Screencap as evidence		
		5	Figure renders and respects inputs for "Group Plots" Facet ncol and nrov inputs	Plot is updated, respecting inputs. Screencap as evidence		
		6	Figure renders and respects inputs for "Group Plots" Scales Free_y inputs	Plot is updated, respecting inputs. Screencap as evidence		
		7	Figure renders and respects inputs for all "Plots Details" and "Change Defaults" boxes	Plot is updated, respecting inputs. Screencap as evidence		

RID	Topic	Test ID	Step Description	Expected Result	Qualification Note(s)	Pass/Fail
		8	Figure specific limits work: Enter the following into "Limit": DOSE<=7	Plot is updated, respecting inputs. Screencap as evidence		
		9	Figure renders and respects changes in Theme Size Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
		10	Figure renders and respects changes in Theme Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
4	Parameter Distribution	1	Create plot panel: Analysis Selection -> Model figures ->Parameter Distribution to 1	paramDist panel created in Figures		
		2	Figure renders and respects inputs for all "Group Plots" inputs	Plot is updated, respecting inputs. Screencap as evidence		
		3	Figure renders and respects inputs for all "Plots Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		4	Figure renders and respects inputs for all "Change Defaults" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		5	Figure specific limits work: Enter the following into "Limit": DOSE<=7	Plot is updated, respecting inputs. Screencap as evidence		
		6	Figure renders and respects changes in Theme Size and Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
5	Categorical Covariance	1	Create plot panel: Analysis Selection -> Model figures -> Categorical covariance to 1	covCat panel created in Figures		
		2	Figure renders and respects inputs for all "Plots Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		3	Figure renders and respects inputs for all "Change Defaults" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		4	Figure specific limits work: Enter the following into "Limit": DOSE<=7	Plot is updated, respecting inputs. Screencap as evidence		
		5	Figure renders and respects changes in Theme Size and Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
6	Continuous Covariance	1	Create plot panel: Analysis Selection -> Model figures -> Continuous covariance to 1	covCon panel created in Figures		
		2	Figure renders and respects inputs for all "Plots Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		3	Figure renders and respects inputs for all "Change Defaults" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		4	Figure specific limits work: Enter the following into "Limit": DOSE<=7	Plot is updated, respecting inputs. Screencap as evidence		
		5	Figure renders and respects changes in Theme Size and Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
7	Correlation Pairs	1	Create plot panel: Analysis Selection -> Model figures -> Correlation Pairs to 1	corPairs panel created in Figures		
		2	Figure renders and respects inputs for all "Plots Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		3	Figure renders and respects inputs for all "Change Defaults" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		4	Figure specific limits work: Enter the following into "Limit": DOSE<=7	Plot is updated, respecting inputs. Screencap as evidence		
		5	Figure renders and respects changes in Theme Size and Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
8	Quantile Plot	1	Create plot panel: Analysis Selection -> Model figures -> QQ Plot to 1	QQplot panel created in Figures		
		2	Figure renders and respects "Group Plots" facet by input	Plot is updated, respecting inputs. Screencap as evidence		
		3	Figure renders and respects inputs for "Group Plots" Facet ncol and nrow inputs	Plot is updated, respecting inputs. Screencap as evidence		

RID	Topic	Test ID	Step Description	Expected Result	Qualification Note(s)	Pass/Fail
		4	Figure renders and respects inputs for all "Plots Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		5	Figure renders and respects inputs for all "Change Defaults" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		6	Figure specific limits work: Enter the following into "Limit": DOSE<=7	Plot is updated, respecting inputs. Screencap as evidence		
		7	Figure renders and respects changes in Theme Size and Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
9	Goodness of Fit	1	Create plot panel: Analysis Selection -> Model figures -> GOF to 1	GOF panel created in Figures		
		2	Figure renders and respects inputs for "Group Plots" Marky by discrete	Plot is updated, respecting inputs. Screencap as evidence		
		3	Figure renders and respects inputs for "Group Plots" Marky by continuous	Plot is updated, respecting inputs. Screencap as evidence		
		4	Figure renders and respects inputs for "Group Plots" plot loess	Plot is updated, respecting inputs. Screencap as evidence		
		5	Figure renders and respects inputs for all "Plot Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		6	Figure renders and respects inputs for all "IPRED Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		7	Figure renders and respects inputs for all "PRED Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		8	Figure renders and respects inputs for all "DV Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		9	Figure renders and respects inputs for all "RESID Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		10	Figure renders and respects inputs for all "NPDE Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		11	Figure specific limits work: Enter the following into "Limit": DOSE<=7	Plot is updated, respecting inputs. Screencap as evidence		
		12	Figure renders and respects changes in Theme Size and Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
10	Variable Distribution	1	Create plot panel: Analysis Selection -> Model figures -> distMult to 1	distMult panel created in Figures		
		2	Figure renders and respects inputs for all "Plot Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		3	Figure renders and respects inputs for all "Manipulate Data" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		4	Figure renders and respects changes in Theme Size and Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
11	Bar Charts	1	Create plot panel: Analysis Selection -> Model figures -> barchartMult to 1	barchartMult panel created in Figures		
		2	Figure renders and respects inputs for all "Plot Details" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		3	Figure renders and respects inputs for all "Manipulate Data" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		4	Figure renders and respects changes in Theme Size and Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		
12	VPC	1	Simulation data can be loaded, merged with source data, and displayed on screen. The mi210 510 and 511 runs will be used for this RID. Verify that the data parser runs on the VPC data.			
		2	Additional csv dataset can be loaded and displayed. Use the parser to demonstrate that it runs on the additional data.			
		3	Figure renders and respects inputs for all figures of the shading type "simulated percentiles"			
		4	Figure renders and respects inputs for all figures of the shading type "predicted median"			
		5	Figure renders and respects inputs for all figures of the shading type "none"			
		6	Figure renders and respects inputs for all figures of the shading type "prediction interval"			

RID	Topic	Test ID	Step Description	Expected Result	Qualification Note(s)	Pass/Fail
		7	Figure renders and respects inputs for all "Manipulate Data" boxes	Plot is updated, respecting inputs. Screencap as evidence		
		8	Figure renders and respects changes in Theme Size and Colour Manipulation	Plot is updated, respecting inputs. Screencap as evidence		

RID	Topic	Test ID	Step Description	Expected Result	Qualification Note(s)	Pass/Fail
13	Hard reset button gives an environment with no input retained from previous sessions	1	Pressing "Hard reset" button, check input fields to verify they have been reset to the defaults	Input fields are reset to the defaults		

RID	Topic	Test ID	Step Description	Expected Result	Qualification Note(s)	Pass/Fail
14	The app creates RTF output for all specified figure, table, and listings	1	Load the attached validation template into the application (510-template.R)	Template is loaded		
		2	Select ordering of objects to printed in TFL	Scrrenshot which RTF will be checked against		
		3	Generate the RTF and write the companion R script: In "Save and Export" select "Construct *.Doc" and "Reveal Function Text". In filename enter "validation" Press save	validation doc and R script are created		
		4	All objects are located in the RTF, and ordering respects that of the user	Yes. Attach the doc file		
15	The app creates an R script that can reproduce the analysis outside of the app	1	Using the R script created in step 35.3, run the file in R to recreate the RTF file. Verify that the RTF matches that generated in 35.3	Matches. Attach the doc file and R script.		

RID	Topic	Test ID	Step Description	Expected Result	Qualification Note(s)	Pass/Fail
16	The app is under version control	1	Record commit ID for tagged release	git commit ID		
17	Installation package and instructions work to create new app on a new Envision workflow	1	Launch a new Envision workflow	Launch successful		
		2	Upload installation package to Envision workflow via Rstudio	Upload successful		
		3	Update nginx by running: cd script sudo ./nginx-update.sh Report output of: nginx -v	>= 1.10.1		
		4	As user, run pkgSetup.R: cd script R CMD BATCH pkgSetup.R	No errors in pkgSetup.Rout		
		5	Copy shiny-server config file to correct location: sudo cp script/shiny-server.conf /etc/shiny-server/shiny-server.conf	Copy successful		
		6	Ensure application is running: Log in to Metworx dashboard, click "Envision", click "TFL Generator",	Application is running		