Residuals scaling

- Scaling for residuals (linear or logarithmic) can be optionally set for each model output of interest.

- If not set: logarithmic scaling is used.

- Examples:

```
outA  <- Output$new("Organism|A", dataSelection = "x='A'", dataDisplayName = "Data A",
residualScale = ResidualScales$Linear)

outB  <- Output$new("Organism|B", dataSelection = "x='B'", dataDisplayName = "Data B",
residualScale = ResidualScales$Logarithmic)

outC  <- Output$new("Organism|C", dataSelection = "x='C'", dataDisplayName = "Data C")
```

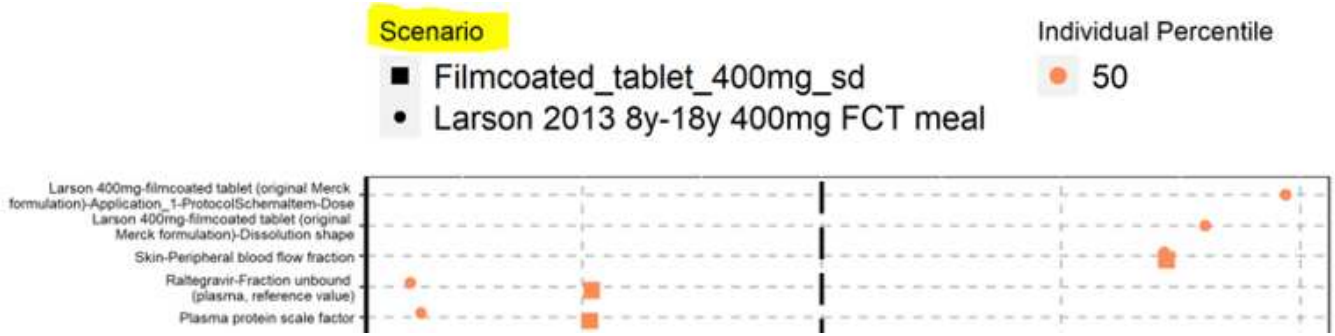
Simulation Set Descriptor

- New Workflow property: Simulation Set Descriptor

As per default, simulation sets are called “Population” (for population workflows) or “Simulation / Simulation Set” (for mean model workflows) in reports, e.g.:

- This can be overwritten by the simulation set descriptor, e.g.

```
popWorkFlow <- PopulationWorkflow$new(workflowType = PopulationWorkflowTypes$pediatric, simulationSets = list(simSet1, simSet2), workflowFolder = outputDir, simulationSetDescriptor = "Scenario")
```



Numbers Formatting

- Settings for number format within reports are now available. They can be updated in global settings using `setDefaultNumericFormat` or within specific tasks through their `$settings` property.

- Example: set global number format for all (plotting) tasks (s. package documentation for details):

```
setDefaultNumericFormat(digits = 2)

setDefaultNumericFormat(digits = 5, nsmall = 2)

setDefaultNumericFormat(digits = 5, scientific = TRUE)
```

- Example: set task-specific number format

```
meanModelWorkflow$plotPKParameters$settings$digits = 5

meanModelWorkflow$plotPKParameters$settings$scientific = TRUE
```

Switching Application ranges on/off

- As per default, time profiles and residuals task for multiple administration simulations creates every plot for the 3 time ranges: total simulation range, first application range and last application range. Some of those ranges can be now turned off. Examples:

```
simulationSet1 <- SimulationSet$new(simulationSetName = 'Set1',
simulationFile = "MultiAdminSim1.pkml", outputs = outputVenousBlood,
observedDataFile = dataFile, observedMetaDataFile = dictionaryFile)


simulationSet2 <- SimulationSet$new(simulationSetName = 'Set2',
simulationFile = "MultiAdminSim2.pkml", outputs = outputVenousBlood,
observedDataFile = dataFile, observedMetaDataFile = dictionaryFile,
applicationRanges = c(ApplicationRanges$total,ApplicationRanges$firstApplication))


simulationSet3 <- SimulationSet$new(simulationSetName = 'Set3',
simulationFile = "MultiAdminSim3.pkml", outputs = outputVenousBlood,
observedDataFile = dataFile, observedMetaDataFile = dictionaryFile,
applicationRanges = c(ApplicationRanges$firstApplication, ApplicationRanges$lastApplication))
```

Nonmem units

- It is possible to define observed data units (time, measurement) in separate Nonmem columns. Thus 2 options for the definition of units are available:

1. Providing units using only the dictionary: for '**time**' and '**dv**' the column '**nonmemUnit**' must be filled with the corresponding unit ('**lloq**' is assumed to have the same unit as '**dv**').

2. (NEW) Providing units within the observed data. The dictionary must include the following new variables in '**ID**': '**time_unit**' and '**dv_unit**'. The dictionary must also include the mapping to the variable names in the dataset using '**nonmenColumn**'. Example (left: dictionary, right: data file)

ID	type	nonmenColumn	nonmemUnit
time	timeprofile	TIME	
dv	timeprofile	DV	
time_unit	timeprofile	XUNIT	
dv_unit	timeprofile	YUNIT	

TIME	DV	XUNIT	YUNIT
2	5	h	ng/ml
4	4	h	ng/ml
325	2	min	ng/ml
8	0.1	h	µg/ml

- Mixing is possible (e.g. time unit defined in the data dictionary and dv unit defined in the Nonmem file)

ID	type	nonmenColumn	nonmemUnit
time	timeprofile	TIME	h
dv	timeprofile	DV	
dv_unit	timeprofile	YUNIT	

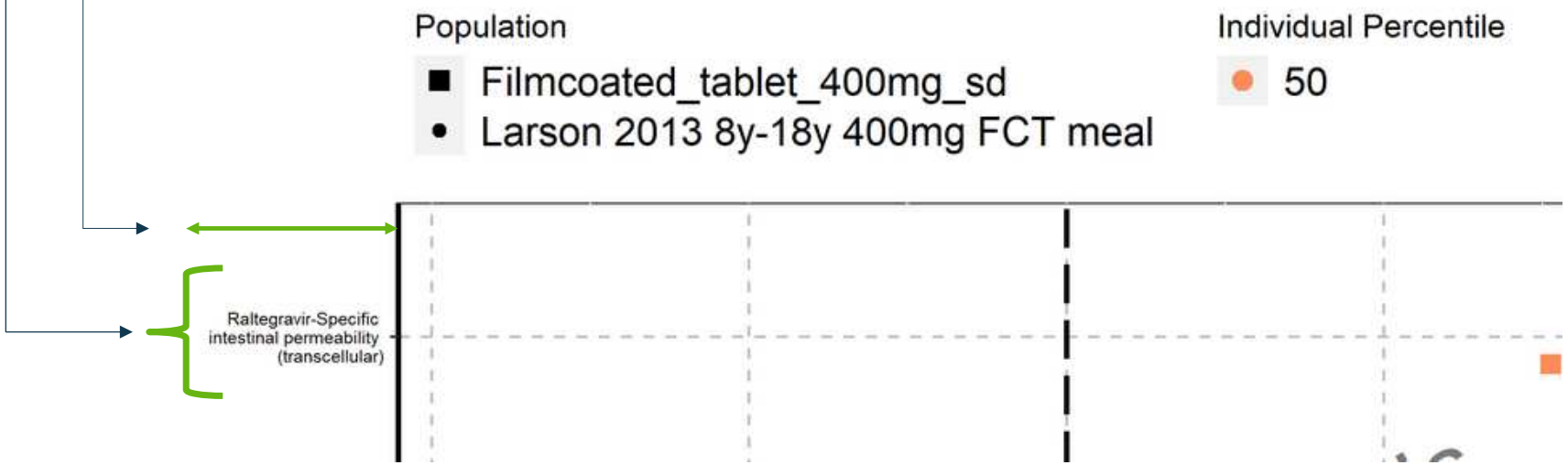
TIME	DV	YUNIT
2	5	ng/ml
4	4	ng/ml
8	0.1	µg/ml

Additional sensitivity legend settings

- Plot sensitivity task settings provides 2 new options
  - `maxLinesPerParameter` is the maximum number of lines for the legend. Default is 3 lines.
  - `maxWidthPerParameter` is the maximum width for the legend. Parameters longer than that will have line breaks. Default is 25 characters.
  - If parameters are longer than `maxLinesPerParameter*maxWidthPerParameter`, they legend will only respect the maximum number of allowed lines.

```
popWorkFlow$plotSensitivity$settings$maxLinesPerParameter = 3

popWorkFlow$plotSensitivity$settings$maxWidthPerParameter = 25
```



Override default parameter display names

- It is possible to override default parameter display names used in different plotting tasks (Population workflows: Demography / PK parameters / Sensitivity; Mean Model workflows: Sensitivity). 2 functions provided
  - `setWorkflowParameterDisplayPathsFromFile`
  - `setWorkflowParameterDisplayPaths`
- S. R package documentation for details
- NOTE: Currently it does NOT work for sensitivity plots

parameter	displayPath
Organism|Height	Body height
Organism|Weight	Body weight
Organism|BMI	Body-Mass-Index
Raltegravir|Specific intestinal permeability (transcellular)	Intestinal permeability
Raltegravir-UGT1A9-Kassahun 2007|In vitro Vmax for liver microsomes	UGT1A9 Vmax
Raltegravir-UGT1A1-Kassahun 2007|In vitro Vmax for liver microsomes	UGT1A1 Vmax