
PEtab

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PEtab

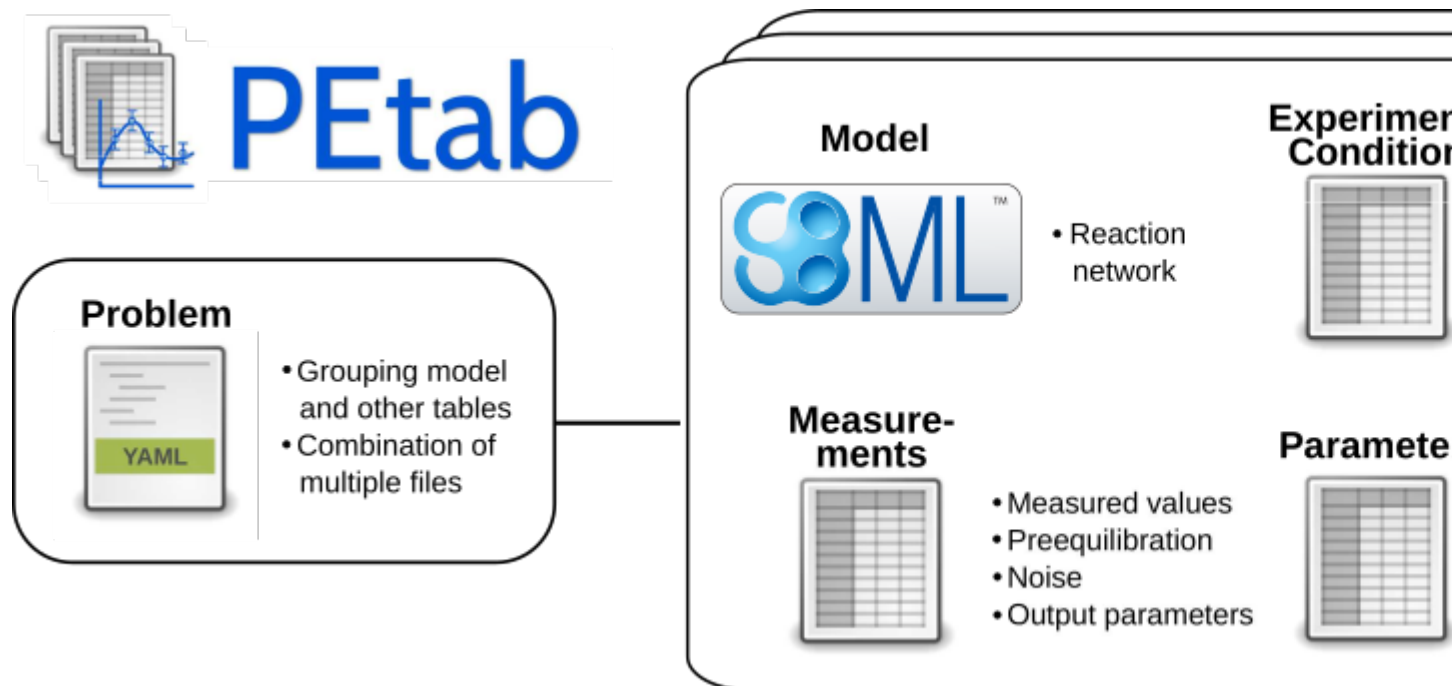
PEtab is a data format for specifying parameter estimation problems in systems biology. This repository provides extensive documentation and a Python library for easy access and validation of *PEtab* files.

CHAPTER 1

About PEtab

PEtab is built around [SBML](#) and based on tab-separated values (TSV) files. It is meant as a standardized way to provide information for parameter estimation, which is out of the current scope of SBML. This includes for example:

- Specifying and linking measurements to models
 - Defining model outputs
 - Specifying noise models
- Specifying parameter bounds for optimization
- Specifying multiple simulation condition with potentially shared parameters



CHAPTER 2

Documentation

Documentation of the PExab data format and Python library is available at <https://petab.readthedocs.io/en/latest/>.

CHAPTER 3

Examples

A wide range of PTab examples can be found in the systems biology parameter estimation [benchmark problem collection](#).

PEtab support in systems biology tools

Where PEOab is supported (in alphabetical order):

- AMICI (Example)
- A PEOab -> COPASI converter
- d2d (HOWTO)
- dMod (HOWTO)
- MEIGO (HOWTO)
- parPE
- pyABC (Example)
- pyPESTO (Example)

If your project or tool is using PEOab, and you would like to have it listed here, please [let us know](#).

4.1 PEOab features supported in different tools

The following list provides an overview of supported PEOab features in different tools, based on passed test cases of the [PEtab test suite](#):

ID	Test	AM- ICI>=0. 10.20	Co- pasi	D2D	dMod	MEIC	parPEdev	pyABC>=0 10.1	pyPESTO>=0. 0.11
1	Basic simulation	+++	+-	+++	+++	+++	-+	+++	+++
2	Multiple simulation conditions	+++	+-	+++	+++	+++	-+	+++	+++
3	Numeric observable parameter overrides in measurement table	+++	+-	+++	+++	+++	-+	+++	+++
4	Parametric observable parameter overrides in measurement table	+++	+-	+++	+++	+++	-+	+++	+++
5	Parametric overrides in condition table	+++	+-	+++	+++	+++	-+	+++	+++
6	Time-point specific overrides in the measurement table	—	—	+++	+++	+++	—	—	—
7	Observable transformations to log10 scale	+-+	+-	+++	+-	+++	-+	+-+	+-+
8	Replicate measurements	+++	+-	+++	+++	+++	-+	+++	+++
9	Pre-equilibration	+++	+-	+++	+++	+++	-+	+++	+++
10	Partial pre-equilibration	+++	—	+++	+++	+++	-+	+++	+++
11	Numeric initial concentration in condition table	+++	+-	+++	+++	+++	-+	+++	+++
12	Numeric initial compartment sizes in condition table	—	+-	+++	+++	+++	—	—	—
13	Parametric initial concentrations in condition table	+++	+-	+++	+++	+++	-+	+++	+++
14	Numeric noise parameter overrides in measurement table	+++	+-	+++	+++	+++	-+	+++	+++
15	Parametric noise parameter overrides in measurement table	+++	+-	+++	+++	+++	-+	+++	+++
16	Observable transformations to log scale	+-+	+-	+++	+-	+++	-+	+-+	+-+

Legend:

- First character indicates whether computing simulated data is supported and simulations are correct (+) or not (-).
- Second character indicates whether computing chi2 values of residuals are supported and correct (+) or not (-).
- Third character indicates whether computing likelihoods is supported and correct (+) or not (-).

If you would like to use PEstab yourself, please have a look at [doc/documentation_data_format.rst](#) or at the example models provided in the [benchmark collection](#).

To convert your existing parameter estimation problem to the PEstab format, you will have to:

1. Specify your model in SBML.
2. Create a condition table.
3. Create a table of observables.
4. Create a table of measurements.
5. Create a parameter table.

If you are using Python, some handy functions of the [PEstab library](#) can help you with that. This include also a PEstab validator called `petablint` which you can use to check if your files adhere to the PEstab standard. If you have further questions regarding PEstab, feel free to post an [issue](#) at our github repository.

PEtab comes with a Python package for creating, checking, visualizing and working with PEtAb files. This library is available on [pypi](#) and the easiest way to install it is running

It will require Python \geq 3.6 to run.

Development versions of the PEtAb library can be installed using

(replace `develop` by the branch or commit you would like to install).

When setting up a new parameter estimation problem, the most useful tools will be:

- The **PEtab validator**, which is now automatically installed using Python entrypoints to be available as a shell command from anywhere called `petablint`
- `petab.create_parameter_df` to create the parameter table, once you have set up the model, condition table, observable table and measurement table
- `petab.create_combine_archive` to create a [COMBINE Archive](#) from PEtAb files

6.1 Library examples

Examples for PEtAb Python library usage:

- [Validation](#)
- [Visualization](#)

CHAPTER 7

Getting help

If you have any question or problems with PEtab, feel free to post them at our [GitHub issue tracker](#).

Contributions and feedback to PEstab are very welcome, see our [contribution guide](#).

8.1 PEstab data format specification

Format version: 1

This document explains the PEstab data format.

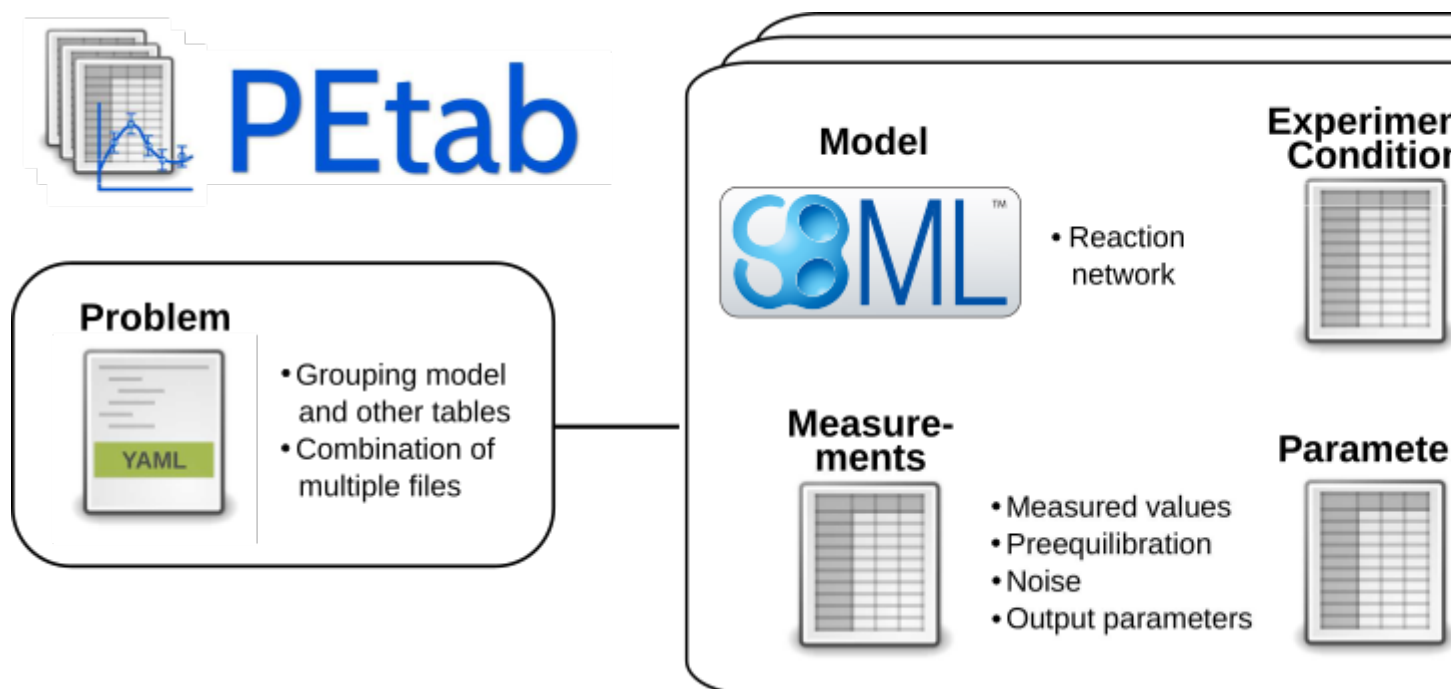
8.1.1 Purpose

Providing a standardized way for specifying parameter estimation problems in systems biology, especially for the case of Ordinary Differential Equation (ODE) models.

8.1.2 Overview

The PEstab data format specifies a parameter estimation problem using a number of text-based files ([Systems Biology Markup Language \(SBML\)](#) and [Tab-Separated Values \(TSV\)](#)), i.e.

- An SBML model [SBML]
- A measurement file to fit the model to [TSV]
- A condition file specifying model inputs and condition-specific parameters [TSV]
- An observable file specifying the observation model [TSV]
- A parameter file specifying optimization parameters and related information [TSV]
- (optional) A simulation file, which has the same format as the measurement file, but contains model simulations [TSV]
- (optional) A visualization file, which contains specifications how the data and/or simulations should be plotted by the visualization routines [TSV]



The following sections will describe the minimum requirements of those components in the core standard, which should provide all information for defining the parameter estimation problem.

Extensions of this format (e.g. additional columns in the measurement table) are possible and intended. However, while those columns may provide extra information for example for plotting, downstream analysis, or for more efficient parameter estimation, they should not affect the optimization problem as such.

General remarks

- All model entities, column names and row names are case-sensitive
- All identifiers must consist only of upper and lower case letters, digits and underscores, and must not start with a digit.
- Fields in “[]” are optional and may be left empty.

8.1.3 SBML model definition

The model must be specified as valid SBML. There are no further restrictions.

8.1.4 Condition table

The condition table specifies parameters, or initial values of species and compartments for specific simulation conditions (generally corresponding to different experimental conditions).

This is specified as a tab-separated value file in the following way:

conditionId	[condition-Name]	parameterOrSpeciesOrCompartmentId1	...	parameterOrSpeciesOrCompartmentId{n}
STRING	[STRING]	NUMERIC STRING	...	NUMERIC STRING
e.g.				
conditionId1	[condition-Name1]	0.42	...	parameterId
conditionId2
...	

Row- and column-ordering are arbitrary, although specifying `conditionId` first may improve human readability.

Additional columns are *not* allowed.

Detailed field description

- `conditionId` [STRING, NOT NULL]

Unique identifier for the simulation/experimental condition, to be referenced by the measurement table described below.

- `conditionName` [STRING, OPTIONAL]

Condition names are arbitrary strings to describe the given condition. They may be used for reporting or visualization.

- `${parameterOrSpeciesOrCompartmentId1}`

Further columns may be global parameter IDs, IDs of species or compartments as defined in the SBML model. Only one column is allowed per ID. Values for these condition parameters may be provided either as numeric values, or as IDs defined in the SBML model, the parameter table or both.

- `${parameterId}`

The values will override any parameter values specified in the model.

- `${speciesId}`

If a species ID is provided, it is interpreted as the initial concentration/amount of that species and will override the initial concentration/amount given in the SBML model or given by a preequilibration condition. If NaN is provided for a condition, the result of the preequilibration (or initial concentration/amount from the SBML model, if no preequilibration is defined) is used.

- `${compartmentId}`

If a compartment ID is provided, it is interpreted as the initial compartment size.

8.1.5 Measurement table

A tab-separated values files containing all measurements to be used for model training or validation.

Expected to have the following named columns in any (but preferably this) order:

observableId	[preequilibrationConditionId]	simulationConditionId	measurement	time
observableId	[conditionId]	conditionId	NUMERIC	NUMERIC inf
...

(wrapped for readability)

...	[observableParameters]	[noiseParameters]
...	[parameterId NUMERIC[:parameterId NUMERIC]][...]	[parameterId NUMERIC[:parameterId NUMERIC]][...]
...

Additional (non-standard) columns may be added. If the additional plotting functionality of PEO should be used, such columns could be

...	[datasetId]	[replicateId]
...	[datasetId]	[replicateId]
...

where `datasetId` is a necessary column to use particular plotting functionality, and `replicateId` is optional, which can be used to group replicates and plot error bars.

Detailed field description

- `observableId` [STRING, NOT NULL, REFERENCES(observables.observableID)]
Observable ID as defined in the observables table described below.
- `preequilibrationConditionId` [STRING OR NULL, REFERENCES(conditionsTable.conditionID), OPTIONAL]
The `conditionId` to be used for preequilibration. E.g. for drug treatments, the model would be preequilibrated with the no-drug condition. Empty for no preequilibration.
- `simulationConditionId` [STRING, NOT NULL, REFERENCES(conditionsTable.conditionID)]
`conditionId` as provided in the condition table, specifying the condition-specific parameters used for simulation.
- `measurement` [NUMERIC, NOT NULL]
The measured value in the same units/scale as the model output.
- `time` [NUMERIC OR STRING, NOT NULL]
Time point of the measurement in the time unit specified in the SBML model, numeric value or `inf` (lower-case) for steady-state measurements.
- `observableParameters` [NUMERIC, STRING OR NULL, OPTIONAL]
This field allows overriding or introducing condition-specific versions of output parameters defined in the observation model. The model can define observables (see below) containing place-holder parameters which can be replaced by condition-specific dynamic or constant parameters. Placeholder parameters must be named `observableParameter${n}__${observableId}` with `n` ranging from 1 (not 0) to the number of placeholders for the given observable, without gaps. If the observable specified under `observableId` contains no placeholders, this field must be empty. If it contains `n > 0` placeholders, this field must hold `n` semicolon-separated numeric values or parameter names. No trailing semicolon must be added.

Different lines for the same `observableId` may specify different parameters. This may be used to account for condition-specific or batch-specific parameters. This will translate into an extended optimization parameter vector.

All placeholders defined in the observation model must be overwritten here. If there are no placeholders used, this column may be omitted.

- `noiseParameters` [NUMERIC, STRING OR NULL, OPTIONAL]

The measurement standard deviation or NaN if the corresponding sigma is a model parameter.

Numeric values or parameter names are allowed. Same rules apply as for `observableParameters` in the previous point.

- `datasetId` [STRING, OPTIONAL]

The `datasetId` is used to group certain measurements to datasets. This is typically the case for data points which belong to the same observable, the same simulation and preequilibration condition, the same noise model, the same observable transformation and the same observable parameters. This grouping makes it possible to use the plotting routines which are provided in the PETA repository.

- `replicateId` [STRING, OPTIONAL]

The `replicateId` can be used to discern replicates with the same `datasetId`, which is helpful for plotting e.g. error bars.

8.1.6 Observables table

Parameter estimation requires linking experimental observations to the model of interest. Therefore, one needs to define observables (model outputs) and respective noise models, which represent the measurement process. Since parameter estimation is beyond the scope of SBML, there exists no standard way to specify observables (model outputs) and respective noise models. Therefore, in PETA observables are specified in a separate table as described in the following. This allows for a clear separation of the observation model and the underlying dynamic model, which allows, in most cases, to reuse any existing SBML model without modifications.

The observable table has the following columns:

<code>observableId</code>	<code>[observableName]</code>	<code>observableFormula</code>
STRING	[STRING]	STRING
e.g.		
<code>relativeTotalProtein1</code>	Relative abundance of Protein1	<code>observableParameter1_relativeTotalProtein1 * (protein1 + phospho_protein1)</code>
...

(wrapped for readability)

...	<code>[observableTransformation]</code>	<code>noiseFormula</code>	<code>[noiseDistribution]</code>
...	<code>[lin(default)llogllog10]</code>	STRING NUMBER	<code>[laplace normal]</code>
...	e.g.		
...	lin	<code>noiseParameter1_relativeTotalProtein1</code>	normal
...

Detailed field description

- `observableId` [STRING]

Any identifier which would be a valid identifier in SBML. This is referenced by the `observableId` column in the measurement table. Must be different from any existing model entity or parameter introduced elsewhere.

- `[observableName]` [STRING, OPTIONAL]

Name of the observable. Only used for output, not for identification.

- `observableFormula` [STRING]

Observation function as plain text formula expression. May contain any symbol defined in the SBML model (including model time `time`) or parameter table. In the simplest case just an SBML species ID or an `AssignmentRule` target.

May introduce new parameters of the form `observableParameter${n}_${observableId}`, which are overridden by `observableParameters` in the measurement table (see description there).

- `observableTransformation` [STRING, OPTIONAL]

Transformation of the observable and measurement for computing the objective function. Must be one of `lin`, `log` or `log10`. Defaults to `lin`. The measurements and model outputs are both assumed to be provided in linear space.

- `noiseFormula` [NUMERIC|STRING]

Measurement noise can be specified as a numerical value which will default to a Gaussian noise model if not specified differently in `noiseDistribution` with standard deviation as provided here. In this case, the same standard deviation is assumed for all measurements for the given observable.

Alternatively, some formula expression can be provided to specify more complex noise models. A noise model which accounts for relative and absolute contributions could, e.g., be defined as:

```
noiseParameter1_observable_pErk + noiseParameter2_observable_pErk*pErk
```

with `noiseParameter1_observable_pErk` denoting the absolute and `noiseParameter2_observable_pErk` the relative contribution for the observable `observable_pErk` corresponding to species `pErk`. IDs of noise parameters that need to have different values for different measurements have the structure: `noiseParameter${indexOfNoiseParameter}_${observableId}` to facilitate automatic recognition. The specific values or parameters are assigned in the `noiseParameters` field of the *measurement table* (see above). Any parameters named `noiseParameter${1..n}_${observableId}` must be overwritten in the measurement table.

- `noiseDistribution` [STRING: ‘normal’ or ‘laplace’, OPTIONAL]

Assumed noise distribution for the given measurement. Only normally or Laplace distributed noise is currently allowed (log-normal and log-Laplace are obtained by setting `observableTransformation` to `log`, similarly for `log10`). Defaults to `normal`. If `normal`, the specified `noiseParameters` will be interpreted as standard deviation (*not* variance). If `Laplace` is specified, the specified `noiseParameter` will be interpreted as the scale, or diversity, parameter.

Noise distributions

For `noiseDistribution`, `normal` and `laplace` are supported. For `observableTransformation`, `lin`, `log` and `log10` are supported. Denote by y the simulation, m the measurement, and σ the standard deviation of a normal, or the scale parameter of a laplace model, as given via the `noiseFormula` field. Then we have the following effective noise distributions.

- Normal distribution:

$$\pi(m|y, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(m-y)^2}{2\sigma^2}\right)$$

- Log-normal distribution (i.e. $\log(m)$ is normally distributed):

$$\pi(m|y, \sigma) = \frac{1}{\sqrt{2\pi}\sigma m} \exp\left(-\frac{(\log m - \log y)^2}{2\sigma^2}\right)$$

- Log10-normal distribution (i.e. $\log_{10}(m)$ is normally distributed):

$$\pi(m|y, \sigma) = \frac{1}{\sqrt{2\pi\sigma m \log(10)}} \exp\left(-\frac{(\log_{10} m - \log_{10} y)^2}{2\sigma^2}\right)$$

- Laplace distribution:

$$\pi(m|y, \sigma) = \frac{1}{2\sigma} \exp\left(-\frac{|m - y|}{\sigma}\right)$$

- Log-Laplace distribution (i.e. $\log(m)$ is Laplace distributed):

$$\pi(m|y, \sigma) = \frac{1}{2\sigma m} \exp\left(-\frac{|\log m - \log y|}{\sigma}\right)$$

- Log10-Laplace distribution (i.e. $\log_{10}(m)$ is Laplace distributed):

$$\pi(m|y, \sigma) = \frac{1}{2\sigma m \log(10)} \exp\left(-\frac{|\log_{10} m - \log_{10} y|}{\sigma}\right)$$

The distributions above are for a single data point. For a collection $D = \{m_i\}_i$ of data points and corresponding simulations $Y = \{y_i\}_i$ and noise parameters $\Sigma = \{\sigma_i\}_i$, the current specification assumes independence, i.e. the full distributions is

$$\pi(D|Y, \Sigma) = \prod_i \pi(m_i|y_i, \sigma_i)$$

8.1.7 Parameter table

A tab-separated value text file containing information on model parameters.

This table *must* include the following parameters:

- Named parameter overrides introduced in the *conditions table*, unless defined in the SBML model
- Named parameter overrides introduced in the *measurement table*

and *must not* include:

- Placeholder parameters (see `observableParameters` and `noiseParameters` above)
- Parameters included as column names in the *condition table*
- Parameters that are `AssignmentRule` targets in the SBML model

it *may* include:

- Any SBML model parameter that was not excluded above
- Named parameter overrides introduced in the *conditions table*

One row per parameter with arbitrary order of rows and columns:

parameterId	[parameter-Name]	parameter-Scale	lower-Bound	upper-Bound	nominal-Value	estimate	...
STRING	[STRING]	log10 lin log	NUMERIC	NUMERIC	NUMERIC	0 1	...
...

(wrapped for readability)

...	[initializationPriorType]	[initializationPriorParameters]	[objectivePriorType]	[objectivePriorParameters]
...	<i>see below</i>	<i>see below</i>	<i>see below</i>	<i>see below</i>
...

Additional columns may be added.

Detailed field description

- `parameterId` [STRING, NOT NULL]

The `parameterId` of the parameter described in this row. This has to match the ID of a parameter specified in the SBML model, a parameter introduced as override in the condition table, or a parameter occurring in the `observableParameters` or `noiseParameters` column of the measurement table (see above).

- `parameterName` [STRING, OPTIONAL]

Parameter name to be used e.g. for plotting etc. Can be chosen freely. May or may not coincide with the SBML parameter name.

- `parameterScale` [lin|log|log10]

Scale of the parameter to be used during parameter estimation.

- `lowerBound` [NUMERIC]

Lower bound of the parameter used for optimization. Optional, if `estimate==0`. Must be provided in linear space, independent of `parameterScale`.

- `upperBound` [NUMERIC]

Upper bound of the parameter used for optimization. Optional, if `estimate==0`. Must be provided in linear space, independent of `parameterScale`.

- `nominalValue` [NUMERIC]

Some parameter value to be used if the parameter is not subject to estimation (see `estimate` below). Must be provided in linear space, independent of `parameterScale`. Optional, unless `estimate==0`.

- `estimate` [BOOL 0|1]

1 or 0, depending on, if the parameter is estimated (1) or set to a fixed value(0) (see `nominalValue`).

- `initializationPriorType` [STRING, OPTIONAL]

Prior types used for sampling of initial points for optimization. Sampled points are clipped to lie inside the parameter boundaries specified by `lowerBound` and `upperBound`. Defaults to `parameterScaleUniform`.

Possible prior types are:

- *uniform*: flat prior on linear parameters
- *normal*: Gaussian prior on linear parameters
- *laplace*: Laplace prior on linear parameters
- *logNormal*: exponentiated Gaussian prior on linear parameters
- *logLaplace*: exponentiated Laplace prior on linear parameters
- *parameterScaleUniform* (default): Flat prior on original parameter scale (equivalent to “no prior”)

- *parameterScaleNormal*: Gaussian prior on original parameter scale
- *parameterScaleLaplace*: Laplace prior on original parameter scale
- *initializationPriorParameters* [STRING, OPTIONAL]

Prior parameters used for sampling of initial points for optimization, separated by a semicolon. Defaults to `lowerBound;upperBound`.

So far, only numeric values will be supported, no parameter names. Parameters for the different prior types are:

- *uniform*: lower bound; upper bound
 - *normal*: mean; standard deviation (**not** variance)
 - *laplace*: location; scale
 - *logNormal*: parameters of corresp. normal distribution (see: *normal*)
 - *logLaplace*: parameters of corresp. Laplace distribution (see: *laplace*)
 - *parameterScaleUniform*: lower bound; upper bound
 - *parameterScaleNormal*: mean; standard deviation (**not** variance)
 - *parameterScaleLaplace*: location; scale
 - *objectivePriorType* [STRING, OPTIONAL]
- Prior types used for the objective function during optimization or sampling. For possible values, see *initializationPriorType*.
- *objectivePriorParameters* [STRING, OPTIONAL]
- Prior parameters used for the objective function during optimization. For more detailed documentation, see *initializationPriorParameters*.

8.1.8 Visualization table

A tab-separated value file containing the specification of the visualization routines which come with the PEO repository. Plots are in general collections of different datasets as specified using their `datasetId` (if provided) inside the measurement table.

Expected to have the following columns in any (but preferably this) order:

plotId	[plot-Name]	[plotTypeSimulation]	[plotTypeData]
STRING	[STRING]	[Line-Plot(default) BarPlot ScatterPlot]	[MeanAndSD(default) MeanAndSEM replicate;provided]
...

(wrapped for readability)

...	[datasetId]	[xValues]	[xOffset]	[xLabel]	[xScale]
...	[datasetId]	[time(default) parameterOrStateId]	[NUMERIC]	[STRING]	[lin log log10 order]
...

(wrapped for readability)

...	[yValues]	[yOffset]	[yLabel]	[yScale]	[legendEntry]
...	[observableId]	[NUMERIC]	[STRING]	[lin log log10]	[STRING]
...

Detailed field description

- `plotId` [STRING, NOT NULL]
An ID which corresponds to a specific plot. All datasets with the same `plotId` will be plotted into the same axes object.
- `plotName` [STRING, OPTIONAL]
A name for the specific plot.
- `plotTypeSimulation` [STRING, OPTIONAL]
The type of the corresponding plot, can be `LinePlot`, `BarPlot` and `ScatterPlot`. Default is `LinePlot`.
- `plotTypeData` [STRING, OPTIONAL]
The type how replicates should be handled, can be `MeanAndSD`, `MeanAndSEM`, `replicate` (for plotting all replicates separately), or `provided` (if numeric values for the noise level are provided in the measurement table). Default is `MeanAndSD`.
- `datasetId` [STRING, NOT NULL, REFERENCES(measurementTable.datasetId), OPTIONAL]
The datasets which should be grouped into one plot.
- `xValues` [STRING, OPTIONAL]
The independent variable, which will be plotted on the x-axis. Can be `time` (default, for time resolved data), or it can be `parameterOrStateId` for dose-response plots. The corresponding numeric values will be shown on the x-axis.
- `xOffset` [NUMERIC, OPTIONAL]
Possible data-offsets for the independent variable (default is 0).
- `xLabel` [STRING, OPTIONAL]
Label for the x-axis. Defaults to the entry in `xValues`.
- `xScale` [STRING, OPTIONAL]
Scale of the independent variable, can be `lin`, `log`, `log10` or `order`. The `order` value should be used if values of the independent variable are ordinal. This value can only be used in combination with `LinePlot` value for the `plotTypeSimulation` column. In this case, points on x axis will be placed equidistantly from each other. Default is `lin`.
- `yValues` [observableId, REFERENCES(measurementTable.observableId), OPTIONAL]
The observable which should be plotted on the y-axis.
- `yOffset` [NUMERIC, OPTIONAL]
Possible data-offsets for the observable (default is 0).
- `yLabel` [STRING, OPTIONAL]
Label for the y-axis. Defaults to the entry in `yValues`.
- `yScale` [STRING, OPTIONAL]
Scale of the observable, can be `lin`, `log`, or `log10`. Default is `lin`.

- `legendEntry` [STRING, OPTIONAL]

The name that should be displayed for the corresponding dataset in the legend and which defaults to the value in `datasetId`.

Extensions

Additional columns, such as `Color`, etc. may be specified.

Examples

Examples of the visualization table can be found in the [Benchmark model collection](#), for example in the [Chen_MSB2009](#) model.

8.1.9 YAML file for grouping files

To link the SBML model, measurement table, condition table, etc. in an unambiguous way, we use a [YAML](#) file.

This file also allows specifying a PEtAb version (as the format is not unlikely to change in the future).

Furthermore, this can be used to describe parameter estimation problems comprising multiple models (more details below).

The format is described in the schema `../petab/petab_schema.yaml`, which allows for easy validation.

Parameter estimation problems combining multiple models

Parameter estimation problems can comprise multiple models. For now, PEtAb allows to specify multiple SBML models with corresponding condition and measurement tables, and one joint parameter table. This means that the parameter namespace is global. Therefore, parameters with the same ID in different models will be considered identical.

8.2 API Reference

<code>petab</code>	PEtab global
<code>petab.composite_problem</code>	PEtab problems consisting of multiple models
<code>petab.core</code>	PEtab core functions (or functions that don't fit anywhere else)
<code>petab.conditions</code>	Functions operating on the PEtAb condition table
<code>petab.C</code>	This file contains constant definitions.
<code>petab.lint</code>	Integrity checks and tests for specific features used
<code>petab.measurements</code>	Functions operating on the PEtAb measurement table
<code>petab.parameter_mapping</code>	Functions related to mapping parameter from model to parameter estimation problem
<code>petab.parameters</code>	Functions operating on the PEtAb parameter table
<code>petab.problem</code>	PEtab Problem class
<code>petab.sampling</code>	Functions related to parameter sampling
<code>petab.sbml</code>	Functions for interacting with SBML models
<code>petab.yaml</code>	Code regarding the PEtAb YAML config files

Continued on next page

Table 1 – continued from previous page

<code>petab.visualize.data_overview</code>	Functions for creating an overview report of a PETA problem
<code>petab.visualize.helper_functions</code>	This file should contain the functions, which PETA internally needs for plotting, but which are not meant to be used by non-developers and should hence not be directly visible/usable when using <code>import petab.visualize</code> .
<code>petab.visualize.plot_data_and_simulation(...)</code>	Main function for plotting data and simulations.
<code>petab.visualize.plotting_config</code>	Plotting config

8.2.1 petab

PEtab global

`petab.ENV_NUM_THREADS`

Name of environment variable to set number of threads or processes PETA should use for operations that can be performed in parallel. By default, all operations are performed sequentially.

8.2.2 petab.composite_problem

PEtab problems consisting of multiple models

Classes

<code>CompositeProblem(parameter_df, problems)</code>	Representation of a PETA problem consisting of multiple models
---	--

```
class petab.composite_problem.CompositeProblem (parameter_df: pandas.core.frame.DataFrame = None,
                                                problems: List[petab.problem.Problem] = None)
```

Bases: object

Representation of a PETA problem consisting of multiple models

problems

List petab.Problems

parameter_df

PEtab parameter DataFrame

```
static from_yaml (yaml_config: Union[Dict[KT, VT], str]) → petab.composite_problem.CompositeProblem
```

Create from YAML file

Factory method to create a CompositeProblem instance from a PETA YAML config file

Parameters `yaml_config` – PETA configuration as dictionary or YAML file name

8.2.3 petab.core

PEtab core functions (or functions that don't fit anywhere else)

Functions

<code>concat_tables</code> (tables, ...)	Concatenate DataFrames provided as DataFrames or filenames, and a parser
<code>create_combine_archive</code> (yaml_file, filename, ...)	Create COMBINE archive (http://co.mbine.org/documents/archive) based on PETab YAML file.
<code>flatten_timepoint_specific_output_overrides</code> (petab_problem)	Flatten timepoint-specific output parameter overrides.
<code>get_notnull_columns</code> (df, candidates)	Return list of df-columns in candidates which are not all null/nan.
<code>get_observable_id</code> (parameter_id)	Get PETab observable ID from PETab-style sigma or observable <i>AssignmentRule</i> -target <i>parameter_id</i> .
<code>get_simulation_df</code> (simulation_file)	Read PETab simulation table
<code>get_visualization_df</code> (visualization_file)	Read PETab visualization table
<code>is_empty</code> (val)	Check if the value <i>val</i> , e.g.
<code>to_float_if_float</code> (x)	Return input as float if possible, otherwise return as is
<code>unique_preserve_order</code> (seq)	Return a list of unique elements in Sequence, keeping only the first occurrence of each element
<code>write_simulation_df</code> (df, filename)	Write PETab simulation table
<code>write_visualization_df</code> (df, filename)	Write PETab visualization table

`petab.core.concat_tables` (tables: *Union[str, pandas.core.frame.DataFrame, Iterable[Union[pandas.core.frame.DataFrame, str]]]*, file_parser: *Optional[Callable] = None*) → *pandas.core.frame.DataFrame*
Concatenate DataFrames provided as DataFrames or filenames, and a parser

Parameters

- **tables** – Iterable of tables to join, as DataFrame or filename.
- **file_parser** – Function used to read the table in case filenames are provided, accepting a filename as only argument.

Returns The concatenated DataFrames

`petab.core.create_combine_archive` (yaml_file: *str*, filename: *str*, family_name: *Optional[str] = None*, given_name: *Optional[str] = None*, email: *Optional[str] = None*, organization: *Optional[str] = None*) → *None*
Create COMBINE archive (<http://co.mbine.org/documents/archive>) based on PETab YAML file.

Parameters

- **yaml_file** – Path to PETab YAML file
- **family_name** – Family name of archive creator
- **given_name** – Given name of archive creator
- **email** – E-mail address of archive creator
- **organization** – Organization of archive creator

`petab.core.flatten_timepoint_specific_output_overrides` (petab_problem: *petab.problem.Problem*) → *None*
Flatten timepoint-specific output parameter overrides.

If the PETab problem definition has timepoint-specific *observableParameters* or *noiseParameters* for the same observable, replace those by replicating the respective observable.

This is a helper function for some tools which may not support such timepoint-specific mappings. The observable table and measurement table are modified in place.

Parameters `petab_problem` – PEtAb problem to work on

`petab.core.get_notnull_columns(df: pandas.core.frame.DataFrame, candidates: Iterable[T_co])`
Return list of df-columns in candidates which are not all null/nan.

The output can e.g. be used as input for `pandas.DataFrame.groupby`.

Parameters

- **df** – Dataframe
- **candidates** – Columns of df to consider

`petab.core.get_observable_id(parameter_id: str) → str`
Get PEtAb observable ID from PEtAb-style sigma or observable *AssignmentRule*-target `parameter_id`.
e.g. for ‘observable_obs1’ -> ‘obs1’, for ‘sigma_obs1’ -> ‘obs1’

Parameters `parameter_id` – Some parameter ID

Returns Observable ID

`petab.core.get_simulation_df(simulation_file: str) → pandas.core.frame.DataFrame`
Read PEtAb simulation table

Parameters `simulation_file` – URL or filename of PEtAb simulation table

Returns Simulation DataFrame

`petab.core.get_visualization_df(visualization_file: str) → pandas.core.frame.DataFrame`
Read PEtAb visualization table

Parameters `visualization_file` – URL or filename of PEtAb visualization table

Returns Visualization DataFrame

`petab.core.is_empty(val) → bool`
Check if the value *val*, e.g. a table entry, is empty.

Parameters `val` – The value to check.

Returns Whether the field is to be considered empty.

Return type `empty`

`petab.core.to_float_if_float(x: Any) → Any`
Return input as float if possible, otherwise return as is

Parameters `x` – Anything

Returns `x` as float if possible, otherwise `x`

`petab.core.unique_preserve_order(seq: Sequence[T_co]) → List[T]`
Return a list of unique elements in Sequence, keeping only the first occurrence of each element
`seq`: Sequence to prune

Returns List of unique elements in `seq`

`petab.core.write_simulation_df(df: pandas.core.frame.DataFrame, filename: str) → None`
Write PEtAb simulation table

Parameters

- **df** – PEtAb simulation table

- **filename** – Destination file name

`petab.core.write_visualization_df(df: pandas.core.frame.DataFrame, filename: str) → None`
Write PETab visualization table

Parameters

- **df** – PETab visualization table
- **filename** – Destination file name

8.2.4 petab.conditions

Functions operating on the PETab condition table

Functions

<code>create_condition_df(parameter_ids, condition_ids)</code>	Create empty condition DataFrame
<code>get_condition_df(condition_file, ...)</code>	Read the provided condition file into a pandas.DataFrame
<code>get_parametric_overrides(condition_df)</code>	Get parametric overrides from condition table
<code>write_condition_df(df, filename)</code>	Write PETab condition table

`petab.conditions.create_condition_df(parameter_ids: Iterable[str], condition_ids: Optional[Iterable[str]] = None) → pandas.core.frame.DataFrame`
Create empty condition DataFrame

Parameters

- **parameter_ids** – the columns
- **condition_ids** – the rows

Returns A pandas.DataFrame with empty given rows and columns and all nan values

`petab.conditions.get_condition_df(condition_file: Union[str, pandas.core.frame.DataFrame, None]) → pandas.core.frame.DataFrame`
Read the provided condition file into a pandas.DataFrame

Conditions are rows, parameters are columns, conditionId is index.

Parameters **condition_file** – File name of PETab condition file or pandas.DataFrame

`petab.conditions.get_parametric_overrides(condition_df: pandas.core.frame.DataFrame) → List[str]`
Get parametric overrides from condition table

Parameters **condition_df** – PETab condition table

Returns List of parameter IDs that are mapped in a condition-specific way

`petab.conditions.write_condition_df(df: pandas.core.frame.DataFrame, filename: str) → None`
Write PETab condition table

Parameters

- **df** – PETab condition table

- **filename** – Destination file name

8.2.5 petab.C

This file contains constant definitions.

8.2.6 petab.lint

Integrity checks and tests for specific features used

Functions

<code>assert_all_parameters_present_in_parameter_table(...)</code>	Ensure all required parameters are contained in the parameter table with no additional ones
<code>assert_measured_observables_defined(...)</code>	Check if all observables in the measurement table have been defined in the observable table
<code>assert_measurement_conditions_present_in_condition_table(...)</code>	Ensure that all entries from measurement_df.simulationConditionId and measurement_df.preequilibrationConditionId are present in condition_df.index.
<code>assert_model_parameters_in_condition_or_measurement_table(...)</code>	Model parameters that are targets of AssignmentRule must not be present in parameter table or in condition table columns.
<code>assert_no_leading_trailing_whitespace(...)</code>	Check that there is no trailing whitespace in elements of Iterable
<code>assert_noise_distributions_valid(observable_df)</code>	Ensure that noise distributions and transformations for observables are valid.
<code>assert_parameter_bounds_are_numeric(parameter_df)</code>	Check if all entries in the lowerBound and upperBound columns of the parameter table are numeric.
<code>assert_parameter_estimate_is_boolean(...)</code>	Check if all entries in the estimate column of the parameter table are 0 or 1.
<code>assert_parameter_id_is_string(parameter_df)</code>	Check if all entries in the parameterId column of the parameter table are string and not empty.
<code>assert_parameter_prior_parameters_are_valid(...)</code>	Check that the prior parameters are valid.
<code>assert_parameter_prior_type_is_valid(...)</code>	Check that valid prior types have been selected
<code>assert_parameter_scale_is_valid(parameter_df)</code>	Check if all entries in the parameterScale column of the parameter table are 'lin' for linear, 'log' for natural logarithm or 'log10' for base 10 logarithm.
<code>assert_unique_observable_ids(observable_df)</code>	Check if the observableId column of the observable table is unique.
<code>assert_unique_parameter_ids(parameter_df)</code>	Check if the parameterId column of the parameter table is unique.
<code>check_condition_df(df, sbml_model)</code>	Run sanity checks on PETA condition table
<code>check_ids(ids, kind)</code>	Check IDs are valid
<code>check_measurement_df(df, observable_df)</code>	Run sanity checks on PETA measurement table
<code>check_observable_df(observable_df)</code>	Check validity of observable table
<code>check_parameter_bounds(parameter_df)</code>	Check if all entries in the lowerBound are smaller than upperBound column in the parameter table and that bounds are positive for parameterScale loglog10.

Continued on next page

Table 5 – continued from previous page

<code>check_parameter_df(df, sbml_model, ...)</code>	Run sanity checks on PEtAb parameter table
<code>condition_table_is_parameter_free(condition_df)</code>	Check if all entries in the condition table are numeric (no parameter IDs)
<code>get_non_unique(values)</code>	
<code>is_valid_identifier(x)</code>	Check whether x is a valid identifier
<code>lint_problem(problem)</code>	Run PEtAb validation on problem
<code>measurement_table_has_observable_parameters_to_override(measurement_df)</code>	Are there any numbers to override observable parameters?
<code>measurement_table_has_timepoint_specific_assignments(measurement_df)</code>	Are there time (point) or replicate specific parameter assignments in the measurement table.

`petab.lint._check_df(df: pandas.core.frame.DataFrame, req_cols: Iterable[T_co], name: str) → None`
Check if given columns are present in DataFrame

Parameters

- **df** – Dataframe to check
- **req_cols** – Column names which have to be present
- **name** – Name of the DataFrame to be included in error message

Raises `AssertionError` – if a column is missing

`petab.lint.assert_all_parameters_present_in_parameter_df(parameter_df: pandas.core.frame.DataFrame, sbml_model: libsbml.Model, observable_df: pandas.core.frame.DataFrame, measurement_df: pandas.core.frame.DataFrame, condition_df: pandas.core.frame.DataFrame) → None`
Ensure all required parameters are contained in the parameter table with no additional ones

Parameters

- **parameter_df** – PEtAb parameter DataFrame
- **sbml_model** – PEtAb SBML Model
- **observable_df** – PEtAb observable table
- **measurement_df** – PEtAb measurement table
- **condition_df** – PEtAb condition table

Raises `AssertionError` – in case of problems

`petab.lint.assert_measured_observables_defined(measurement_df: pandas.core.frame.DataFrame, observable_df: pandas.core.frame.DataFrame) → None`
Check if all observables in the measurement table have been defined in the observable table

Parameters

- **measurement_df** – PEtAb measurement table

- **observable_df** – PETab observable table

Raises `AssertionError` – in case of problems

```
petab.lint.assert_measurement_conditions_present_in_condition_table(measurement_df:
                                                                    pan-
                                                                    das.core.frame.DataFrame,
                                                                    condi-
                                                                    tion_df:
                                                                    pan-
                                                                    das.core.frame.DataFrame)
                                                                    → None
Ensure that all entries from measurement_df.simulationConditionId and measure-
ment_df.preequilibrationConditionId are present in condition_df.index.
```

Parameters

- **measurement_df** – PETab measurement table
- **condition_df** – PETab condition table

Raises `AssertionError` – in case of problems

```
petab.lint.assert_model_parameters_in_condition_or_parameter_table(sbml_model:
                                                                    libs-
                                                                    bml.Model,
                                                                    condi-
                                                                    tion_df:
                                                                    pan-
                                                                    das.core.frame.DataFrame,
                                                                    param-
                                                                    eter_df:
                                                                    pan-
                                                                    das.core.frame.DataFrame)
                                                                    → None
Model parameters that are targets of AssignmentRule must not be present in parameter table or in condition
table columns. Other parameters must only be present in either in parameter table or condition table columns.
Check that.
```

Parameters

- **parameter_df** – PETab parameter DataFrame
- **sbml_model** – PETab SBML Model
- **condition_df** – PETab condition table

Raises `AssertionError` – in case of problems

```
petab.lint.assert_no_leading_trailing_whitespace(names_list: Iterable[str], name: str)
                                                                    → None
Check that there is no trailing whitespace in elements of Iterable
```

Parameters

- **names_list** – strings to check for whitespace
- **name** – name of *names_list* for error messages

Raises `AssertionError` – if there is trailing whitespace

```
petab.lint.assert_noise_distributions_valid(observable_df:
                                                                    pan-
                                                                    das.core.frame.DataFrame) → None
Ensure that noise distributions and transformations for observables are valid.
```

Parameters `observable_df` – PEtAb observable table

Raises `AssertionError` – in case of problems

`petab.lint.assert_parameter_bounds_are_numeric` (*parameter_df: pandas.core.frame.DataFrame*) → `None`

Check if all entries in the `lowerBound` and `upperBound` columns of the parameter table are numeric.

Parameters `parameter_df` – PEtAb parameter DataFrame

Raises `AssertionError` – in case of problems

`petab.lint.assert_parameter_estimate_is_boolean` (*parameter_df: pandas.core.frame.DataFrame*) → `None`

Check if all entries in the `estimate` column of the parameter table are 0 or 1.

Parameters `parameter_df` – PEtAb parameter DataFrame

Raises `AssertionError` – in case of problems

`petab.lint.assert_parameter_id_is_string` (*parameter_df: pandas.core.frame.DataFrame*) → `None`

Check if all entries in the `parameterId` column of the parameter table are string and not empty.

Parameters `parameter_df` – PEtAb parameter DataFrame

Raises `AssertionError` – in case of problems

`petab.lint.assert_parameter_prior_parameters_are_valid` (*parameter_df: pandas.core.frame.DataFrame*) → `None`

Check that the prior parameters are valid.

Parameters `parameter_df` – PEtAb parameter table

Raises `AssertionError` in case of invalide prior parameters

`petab.lint.assert_parameter_prior_type_is_valid` (*parameter_df: pandas.core.frame.DataFrame*) → `None`

Check that valid prior types have been selected

Parameters `parameter_df` – PEtAb parameter table

Raises `AssertionError` in case of invalid prior

`petab.lint.assert_parameter_scale_is_valid` (*parameter_df: pandas.core.frame.DataFrame*) → `None`

Check if all entries in the `parameterScale` column of the parameter table are ‘lin’ for linear, ‘log’ for natural logarithm or ‘log10’ for base 10 logarithm.

Parameters `parameter_df` – PEtAb parameter DataFrame

Raises `AssertionError` – in case of problems

`petab.lint.assert_unique_observable_ids` (*observable_df: pandas.core.frame.DataFrame*) → `None`

Check if the `observableId` column of the observable table is unique.

Parameters `observable_df` – PEtAb observable DataFrame

Raises `AssertionError` – in case of problems

`petab.lint.assert_unique_parameter_ids` (*parameter_df: pandas.core.frame.DataFrame*) → `None`

Check if the `parameterId` column of the parameter table is unique.

Parameters `parameter_df` – PEtAb parameter DataFrame

Raises `AssertionError` – in case of problems

`petab.lint.check_condition_df` (*df*: `pandas.core.frame.DataFrame`, *sbml_model*: `Optional[libsbml.Model]`) → None

Run sanity checks on PEtAb condition table

Parameters

- **df** – PEtAb condition DataFrame
- **sbml_model** – SBML Model for additional checking of parameter IDs

Raises `AssertionError` – in case of problems

`petab.lint.check_ids` (*ids*: `Iterable[str]`, *kind*: `str` = "") → None

Check IDs are valid

Parameters

- **ids** – Iterable of IDs to check
- **kind** – Kind of IDs, for more informative error message

Raises `ValueError` - in case of invalid IDs

`petab.lint.check_measurement_df` (*df*: `pandas.core.frame.DataFrame`, *observable_df*: `Optional[pandas.core.frame.DataFrame]` = None) → None

Run sanity checks on PEtAb measurement table

Parameters

- **df** – PEtAb measurement DataFrame
- **observable_df** – PEtAb observable DataFrame for checking if measurements are compatible with observable transformations.

Raises `AssertionError`, `ValueError` – in case of problems

`petab.lint.check_observable_df` (*observable_df*: `pandas.core.frame.DataFrame`) → None

Check validity of observable table

Parameters `observable_df` – PEtAb observable DataFrame

Raises `AssertionError` – in case of problems

`petab.lint.check_parameter_bounds` (*parameter_df*: `pandas.core.frame.DataFrame`) → None

Check if all entries in the lowerBound are smaller than upperBound column in the parameter table and that bounds are positive for parameterScale loglog10.

Parameters `parameter_df` – PEtAb parameter DataFrame

Raises `AssertionError` – in case of problems

`petab.lint.check_parameter_df` (*df*: `pandas.core.frame.DataFrame`, *sbml_model*: `Optional[libsbml.Model]` = None, *observable_df*: `Optional[pandas.core.frame.DataFrame]` = None, *measurement_df*: `Optional[pandas.core.frame.DataFrame]` = None, *condition_df*: `Optional[pandas.core.frame.DataFrame]` = None) → None

Run sanity checks on PEtAb parameter table

Parameters

- **df** – PEtAb condition DataFrame
- **sbml_model** – SBML Model for additional checking of parameter IDs

- **observable_df** – PETab observable table for additional checks
- **measurement_df** – PETab measurement table for additional checks
- **condition_df** – PETab condition table for additional checks

Raises `AssertionError` – in case of problems

`petab.lint.condition_table_is_parameter_free(condition_df: pan-das.core.frame.DataFrame) → bool`

Check if all entries in the condition table are numeric (no parameter IDs)

Parameters `condition_df` – PETab condition table

Returns True if there are no parameter overrides in the condition table, False otherwise.

`petab.lint.is_valid_identifier(x: str) → bool`

Check whether `x` is a valid identifier

Check whether `x` is a valid identifier for conditions, parameters, observables. . . . Identifiers may contain upper and lower case letters, digits and underscores, but must not start with a digit.

Parameters `x` – string to check

Returns True if valid, False otherwise

`petab.lint.lint_problem(problem: petab.problem.Problem) → bool`

Run PETab validation on problem

Parameters `problem` – PETab problem to check

Returns True is errors occurred, False otherwise

`petab.lint.measurement_table_has_observable_parameter_numeric_overrides(measurement_df: pan-das.core.frame.DataFrame) → bool`

Are there any numbers to override observable parameters?

Parameters `measurement_df` – PETab measurement table

Returns True if there any numbers to override observable parameters, False otherwise.

`petab.lint.measurement_table_has_timepoint_specific_mappings(measurement_df: pan-das.core.frame.DataFrame) → bool`

Are there time-point or replicate specific parameter assignments in the measurement table.

Parameters `measurement_df` – PETab measurement table

Returns True if there are time-point or replicate specific parameter assignments in the measurement table, False otherwise.

8.2.7 petab.measurements

Functions operating on the PETab measurement table

Functions

<code>assert_overrides_match_parameter_count(measurement_df, observable_df)</code>	Ensure that number of parameters in the observable definition matches the number of overrides in measurement_df
<code>create_measurement_df()</code>	Create empty measurement dataframe
<code>get_measurement_df(measurement_file, str, ...)</code>	Read the provided measurement file into a pandas .Dataframe.
<code>get_measurement_parameter_ids(measurement_df)</code>	Return list of ID of parameters which occur in measurement table as observable or noise parameter overrides.
<code>get_noise_distributions(measurement_df)</code>	Returns dictionary of cost definitions per observable, if specified.
<code>get_rows_for_condition(measurement_df, ...)</code>	Extract rows in <i>measurement_df</i> for <i>condition</i> according to 'preequilibrationConditionId' and 'simulationConditionId' in <i>condition</i> .
<code>get_simulation_conditions(measurement_df)</code>	Create a table of separate simulation conditions.
<code>measurements_have_replicates(measurement_df)</code>	Tests whether the measurements come with replicates
<code>split_parameter_replacement_list(...)</code>	Split values in observableParameters and noiseParameters in measurement table.
<code>write_measurement_df(df, filename)</code>	Write PEtAb measurement table

`petab.measurements.assert_overrides_match_parameter_count` (*measurement_df*: *pandas.core.frame.DataFrame*,
observable_df: *pandas.core.frame.DataFrame*)
→ None
Ensure that number of parameters in the observable definition matches the number of overrides in measurement_df

Parameters

- **measurement_df** – PEtAb measurement table
- **observable_df** – PEtAb observable table

`petab.measurements.create_measurement_df()` → *pandas.core.frame.DataFrame*
Create empty measurement dataframe

Returns

Created DataFrame

`petab.measurements.get_measurement_df` (*measurement_file*: *Union[None, str, pandas.core.frame.DataFrame]*) → *pandas.core.frame.DataFrame*
Read the provided measurement file into a pandas.DataFrame.

Parameters *measurement_file* – Name of file to read from or pandas.DataFrame

Returns Measurement DataFrame

`petab.measurements.get_measurement_parameter_ids` (*measurement_df*: *pandas.core.frame.DataFrame*) → *List[str]*
Return list of ID of parameters which occur in measurement table as observable or noise parameter overrides.

Parameters *measurement_df* – PEtAb measurement DataFrame

Returns List of parameter IDs

`petab.measurements.get_noise_distributions` (*measurement_df*: *pandas.core.frame.DataFrame*) → *dict*
Returns dictionary of cost definitions per observable, if specified.

Looks through all parameters satisfying *sbml_parameter_is_cost* and return as dictionary.

Parameters *measurement_df* – PETab measurement table

Returns Dictionary with *observableId* => *cost definition*

```
petab.measurements.get_rows_for_condition (measurement_df:      pandas
                                           das.core.frame.DataFrame, condition:
                                           Union[pandas.core.series.Series, pandas
                                           das.core.frame.DataFrame, Dict[KT, VT]])
                                           → pandas.core.frame.DataFrame
```

Extract rows in *measurement_df* for *condition* according to 'preequilibrationConditionId' and 'simulationConditionId' in *condition*.

Parameters

- **measurement_df** – PETab measurement DataFrame
- **condition** – DataFrame with single row (or Series) and columns 'preequilibrationConditionId' and 'simulationConditionId'. Or dictionary with those keys.

Returns The subselection of rows in *measurement_df* for the condition

condition.

```
petab.measurements.get_simulation_conditions (measurement_df:      pandas
                                              das.core.frame.DataFrame) → pandas
                                              das.core.frame.DataFrame
```

Create a table of separate simulation conditions. A simulation condition is a specific combination of simulationConditionId and preequilibrationConditionId.

Parameters *measurement_df* – PETab measurement table

Returns Dataframe with columns 'simulationConditionId' and 'preequilibrationConditionId'. All-null columns will be omitted. Missing 'preequilibrationConditionId's will be set to '' (empty string).

```
petab.measurements.measurements_have_replicates (measurement_df:      pandas
                                                  das.core.frame.DataFrame) →
                                                  bool
```

Tests whether the measurements come with replicates

Parameters *measurement_df* – Measurement table

Returns True if there are replicates, False otherwise

```
petab.measurements.split_parameter_replacement_list (list_string: Union[str, numbers
                                                                           .Number], delim: str = ';')
                                                     → List[Union[str, float]]
```

Split values in observableParameters and noiseParameters in measurement table.

Parameters

- **list_string** – delim-separated stringified list
- **delim** – delimiter

Returns List of split values. Numeric values converted to float.

```
petab.measurements.write_measurement_df (df: pandas.core.frame.DataFrame, filename: str)
                                         → None
```

Write PETab measurement table

Parameters

- **df** – PETab measurement table

- **filename** – Destination file name

8.2.8 petab.parameter_mapping

Functions related to mapping parameter from model to parameter estimation problem

Functions

<code>get_optimization_to_simulation_parameter_mapping(...)</code>	Create list of mapping dicts from PETab-problem to SBML parameters.
<code>get_parameter_mapping_for_condition(...)</code>	Create dictionary of parameter value and parameter scale mappings from PETab-problem to SBML parameters for the given condition.
<code>handle_missing_overrides(...)</code>	Find all observable parameters and noise parameters that were not mapped and set their mapping to np.nan.
<code>merge_preeq_and_sim_pars(parameter_mappings, ...)</code>	Merge preequilibration and simulation parameters and scales for a list of conditions while checking for compatibility.
<code>merge_preeq_and_sim_pars_condition(...)</code>	Merge preequilibration and simulation parameters and scales for a single condition while checking for compatibility.

`petab.parameter_mapping._apply_condition_parameters` (*par_mapping*: Dict[str, Union[str, numbers.Number]], *scale_mapping*: Dict[str, str], *condition_id*: str, *condition_df*: pandas.core.frame.DataFrame, *sbml_model*: libsbml.Model) → None

Replace parameter IDs in parameter mapping dictionary by condition table parameter values (in-place).

Parameters

- **par_mapping** – see `get_parameter_mapping_for_condition`
- **condition_id** – ID of condition to work on
- **condition_df** – PETab condition table

`petab.parameter_mapping._apply_output_parameter_overrides` (*mapping*: Dict[str, Union[str, numbers.Number]], *cur_measurement_df*: pandas.core.frame.DataFrame) → None

Apply output parameter overrides to the parameter mapping dict for a given condition as defined in the measurement table (`observableParameter`, `noiseParameters`).

Parameters

- **mapping** – parameter mapping dict as obtained from `get_parameter_mapping_for_condition`
- **cur_measurement_df** – Subset of the measurement table for the current condition

```
petab.parameter_mapping._apply_overrides_for_observable(mapping: Dict[str, Union[str, numbers.Number]], observable_id: str, override_type: str, overrides: List[str]) → None
```

Apply parameter-overrides for observables and noises to mapping matrix.

Parameters

- **mapping** – mapping dict to which to apply overrides
- **observable_id** – observable ID
- **override_type** – ‘observable’ or ‘noise’
- **overrides** – list of overrides for noise or observable parameters

```
petab.parameter_mapping._apply_parameter_table(par_mapping: Dict[str, Union[str, numbers.Number]], scale_mapping: Dict[str, str], parameter_df: Optional[pandas.core.frame.DataFrame] = None, scaled_parameters: bool = False, fill_fixed_parameters: bool = True) → None
```

Replace parameters from parameter table in mapping list for a given condition and set the corresponding scale.

Replace non-estimated parameters by `nominalValues` (un-scaled / lin-scaled), replace estimated parameters by the respective ID.

Parameters

- **par_mapping** – mapping dict obtained from `get_parameter_mapping_for_condition`
- **parameter_df** – PEtab parameter table

```
petab.parameter_mapping._map_condition(packed_args)
```

Helper function for parallel condition mapping.

For arguments see `get_optimization_to_simulation_parameter_mapping`

```
petab.parameter_mapping._map_condition_arg_packer(simulation_conditions, measurement_df, condition_df, parameter_df, sbml_model, simulation_parameters, warn_unmapped, scaled_parameters, fill_fixed_parameters)
```

Helper function to pack extra arguments for `_map_condition`

```
petab.parameter_mapping._output_parameters_to_nan(mapping: Dict[str, Union[str, numbers.Number]]) → None
```

Set output parameters in mapping dictionary to nan

```
petab.parameter_mapping._perform_mapping_checks(measurement_df: pandas.core.frame.DataFrame) → None
```

Check for PEtab features which we can’t account for during parameter mapping.

```

petab.parameter_mapping.get_optimization_to_simulation_parameter_mapping(
    condition_df:
        pandas.core.frame.DataFrame
    measurement_df:
        pandas.core.frame.DataFrame
    parameter_df:
        Optional[pandas.core.frame.
            DataFrame] =
        None,
    observable_df:
        Optional[pandas.core.frame.
            DataFrame] =
        None,
    sbml_model:
        sbml.Model
    simulation_conditions:
        Optional[pandas.core.frame.
            DataFrame] =
        None,
    warn_unmapped:
        Optional[bool] =
        True,
    scaled_parameters:
        bool =
        False,
    fill_fixed_parameters:
        bool =
        True)
    →
    List[Tuple[Dict[str,
        Union[str,
            numbers.Number]],
        Dict[str,
            Union[str,
                numbers.Number]],
        Dict[str,
            Union[str,
                numbers.Number]],
        Dict[str,
            Union[str,
                numbers.Number]]]]

```

Create list of mapping dicts from PEtAb-problem to SBML parameters.

Mapping can be performed in parallel. The number of threads is controlled by the environment variable with the name of `petab.ENV_NUM_THREADS`.

Parameters

- **measurement_df, parameter_df, observable_df** (*condition_df*,) – The dataframes in the PEtAb format.
- **sbml_model** – The sbml model with observables and noise specified according to the PEtAb format.
- **simulation_conditions** – Table of simulation conditions as created by `petab.get_simulation_conditions`.
- **warn_unmapped** – If `True`, log warning regarding unmapped parameters
- **scaled_parameters** – Whether parameter values should be scaled.
- **fill_fixed_parameters** – Whether to fill in nominal values for fixed parameters (`estimate=0` in parameters table).

Returns

Parameter value and parameter scale mapping for all conditions.

The length of the returned array is the number of unique combinations of `simulationConditionId`'s and `preequilibrationConditionId`'s from the measurement table. Each entry is a tuple of four dicts of length equal to the number of model parameters. The first two dicts map simulation parameter IDs to optimization parameter IDs or values (where values are fixed) for preequilibration and simulation condition, respectively. The last two dicts map simulation parameter IDs to the parameter scale of the respective parameter, again for preequilibration and simulation condition. If no preequilibration condition is defined, the respective dicts will be empty. `NaN` is used where no mapping exists.

```
petab.parameter_mapping.get_parameter_mapping_for_condition(condition_id: str,
                                                            is_preeq: bool,
                                                            cur_measurement_df:
                                                                pandas.core.frame.DataFrame,
                                                            sbml_model:
                                                                libsbml.Model,
                                                            condition_df: pandas.
                                                                core.frame.DataFrame,
                                                            parameter_df: pandas.
                                                                core.frame.DataFrame
                                                            = None, simulation_
                                                                parameters:
                                                                Optional[Dict[str,
                                                                str]] = None,
                                                            warn_unmapped:
                                                                bool = True,
                                                            scaled_parameters:
                                                                bool = False,
                                                            fill_fixed_parameters:
                                                                bool = True) →
                                                                Tuple[Dict[str,
                                                                Union[str, num-
                                                                bers.Number]],
                                                                Dict[str, str]]
```

Create dictionary of parameter value and parameter scale mappings from PETA-problem to SBML parameters for the given condition.

Parameters

- **condition_id** – Condition ID for which to perform mapping
- **is_preeq** – If True, output parameters will not be mapped
- **cur_measurement_df** – Measurement sub-table for current condition
- **condition_df** – PETA condition DataFrame
- **parameter_df** – PETA parameter DataFrame
- **sbml_model** – The sbml model with observables and noise specified according to the PETA format used to retrieve simulation parameter IDs.
- **simulation_parameters** – Model simulation parameter IDs mapped to parameter values (output of `petab.sbml.get_model_parameters(..., with_values=True)`). Optional, saves time if precomputed.
- **warn_unmapped** – If True, log warning regarding unmapped parameters
- **fill_fixed_parameters** – Whether to fill in nominal values for fixed parameters (estimate=0 in parameters table).

Returns Tuple of two dictionaries. First dictionary mapping model parameter IDs to mapped parameters IDs to be estimated or to filled-in values in case of non-estimated parameters. Second dictionary mapping model parameter IDs to their scale. NaN is used where no mapping exists.


```
petab.parameter_mapping.handle_missing_overrides(mapping_par_opt_to_par_sim:
                                                Dict[str, Union[str, num-
                                                bers.Number]], warn: bool =
                                                True, condition_id: str = None) →
                                                None
```

Find all observable parameters and noise parameters that were not mapped and set their mapping to np.nan.

Assumes that parameters matching “(noise|observable)Parameter[0-9]+_” were all supposed to be overwritten.

Parameters

- **mapping_par_opt_to_par_sim** – Output of get_parameter_mapping_for_condition
- **warn** – If True, log warning regarding unmapped parameters
- **condition_id** – Optional condition ID for more informative output

```
petab.parameter_mapping.merge_preeq_and_sim_pars(parameter_mappings:
                                                Iterable[Tuple[Dict[str,
                                                Union[str,
                                                numbers.Number]],
                                                Dict[str,
                                                Union[str,
                                                numbers.Number]]]],
                                                scale_mappings:
                                                Iterable[Tuple[Dict[str,
                                                str],
                                                Dict[str,
                                                str]]]) → Tuple[List[Tuple[Dict[str,
                                                Union[str,
                                                numbers.Number]],
                                                Dict[str,
                                                Union[str,
                                                num-
                                                bers.Number]]],
                                                List[Tuple[Dict[str,
                                                str],
                                                Dict[str,
                                                str]]]]]
```

Merge preequilibration and simulation parameters and scales for a list of conditions while checking for compatibility.

Parameters

- **parameter_mappings** – As returned by petab.get_optimization_to_simulation_parameter_mapping
- **scale_mappings** – As returned by petab.get_optimization_to_simulation_scale_mapping

Returns The parameter and scale simulation mappings, modified and checked.

```
petab.parameter_mapping.merge_preeq_and_sim_pars_condition(condition_map_preeq:
                                                            Dict[str,
                                                            Union[str,
                                                            numbers.Number]],
                                                            condition_map_sim:
                                                            Dict[str,
                                                            Union[str,
                                                            num-
                                                            bers.Number]],
                                                            condition_scale_map_preeq:
                                                            Dict[str,
                                                            str],
                                                            condition_scale_map_sim:
                                                            Dict[str,
                                                            str],
                                                            condition:
                                                            Any) →
                                                            None
```

Merge preequilibration and simulation parameters and scales for a single condition while checking for compatibility.

This function is meant for the case where we cannot have different parameters (and scales) for preequilibration and simulation. Therefore, merge both and ensure matching scales and parameters. condition_map_sim and condition_scale_map_sim will ne modified in place.

Parameters

- **condition_map_sim**(*condition_map_preeq*,) – Parameter mapping as obtained from *get_parameter_mapping_for_condition*
- **condition_scale_map_sim** (*condition_scale_map_preeq*,) – Parameter scale mapping as obtained from *get_get_scale_mapping_for_condition*
- **condition** – Condition identifier for more informative error messages

8.2.9 petab.parameters

Functions operating on the PETab parameter table

Functions

<code>create_parameter_df(sbml_model, ...)</code>	Create a new PETab parameter table
<code>get_optimization_parameter_scaling(parameter_df)</code>	Get dictionary with optimization parameter IDs mapped to parameter scaling strings.
<code>get_optimization_parameters(parameter_df)</code>	Get list of optimization parameter IDs from parameter table.
<code>get_parameter_df(parameter_file, List[str], ...)</code>	Read the provided parameter file into a pandas.DataFrame.
<code>get_priors_from_df(parameter_df, mode)</code>	Create list with information about the parameter priors
<code>get_required_parameters_for_parameter_table(parameter_df)</code>	Get set of parameters which need to go into the parameter table
<code>get_valid_parameters_for_parameter_table(parameter_df)</code>	Get set of parameters which may be present inside the parameter table
<code>map_scale(parameters, scale_strs)</code>	As <code>scale()</code> , but for Iterables
<code>normalize_parameter_df(parameter_df)</code>	Add missing columns and fill in default values.
<code>scale(parameter, scale_str)</code>	Scale parameter according to <code>scale_str</code>
<code>unscale(parameter, scale_str)</code>	Unscale parameter according to <code>scale_str</code>
<code>write_parameter_df(df, filename)</code>	Write PETab parameter table

```
petab.parameters.create_parameter_df (sbml_model: libsbml.Model, condition_df: pandas.core.frame.DataFrame, observable_df: pandas.core.frame.DataFrame, measurement_df: pandas.core.frame.DataFrame, include_optional: bool = False, parameter_scale: str = 'log10', lower_bound: Iterable[T_co] = None, upper_bound: Iterable[T_co] = None) → pandas.core.frame.DataFrame
```

Create a new PETab parameter table

All table entries can be provided as string or list-like with length matching the number of parameters

Parameters

- **sbml_model** – SBML Model
- **condition_df** – PETab condition DataFrame
- **measurement_df** – PETab measurement DataFrame
- **include_optional** – By default this only returns parameters that are required to be present in the parameter table. If set to True, this returns all parameters that are allowed to be present in the parameter table (i.e. also including parameters specified in the SBML model).

- **parameter_scale** – parameter scaling
- **lower_bound** – lower bound for parameter value
- **upper_bound** – upper bound for parameter value

Returns The created parameter DataFrame

```
petab.parameters.get_optimization_parameter_scaling (parameter_df:      pan-
                                                    das.core.frame.DataFrame)
                                                    → Dict[str, str]
```

Get Dictionary with optimization parameter IDs mapped to parameter scaling strings.

Parameters **parameter_df** – PEtAb parameter DataFrame

Returns Dictionary with optimization parameter IDs mapped to parameter scaling strings.

```
petab.parameters.get_optimization_parameters (parameter_df:      pan-
                                                    das.core.frame.DataFrame) → List[str]
```

Get list of optimization parameter IDs from parameter table.

Parameters **parameter_df** – PEtAb parameter DataFrame

Returns List of IDs of parameters selected for optimization.

```
petab.parameters.get_parameter_df (parameter_file: Union[str, List[str],      pan-
                                                    das.core.frame.DataFrame,      None]) →      pan-
                                                    das.core.frame.DataFrame
```

Read the provided parameter file into a pandas.DataFrame.

Parameters **parameter_file** – Name of the file to read from or pandas.DataFrame.

Returns Parameter DataFrame

```
petab.parameters.get_priors_from_df (parameter_df: pandas.core.frame.DataFrame, mode:
                                                    str) → List[Tuple]
```

Create list with information about the parameter priors

Parameters

- **parameter_df** – PEtAb parameter table
- **mode** – ‘initialization’ or ‘objective’

Returns List with prior information.

```
petab.parameters.get_required_parameters_for_parameter_table (sbml_model:
                                                                libsaml.Model,
                                                                condition_df: pan-
                                                                das.core.frame.DataFrame,
                                                                observ-
                                                                able_df:      pan-
                                                                das.core.frame.DataFrame,
                                                                measure-
                                                                ment_df:      pan-
                                                                das.core.frame.DataFrame)
                                                                → Set[str]
```

Get set of parameters which need to go into the parameter table

Parameters

- **sbml_model** – PEtAb SBML model
- **condition_df** – PEtAb condition table
- **observable_df** – PEtAb observable table

- **measurement_df** – PEtAb measurement table

Returns Set of parameter IDs which PEtAb requires to be present in the parameter table. That is all {observable,noise}Parameters from the measurement table as well as all parametric condition table overrides that are not defined in the SBML model.

```
petab.parameters.get_valid_parameters_for_parameter_table (sbml_model: lib-
                                                           sbml.Model,      con-
                                                           dition_df:      pan-
                                                           das.core.frame.DataFrame,
                                                           observable_df:  pan-
                                                           das.core.frame.DataFrame,
                                                           measurement_df: pandas.core.frame.DataFrame)
                                                           → Set[str]
```

Get set of parameters which may be present inside the parameter table

Parameters

- **sbml_model** – PEtAb SBML model
- **condition_df** – PEtAb condition table
- **observable_df** – PEtAb observable table
- **measurement_df** – PEtAb measurement table

Returns Set of parameter IDs which PEtAb allows to be present in the parameter table.

```
petab.parameters.map_scale (parameters: Iterable[numbers.Number], scale_strs: Iterable[str]) →
                           Iterable[numbers.Number]
```

As scale(), but for Iterables

```
petab.parameters.normalize_parameter_df (parameter_df: pandas.core.frame.DataFrame) →
                                         pandas.core.frame.DataFrame
```

Add missing columns and fill in default values.

```
petab.parameters.scale (parameter: numbers.Number, scale_str: str) → numbers.Number
```

Scale parameter according to scale_str

Parameters

- **parameter** – Parameter to be scaled.
- **scale_str** – One of 'lin' (synonymous with ''), 'log', 'log10'.

Returns The scaled parameter.

Return type parameter

```
petab.parameters.unscale (parameter: numbers.Number, scale_str: str) → numbers.Number
```

Unscale parameter according to scale_str

Parameters

- **parameter** – Parameter to be unscaled.
- **scale_str** – One of 'lin' (synonymous with ''), 'log', 'log10'.

Returns The unscaled parameter.

Return type parameter

```
petab.parameters.write_parameter_df (df: pandas.core.frame.DataFrame, filename: str) →
                                     None
```

Write PEtAb parameter table

Parameters

- **df** – PEtab parameter table
- **filename** – Destination file name

8.2.10 petab.problem

PEtab Problem class

Functions

<code>get_default_condition_file_name(model_name, ...)</code>	Get file name according to proposed convention
<code>get_default_measurement_file_name(...)</code>	Get file name according to proposed convention
<code>get_default_parameter_file_name(model_name, ...)</code>	Get file name according to proposed convention
<code>get_default_sbml_file_name(model_name, folder)</code>	Get file name according to proposed convention

Classes

<code>Problem(sbml_model, sbml_reader, ...)</code>	PEtab parameter estimation problem as defined by
--	--

```
class petab.problem.Problem(sbml_model: libsbml.Model = None, sbml_reader: libsbml.SBMLReader = None, sbml_document: libsbml.SBMLDocument = None, condition_df: pandas.core.frame.DataFrame = None, measurement_df: pandas.core.frame.DataFrame = None, parameter_df: pandas.core.frame.DataFrame = None, visualization_df: pandas.core.frame.DataFrame = None, observable_df: pandas.core.frame.DataFrame = None)
```

Bases: object

PEtab parameter estimation problem as defined by

- SBML model
- condition table
- measurement table
- parameter table
- observables table

Optionally it may contain visualization tables.

condition_df

PEtab condition table

measurement_df

PEtab measurement table

parameter_df

PEtab parameter table

observable_df

PEtab observable table

visualization_df

PEtab visualization table

sbml_reader

Stored to keep object alive.

sbml_document

Stored to keep object alive.

sbml_model

PEtab SBML model

_apply_mask (*v*: List[T], *free*: bool = True, *fixed*: bool = True)

Apply mask of only free or only fixed values.

Parameters

- **v** – The full vector the mask is to be applied to.
- **free** – Whether to return free parameters, i.e. parameters to estimate.
- **fixed** – Whether to return fixed parameters, i.e. parameters not to estimate.

Returns The reduced vector with applied mask.

Return type v

create_parameter_df (*args, **kwargs)

Create a new PEPtab parameter table

See create_parameter_df

static from_combine (filename: str) → petab.problem.Problem

Read PEPtab COMBINE archive (<http://co.mbine.org/documents/archive>).

See also create_combine_archive.

Parameters filename – Path to the PEPtab-COMBINE archive

Returns A petab.Problem instance.

static from_files (sbml_file: str = None, condition_file: str = None, measurement_file: Union[str, Iterable[str]] = None, parameter_file: Union[str, List[str]] = None, visualization_files: Union[str, Iterable[str]] = None, observable_files: Union[str, Iterable[str]] = None) → petab.problem.Problem

Factory method to load model and tables from files.

Parameters

- **sbml_file** – PEPtab SBML model
- **condition_file** – PEPtab condition table
- **measurement_file** – PEPtab measurement table
- **parameter_file** – PEPtab parameter table
- **visualization_files** – PEPtab visualization tables
- **observable_files** – PEPtab observables tables

static from_folder (folder: str, model_name: str = None) → petab.problem.Problem

Factory method to use the standard folder structure and file names, i.e.

```

${model_name}/
+-- experimentalCondition_${model_name}.tsv
+-- measurementData_${model_name}.tsv
+-- model_${model_name}.xml
+-- parameters_${model_name}.tsv

```

Parameters

- **folder** – Path to the directory in which the files are located.
- **model_name** – If specified, overrides the model component in the file names. Defaults to the last component of **folder**.

static from_yaml (*yaml_config: Union[Dict[KT, VT], str]*) → petab.problem.Problem
Factory method to load model and tables as specified by YAML file.

Parameters **yaml_config** – PEtAb configuration as dictionary or YAML file name

get_lb (*free: bool = True, fixed: bool = True, scaled: bool = False*)
Generic function to get lower parameter bounds.

Parameters

- **free** – Whether to return free parameters, i.e. parameters to estimate.
- **fixed** – Whether to return fixed parameters, i.e. parameters not to estimate.
- **scaled** – Whether to scale the values according to the parameter scale, or return them on linear scale.

Returns The lower parameter bounds.

Return type

get_model_parameters ()
See *petab.sbml.get_model_parameters*

get_noise_distributions ()
See *get_noise_distributions*.

get_observable_ids ()
Returns dictionary of observable ids.

get_observables (*remove: bool = False*)
Returns dictionary of observables definitions. See *assignment_rules_to_dict* for details.

get_optimization_parameter_scales ()
Return list of optimization parameter scaling strings.
See *petab.parameters.get_optimization_parameters*.

get_optimization_parameters ()
Return list of optimization parameter IDs.
See *petab.parameters.get_optimization_parameters*.

get_optimization_to_simulation_parameter_mapping (*warn_unmapped: bool = True, scaled_parameters: bool = False*)
See *get_simulation_to_optimization_parameter_mapping*.

get_sigmas (*remove: bool = False*)

Return dictionary of observableId => sigma as defined in the SBML model. This does not include parameter mappings defined in the measurement table.

get_simulation_conditions_from_measurement_df ()

See petab.get_simulation_conditions

get_ub (*free: bool = True, fixed: bool = True, scaled: bool = False*)

Generic function to get upper parameter bounds.

Parameters

- **free** – Whether to return free parameters, i.e. parameters to estimate.
- **fixed** – Whether to return fixed parameters, i.e. parameters not to estimate.
- **scaled** – Whether to scale the values according to the parameter scale, or return them on linear scale.

Returns The upper parameter bounds.

Return type v

get_x_ids (*free: bool = True, fixed: bool = True*)

Generic function to get parameter ids.

Parameters

- **free** – Whether to return free parameters, i.e. parameters to estimate.
- **fixed** – Whether to return fixed parameters, i.e. parameters not to estimate.

Returns The parameter ids.

Return type v

get_x_nominal (*free: bool = True, fixed: bool = True, scaled: bool = False*)

Generic function to get parameter nominal values.

Parameters

- **free** – Whether to return free parameters, i.e. parameters to estimate.
- **fixed** – Whether to return fixed parameters, i.e. parameters not to estimate.
- **scaled** – Whether to scale the values according to the parameter scale, or return them on linear scale.

Returns The parameter nominal values.

Return type v

lb

Parameter table lower bounds.

lb_scaled

Parameter table lower bounds with applied parameter scaling

sample_parameter_startpoints (*n_starts: int = 100*)

Create starting points for optimization

See sample_parameter_startpoints

to_files (*sbml_file: Optional[str] = None, condition_file: Optional[str] = None, measurement_file: Optional[str] = None, parameter_file: Optional[str] = None, visualization_file: Optional[str] = None, observable_file: Optional[str] = None, yaml_file: Optional[str] = None*) → None

Write PEPetab tables to files for this problem

Writes PEPetab files for those entities for which a destination was passed.

NOTE: If this instance was created from multiple measurement or visualization tables, they will be merged and written to a single file.

Parameters

- **sbml_file** – SBML model destination
- **condition_file** – Condition table destination
- **measurement_file** – Measurement table destination
- **parameter_file** – Parameter table destination
- **visualization_file** – Visualization table destination
- **observable_file** – Observables table destination
- **yaml_file** – YAML file destination

Raises

- **ValueError** – If a destination was provided for a non-existing
- **entity**.

ub

Parameter table upper bounds

ub_scaled

Parameter table upper bounds with applied parameter scaling

x_fixed_ids

Parameter table parameter IDs, for fixed parameters.

x_fixed_indices

Parameter table non-estimated parameter indices.

x_free_ids

Parameter table parameter IDs, for free parameters.

x_free_indices

Parameter table estimated parameter indices.

x_ids

Parameter table parameter IDs

x_nominal

Parameter table nominal values

x_nominal_fixed

Parameter table nominal values, for fixed parameters.

x_nominal_fixed_scaled

Parameter table nominal values with applied parameter scaling, for fixed parameters.

x_nominal_free

Parameter table nominal values, for free parameters.

x_nominal_free_scaled

Parameter table nominal values with applied parameter scaling, for free parameters.

x_nominal_scaled

Parameter table nominal values with applied parameter scaling

`petab.problem.get_default_condition_file_name(model_name: str, folder: str = "")`

Get file name according to proposed convention

`petab.problem.get_default_measurement_file_name(model_name: str, folder: str = "")`

Get file name according to proposed convention

`petab.problem.get_default_parameter_file_name(model_name: str, folder: str = "")`

Get file name according to proposed convention

`petab.problem.get_default_sbml_file_name(model_name: str, folder: str = "")`

Get file name according to proposed convention

8.2.11 petab.sampling

Functions related to parameter sampling

Functions

<code>sample_from_prior(prior, list, str, list], ...)</code>	Creates samples for one parameter based on prior
<code>sample_parameter_startpoints(parameter_df, ...)</code>	Create numpy.array with starting points for an optimization

`petab.sampling.sample_from_prior(prior: Tuple[str, list, str, list], n_starts: int) → numpy.array`

Creates samples for one parameter based on prior

Parameters

- **prior** – A tuple as obtained from `petab.parameter.get_priors_from_df`
- **n_starts** – Number of samples

Returns Array with sampled values

`petab.sampling.sample_parameter_startpoints(parameter_df: pandas.core.frame.DataFrame, n_starts: int = 100, seed: int = None) → numpy.array`

Create numpy.array with starting points for an optimization

Parameters

- **parameter_df** – PETab parameter DataFrame
- **n_starts** – Number of points to be sampled
- **seed** – Random number generator seed (see `numpy.random.seed`)

Returns Array of sampled starting points with dimensions `n_startpoints x n_optimization_parameters`

8.2.12 petab.sbml

Functions for interacting with SBML models

Functions

<code>add_global_parameter(sbml_model, ...)</code>	Add new global parameter to SBML model
<code>add_model_output(sbml_model, observable_id, ...)</code>	Add PEtan-style output to model
<code>add_model_output_sigma(sbml_model, ...)</code>	Add PEtan-style sigma for the given observable id
<code>add_model_output_with_sigma(sbml_model, ...)</code>	Add PEtan-style output and corresponding sigma with single (newly created) parameter
<code>assignment_rules_to_dict(sbml_model[, ...])</code>	Turn assignment rules into dictionary.
<code>create_assignment_rule(sbml_model, ...)</code>	Create SBML AssignmentRule
<code>get_model_parameters(sbml_model[, with_values])</code>	Return SBML model parameters which are not AssignmentRule targets for observables or sigmas
<code>get_observables(sbml_model, remove)</code>	Get observables defined in SBML model according to PEtan format.
<code>get_sbml_model(filepath_or_buffer)</code>	Get an SBML model from file or URL or file handle
<code>get_sigmas(sbml_model, remove)</code>	Get sigmas defined in SBML model according to PEtan format.
<code>globalize_parameters(sbml_model, ...)</code>	Turn all local parameters into global parameters with the same properties
<code>is_sbml_consistent(sbml_document, check_units)</code>	Check for SBML validity / consistency
<code>load_sbml_from_file(sbml_file)</code>	Load SBML model from file
<code>load_sbml_from_string(sbml_string)</code>	Load SBML model from string
<code>log_sbml_errors(sbml_document[, ...])</code>	Log libsbml errors
<code>sbml_parameter_is_observable(sbml_parameter)</code>	Returns whether the libsbml.Parameter sbml_parameter matches the defined observable format.
<code>sbml_parameter_is_sigma(sbml_parameter)</code>	Returns whether the libsbml.Parameter sbml_parameter matches the defined sigma format.
<code>write_sbml(sbml_doc, filename)</code>	Write PEtan visualization table

`petab.sbml.add_global_parameter` (*sbml_model*: libsbml.Model, *parameter_id*: str, *parameter_name*: str = None, *constant*: bool = False, *units*: str = 'dimensionless', *value*: float = 0.0) → libsbml.Parameter

Add new global parameter to SBML model

Parameters

- **sbml_model** – SBML model
- **parameter_id** – ID of the new parameter
- **parameter_name** – Name of the new parameter
- **constant** – Is parameter constant?
- **units** – SBML unit ID
- **value** – parameter value

Returns The created parameter

`petab.sbml.add_model_output` (*sbml_model*: libsbml.Model, *observable_id*: str, *formula*: str, *observable_name*: str = None) → None

Add PEtan-style output to model

We expect that all formula parameters are added to the model elsewhere.

Parameters

- **sbml_model** – Model to add output to
- **formula** – Formula string for model output
- **observable_id** – ID without “observable_” prefix
- **observable_name** – Any observable name

```
petab.sbml.add_model_output_sigma(sbml_model: libsbml.Model, observable_id: str, formula: str) → None
```

Add PÉtab-style sigma for the given observable id

We expect that all formula parameters are added to the model elsewhere.

Parameters

- **sbml_model** – Model to add to
- **observable_id** – Observable id for which to add sigma
- **formula** – Formula for sigma

```
petab.sbml.add_model_output_with_sigma(sbml_model: libsbml.Model, observable_id: str,
                                       observable_formula: str, observable_name: str = None) → None
```

Add PÉtab-style output and corresponding sigma with single (newly created) parameter

We expect that all formula parameters are added to the model elsewhere.

Parameters

- **sbml_model** – Model to add output to
- **observable_formula** – Formula string for model output
- **observable_id** – ID without “observable_” prefix
- **observable_name** – Any name

```
petab.sbml.assignment_rules_to_dict(sbml_model: libsbml.Model, filter_function=<function
                                   <lambda>>, remove: bool = False) → Dict[str, Dict[str, Any]]
```

Turn assignment rules into dictionary.

Parameters

- **sbml_model** – a sbml model instance.
- **filter_function** – callback function taking assignment variable as input and returning True/False to indicate if the respective rule should be turned into an observable.
- **remove** – Remove the all matching assignment rules from the model

Returns

```
{
    assigneeId:
    {
        'name': assigneeName,
        'formula': formulaString
    }
}
```

```
petab.sbml.create_assignment_rule (sbml_model: libsbml.Model, assignee_id: str, formula: str,
                                   rule_id: str = None, rule_name: str = None) → libsbml.AssignmentRule
```

Create SBML AssignmentRule

Parameters

- **sbml_model** – Model to add output to
- **assignee_id** – Target of assignment
- **formula** – Formula string for model output
- **rule_id** – SBML id for created rule
- **rule_name** – SBML name for created rule

Returns The created AssignmentRule

```
petab.sbml.get_model_parameters (sbml_model: libsbml.Model, with_values=False) →
                                   Union[List[str], Dict[str, float]]
```

Return SBML model parameters which are not AssignmentRule targets for observables or sigmas

Parameters

- **sbml_model** – SBML model
- **with_values** – If false, returns list of SBML model parameter IDs which
- **not AssignmentRule targets for observables or sigmas. If true, (are) –**
- **a dictionary with those parameter IDs as keys and parameter (returns) –**
- **from the SBML model as values. (values) –**

```
petab.sbml.get_observables (sbml_model: libsbml.Model, remove: bool = False) → dict
```

Get observables defined in SBML model according to PTEtab format.

Returns Dictionary of observable definitions. See *assignment_rules_to_dict* for details.

```
petab.sbml.get_sbml_model (filepath_or_buffer) → Tuple[libsbml.SBMLReader, libsbml.SBMLDocument, libsbml.Model]
```

Get an SBML model from file or URL or file handle

Parameters **filepath_or_buffer** – File or URL or file handle to read the model from

Returns The SBML document, model and reader

```
petab.sbml.get_sigmas (sbml_model: libsbml.Model, remove: bool = False) → dict
```

Get sigmas defined in SBML model according to PTEtab format.

Returns

Dictionary of sigma definitions.

Keys are observable IDs, for values see *assignment_rules_to_dict* for details.

```
petab.sbml.globalize_parameters (sbml_model: libsbml.Model, prepend_reaction_id: bool =
                                   False) → None
```

Turn all local parameters into global parameters with the same properties

Local parameters are currently ignored by other PTEtab functions. Use this function to convert them to global parameters. There may exist local parameters with identical IDs within different kinetic laws. This is not checked here. If in doubt that local parameter IDs are unique, enable *prepend_reaction_id* to create global parameters named `{reaction_id}_{local_parameter_id}`.

Parameters

- **sbml_model** – The SBML model to operate on
- **prepend_reaction_id** – Prepend reaction id of local parameter when creating global parameters

`petab.sbml.is_sbml_consistent` (*sbml_document: libsbml.SBMLDocument*, *check_units: bool = False*) → bool
Check for SBML validity / consistency

Parameters

- **sbml_document** – SBML document to check
- **check_units** – Also check for unit-related issues

Returns False if problems were detected, otherwise True

`petab.sbml.load_sbml_from_file` (*sbml_file: str*) → Tuple[libsbml.SBMLReader, libsbml.SBMLDocument, libsbml.Model]
Load SBML model from file

Parameters **sbml_file** – Filename of the SBML file

Returns The SBML document, model and reader

`petab.sbml.load_sbml_from_string` (*sbml_string: str*) → Tuple[libsbml.SBMLReader, libsbml.SBMLDocument, libsbml.Model]
Load SBML model from string

Parameters **sbml_string** – Model as XML string

Returns The SBML document, model and reader

`petab.sbml.log_sbml_errors` (*sbml_document: libsbml.SBMLDocument*, *minimum_severity=1*) → None
Log libsbml errors

Parameters

- **sbml_document** – SBML document to check
- **minimum_severity** – Minimum severity level to report (see libsbml)

`petab.sbml.sbml_parameter_is_observable` (*sbml_parameter: libsbml.Parameter*) → bool
Returns whether the libsbml.Parameter `sbml_parameter` matches the defined observable format.

`petab.sbml.sbml_parameter_is_sigma` (*sbml_parameter: libsbml.Parameter*) → bool
Returns whether the libsbml.Parameter `sbml_parameter` matches the defined sigma format.

`petab.sbml.write_sbml` (*sbml_doc: libsbml.SBMLDocument*, *filename: str*) → None
Write PETab visualization table

Parameters

- **sbml_doc** – SBML document containing the SBML model
- **filename** – Destination file name

8.2.13 petab.yaml

Code regarding the PETab YAML config files

Functions

add_constructor	
add_implicit_resolver	
add_multi_constructor	
add_multi_representer	
add_path_resolver	
add_representer	
compose	
compose_all	
dump	
dump_all	
emit	
full_load	
full_load_all	
load	
load_all	
load_warning	
parse	
safe_dump	
safe_dump_all	
safe_load	
safe_load_all	
scan	
serialize	
serialize_all	
unsafe_load	
unsafe_load_all	
warnings	Python part of the warnings subsystem.

Classes

YAMLObject
YAMLObjectMetaclass

Exceptions

YAMLLoadWarning

`petab.yaml.assert_single_condition_and_sbml_file` (*problem_config*: *Dict[KT, VT]*) → *None*

Check that there is only a single condition file and a single SBML file specified.

Parameters *problem_config* – Dictionary as defined in the YAML schema inside the *problems* list.

Raises `NotImplementedError` – If multiple condition or SBML files specified.

```
petab.yaml.create_problem_yaml (sbml_files: Union[str, List[str]], condition_files: Union[str,
List[str]], measurement_files: Union[str, List[str]], parameter_file: str, observable_files: Union[str, List[str]], yaml_file:
str, visualization_files: Union[str, List[str], None] = None) →
None
```

Create and write default YAML file for a single PETab problem

Parameters

- **sbml_files** – Path of SBML model file or list of such
- **condition_files** – Path of condition file or list of such
- **measurement_files** – Path of measurement file or list of such
- **parameter_file** – Path of parameter file
- **observable_files** – Path of observable file or list of such
- **yaml_file** – Path to which YAML file should be written
- **visualization_files** – Optional Path to visualization file or list of
- **such** –

```
petab.yaml.is_composite_problem (yaml_config: Union[Dict[KT, VT], str]) → bool
```

Does this YAML file comprise multiple models?

Parameters **yaml_config** – PETab configuration as dictionary or YAML file name

```
petab.yaml.load_yaml (yaml_config: Union[Dict[KT, VT], str]) → Dict[KT, VT]
```

Load YAML

Convenience function to allow for providing YAML inputs as filename, URL or as dictionary.

Parameters **yaml_config** – PETab YAML config as filename or dict or URL.

Returns The unmodified dictionary if **yaml_config** was dictionary. Otherwise the parsed the YAML file.

```
petab.yaml.validate (yaml_config: Union[Dict[KT, VT], str], path_prefix: Optional[str] = None)
```

Validate syntax and semantics of PETab config YAML

Parameters

- **yaml_config** – PETab YAML config as filename or dict.
- **path_prefix** – Base location for relative paths. Defaults to location of YAML file if a filename was provided for **yaml_config** or the current working directory.

```
petab.yaml.validate_yaml_semantics (yaml_config: Union[Dict[KT, VT], str], path_prefix: Op-
tional[str] = None)
```

Validate PETab YAML file semantics

Check for existence of files. Assumes valid syntax.

Version number and contents of referenced files are not yet checked.

Parameters

- **yaml_config** – PETab YAML config as filename or dict.
- **path_prefix** – Base location for relative paths. Defaults to location of YAML file if a filename was provided for **yaml_config** or the current working directory.

Raises `AssertionError` – in case of problems

`petab.yaml.validate_yaml_syntax` (*yaml_config: Union[Dict[KT, VT], str]*, *schema: Union[None, Dict[KT, VT], str] = None*)

Validate PEPab YAML file syntax

Parameters

- **yaml_config** – PEPab YAML file to validate, as file name or dictionary
- **schema** – Custom schema for validation

Raises see `jsonschema.validate`

`petab.yaml.write_yaml` (*yaml_config: Dict[str, Any]*, *filename: str*) → None

Write PEPab YAML file

Parameters

- **yaml_config** – Data to write
- **filename** – File to create

8.2.14 petab.visualize.data_overview

Functions for creating an overview report of a PEPab problem

Functions

<code>create_report</code> (<i>problem</i> , <i>model_name</i>)	Create an HTML overview data / model overview report
<code>get_data_per_observable</code> (<i>measurement_df</i>)	Get table with number of data points per observable and condition
<code>main</code> ()	Data overview generation with example data from the repository for testing

`petab.visualize.data_overview.create_report` (*problem: petab.problem.Problem*, *model_name: str*) → None

Create an HTML overview data / model overview report

Parameters

- **problem** – PEPab problem
- **model_name** – Name of the model, used for file name for report

`petab.visualize.data_overview.get_data_per_observable` (*measurement_df: pandas.core.frame.DataFrame*) → *pandas.core.frame.DataFrame*

Get table with number of data points per observable and condition

Parameters **measurement_df** – PEPab measurement data frame

Returns Pivot table with number of data points per observable and condition

Return type `data_per_observable`

`petab.visualize.data_overview.main`()

Data overview generation with example data from the repository for testing

8.2.15 petab.visualize.helper_functions

This file should contain the functions, which PETab internally needs for plotting, but which are not meant to be used by non-developers and should hence not be directly visible/usable when using *import petab.visualize*.

Functions

<code>check_ex_exp_columns(exp_data, ...)</code>	Check the columns in measurement file, if non-mandatory columns does not exist, create default columns
<code>check_ex_visu_columns(vis_spec, exp_data, ...)</code>	Check the columns in Visu_Spec file, if non-mandatory columns does not exist, create default columns
<code>check_vis_spec_consistency(exp_data, ...)</code>	Helper function for plotting data and simulations, which checks the visualization setting, if no visualization specification file is provided.
<code>create_dataset_id_list(simcond_id_list, ...)</code>	Create dataset id list and corresponding plot legends.
<code>create_figure(uni_plot_ids, plots_to_file)</code>	Helper function for plotting data and simulations, open figure and axes
<code>create_or_update_vis_spec(exp_data, ...)</code>	Helper function for plotting data and simulations, which updates vis_spec file if necessary or creates a default visualization table and updates/creates DATASET_ID column of exp_data.
<code>expand_vis_spec_settings(vis_spec, columns_dict)</code>	only makes sense if DATASET_ID is not in vis_spec.columns?
<code>get_data_to_plot(plot_spec, m_data, ...)</code>	Group the data, which should be plotted and return it as dataframe.
<code>get_default_vis_specs(exp_data, ...)</code>	Helper function for plotting data and simulations, which creates a default visualization table and updates/creates DATASET_ID column of exp_data
<code>get_vis_spec_dependent_columns_dict(...)</code>	Helper function for creating values for columns PLOT_ID, DATASET_ID, LEGEND_ENTRY, Y_VALUES for visualization specification file.
<code>handle_dataset_plot(plot_spec, ax, exp_data, ...)</code>	Handle dataset plot
<code>import_from_files(data_file_path, ...)</code>	Helper function for plotting data and simulations, which imports data from PETab files.
<code>matches_plot_spec(df, col_id, x_value, str], ...)</code>	constructs an index for subsetting of the dataframe according to what is specified in plot_spec.

```
petab.visualize.helper_functions.check_ex_exp_columns (exp_data:      pan-  
                                                         das.core.frame.DataFrame,  
                                                         dataset_id_list:  
                                                         List[List[str]],  
                                                         sim_cond_id_list:  
                                                         List[List[str]],  
                                                         sim_cond_num_list:  
                                                         List[List[int]],      observ-  
                                                         able_id_list:  List[List[str]],  
                                                         observable_num_list:  
                                                         List[List[int]],  
                                                         exp_conditions:      pan-  
                                                         das.core.frame.DataFrame,  
                                                         sim:              Optional[bool]  
                                                         = False)      →  Tu-  
                                                         ple[pandas.core.frame.DataFrame,  
                                                         List[List[str]], Dict[KT, VT]]
```

Check the columns in measurement file, if non-mandatory columns does not exist, create default columns

Returns A tuple of experimental DataFrame, list of datasetIds and dictionary of plot legends, corresponding to the datasetIds

```
petab.visualize.helper_functions.check_ex_visu_columns (vis_spec:      pan-  
                                                         das.core.frame.DataFrame,  
                                                         exp_data:      pan-  
                                                         das.core.frame.DataFrame,  
                                                         exp_conditions: pan-  
                                                         das.core.frame.DataFrame)  
                                                         →      pan-  
                                                         das.core.frame.DataFrame
```

Check the columns in Visu_Spec file, if non-mandatory columns does not exist, create default columns

Returns Updated visualization specification DataFrame

```
petab.visualize.helper_functions.check_vis_spec_consistency (exp_data:      pan-  
                                                         das.core.frame.DataFrame,  
                                                         dataset_id_list: Op-  
                                                         tional[List[List[str]]]  
                                                         =      None,  
                                                         sim_cond_id_list:  
                                                         Op-  
                                                         tional[List[List[str]]]  
                                                         =      None,  
                                                         sim_cond_num_list:  
                                                         Op-  
                                                         tional[List[List[int]]]  
                                                         =      None, observ-  
                                                         able_id_list:  Op-  
                                                         tional[List[List[str]]]  
                                                         =      None, observ-  
                                                         able_num_list: Op-  
                                                         tional[List[List[int]]]  
                                                         =      None) → str
```

Helper function for plotting data and simulations, which checks the visualization setting, if no visualization specification file is provided.

For documentation, see main function `plot_data_and_simulation()`

Returns Specifies the grouping of data to plot.

Return type group_by

```
petab.visualize.helper_functions.create_dataset_id_list (simcond_id_list:
                                                         List[List[str]],      sim-
                                                         cond_num_list:
                                                         List[List[int]],      ob-
                                                         servable_id_list:
                                                         List[List[str]],      ob-
                                                         servable_num_list:
                                                         List[List[int]],
                                                         exp_data:             pan-
                                                         das.core.frame.DataFrame,
                                                         exp_conditions:       pan-
                                                         das.core.frame.DataFrame,
                                                         group_by: str) → Tu-
                                                         ple[pandas.core.frame.DataFrame,
                                                         List[List[str]], Dict[KT,
                                                         VT], Dict[KT, VT]]
```

Create dataset id list and corresponding plot legends. Additionally, update/create DATASET_ID column of exp_data

Parameters group_by – defines grouping of data to plot

Returns A tuple of experimental DataFrame, list of datasetIds and dictionary of plot legends, corresponding to the datasetIds

For additional documentation, see main function plot_data_and_simulation()

```
petab.visualize.helper_functions.create_figure (uni_plot_ids:      numpy.ndarray,
                                                         plots_to_file: bool) → Tu-
                                                         ple[matplotlib.figure.Figure,
                                                         Union[Dict[str,          mat-
                                                         plotlib.axes._subplots.AxesSubplot],
                                                         np.ndarray[plt.Subplot]]]
```

Helper function for plotting data and simulations, open figure and axes

Parameters

- **uni_plot_ids** – Array with unique plot indices
- **plots_to_file** – Indicator if plots are saved to file

Returns

- **fig** (*Figure object of the created plot.*)
- **ax** (*Axis object of the created plot.*)

```

petab.visualize.helper_functions.create_or_update_vis_spec(exp_data:      pandas.core.frame.DataFrame,
                                                           exp_conditions: pandas.core.frame.DataFrame,
                                                           vis_spec:      Optional[pandas.core.frame.DataFrame]
                                                           = None,
                                                           dataset_id_list: Optional[List[List[str]]]
                                                           = None,
                                                           sim_cond_id_list: Optional[List[List[str]]]
                                                           = None,
                                                           sim_cond_num_list: Optional[List[List[int]]]
                                                           = None, observable_id_list: Optional[List[List[str]]]
                                                           = None, observable_num_list: Optional[List[List[int]]]
                                                           = None, plotted_noise: Optional[str]
                                                           = 'MeanAndSD')

```

Helper function for plotting data and simulations, which updates vis_spec file if necessary or creates a default visualization table and updates/creates DATASET_ID column of exp_data. As a result, a visualization specification file exists with columns PLOT_ID, DATASET_ID, Y_VALUES and LEGEND_ENTRY

Returns A tuple of visualization specification DataFrame and experimental DataFrame.

```

petab.visualize.helper_functions.expand_vis_spec_settings(vis_spec,
                                                         columns_dict)

```

only makes sense if DATASET_ID is not in vis_spec.columns?

Returns A visualization specification DataFrame

```

petab.visualize.helper_functions.get_data_to_plot(plot_spec:      pandas.core.series.Series,      m_data:      pandas.core.frame.DataFrame,
                                                  simulation_data: pandas.core.frame.DataFrame,
                                                  condition_ids: numpy.ndarray,
                                                  col_id:      str,      simulation_field: str = 'simulation') → pandas.core.frame.DataFrame

```

Group the data, which should be plotted and return it as dataframe.

Parameters

- **plot_spec** – information about contains defined data format (visualization file)
- **m_data** – contains defined data format (measurement file)
- **simulation_data** – contains defined data format (simulation file)
- **condition_ids** – contains all unique condition IDs which should be plotted in one figure (can be found in measurementData file, column simulationConditionId)

- **col_id** – the name of the column in visualization file, whose entries should be unique (depends on condition in column xValues)
- **simulation_field** – Column name in `simulation_data` that contains the actual simulation result.

Returns Contains the data which should be plotted (Mean and Std)

Return type `data_to_plot`

```
petab.visualize.helper_functions.get_default_vis_specs (exp_data:      pandas.core.frame.DataFrame,
                                                         exp_conditions:      pandas.core.frame.DataFrame,
                                                         dataset_id_list:      Optional[List[List[str]]] =
                                                         None,      sim_cond_id_list:
                                                         Optional[List[List[str]]] =
                                                         None,      sim_cond_num_list:
                                                         Optional[List[List[int]]] =
                                                         None,      observable_id_list:
                                                         Optional[List[List[str]]] =
                                                         None,      observable_num_list:
                                                         Optional[List[List[int]]]
                                                         = None,      plotted_noise:
                                                         Optional[str] =
                                                         'MeanAndSD') → Tuple[
                                                         pandas.core.frame.DataFrame,
                                                         pandas.core.frame.DataFrame]
```

Helper function for plotting data and simulations, which creates a default visualization table and updates/creates DATASET_ID column of `exp_data`

Returns A tuple of visualization specification DataFrame and experimental DataFrame.

For documentation, see main function `plot_data_and_simulation()`

```
petab.visualize.helper_functions.get_vis_spec_dependent_columns_dict (exp_data:
                                                                    pan-
                                                                    das.core.frame.DataFrame,
                                                                    exp_conditions:
                                                                    pan-
                                                                    das.core.frame.DataFrame,
                                                                    dataset_id_list:
                                                                    Op-
                                                                    tional[List[List[str]]]
                                                                    =
                                                                    None,
                                                                    sim_cond_id_list:
                                                                    Op-
                                                                    tional[List[List[str]]]
                                                                    =
                                                                    None,
                                                                    sim_cond_num_list:
                                                                    Op-
                                                                    tional[List[List[int]]]
                                                                    =
                                                                    None,
                                                                    observ-
                                                                    able_id_list:
                                                                    Op-
                                                                    tional[List[List[str]]]
                                                                    =
                                                                    None,
                                                                    observ-
                                                                    able_num_list:
                                                                    Op-
                                                                    tional[List[List[int]]]
                                                                    =
                                                                    None)
                                                                    → Tu-
                                                                    ple[pandas.core.frame.DataFrame,
                                                                    Dict[KT,
                                                                    VT]]
```

Helper function for creating values for columns PLOT_ID, DATASET_ID, LEGEND_ENTRY, Y_VALUES for visualization specification file. DATASET_ID column of exp_data is updated accordingly.

Returns A tuple of experimental DataFrame and a dictionary with values for columns PLOT_ID, DATASET_ID, LEGEND_ENTRY, Y_VALUES for visualization specification file.

```
petab.visualize.helper_functions.handle_dataset_plot (plot_spec:
                                                                    pan-
                                                                    das.core.series.Series,      ax:
                                                                    matplotlib.axes._axes.Axes,
                                                                    exp_data:                    pan-
                                                                    das.core.frame.DataFrame,
                                                                    exp_conditions:              pan-
                                                                    das.core.frame.DataFrame,
                                                                    sim_data:                    pan-
                                                                    das.core.frame.DataFrame)
```

Handle dataset plot

```
petab.visualize.helper_functions.import_from_files (data_file_path:      str,      condi-
                                                    tion_file_path:      str,      sim-
                                                    ulation_file_path:      str,
dataset_id_list:      List[List[str]],
sim_cond_id_list:      List[List[str]],
sim_cond_num_list:
List[List[int]], observable_id_list:
List[List[str]],      observ-
able_num_list:      List[List[int]],
plotted_noise:      str,      visualiza-
tion_file_path: str = None) → Tu-
ple[pandas.core.frame.DataFrame,
pandas.core.frame.DataFrame,
pandas.core.frame.DataFrame,
pandas.core.frame.DataFrame]
```

Helper function for plotting data and simulations, which imports data from PETab files. If *visualization_file_path* is not provided, the visualisation specification DataFrame will be generated automatically.

For documentation, see main function `plot_data_and_simulation()`

Returns A tuple of experimental data, experimental conditions, visualization specification and simulation data DataFrames.

```
petab.visualize.helper_functions.matches_plot_spec (df: pandas.core.frame.DataFrame,
col_id: str, x_value: Union[float,
str],      plot_spec: pandas.core.series.Series) → pan-
das.core.series.Series
```

constructs an index for subsetting of the dataframe according to what is specified in `plot_spec`.

Parameters

- **df** – pandas data frame to subset, can be from measurement file or simulation file
- **col_id** – name of the column that will be used for indexing in x variable
- **x_value** – subsetting x value
- **plot_spec** – visualization spec from the visualization file

Returns Boolean series that can be used for subsetting of the passed dataframe

Return type index

8.2.16 petab.visualize.plot_data_and_simulation

```
petab.visualize.plot_data_and_simulation(exp_data: Union[str, pandas.core.frame.DataFrame], exp_conditions: Union[str, pandas.core.frame.DataFrame], vis_spec: Union[str, pandas.core.frame.DataFrame, None] = None, sim_data: Union[str, pandas.core.frame.DataFrame, None] = None, dataset_id_list: Optional[List[List[str]]] = None, sim_cond_id_list: Optional[List[List[str]]] = None, sim_cond_num_list: Optional[List[List[int]]] = None, observable_id_list: Optional[List[List[str]]] = None, observable_num_list: Optional[List[List[int]]] = None, plotted_noise: Optional[str] = 'MeanAndSD', subplot_file_path: str = '') → Union[Dict[str, matplotlib.axes._subplots.AxesSubplot], np.ndarray[plt.Subplot], None]
```

Main function for plotting data and simulations.

What exactly should be plotted is specified in a visualizationSpecification.tsv file.

Also, the data, simulations and conditions have to be defined in a specific format (see “doc/documentation_data_format.md”).

Parameters

- **exp_data** – measurement DataFrame in the PEOab format or path to the data file.
- **exp_conditions** – condition DataFrame in the PEOab format or path to the condition file.
- **vis_spec** – Visualization specification DataFrame in the PEOab format or path to visualization file.
- **sim_data** – simulation DataFrame in the PEOab format or path to the simulation output data file.
- **dataset_id_list** – A list of lists. Each sublist corresponds to a plot, each subplot contains the datasetIds for this plot. Only to be used if no visualization file was available.
- **sim_cond_id_list** – A list of lists. Each sublist corresponds to a plot, each subplot contains the simulationConditionIds for this plot. Only to be used if no visualization file was available.
- **sim_cond_num_list** – A list of lists. Each sublist corresponds to a plot, each subplot contains the numbers corresponding to the simulationConditionIds for this plot. Only to be used if no visualization file was available.
- **observable_id_list** – A list of lists. Each sublist corresponds to a plot, each subplot contains the observableIds for this plot. Only to be used if no visualization file was available.
- **observable_num_list** – A list of lists. Each sublist corresponds to a plot, each subplot contains the numbers corresponding to the observableIds for this plot. Only to be used if no visualization file was available.
- **plotted_noise** – String indicating how noise should be visualized: [‘MeanAndSD’ (default), ‘MeanAndSEM’, ‘replicate’, ‘provided’]

- **subplot_file_path** – String which is taken as file path to which single subplots are saved. PlotIDs will be taken as file names.

Returns

- **ax** (*Axis object of the created plot.*)
- **None** (*In case subplots are save to file*)

8.2.17 petab.visualize.plotting_config

Plotting config

Functions

<code>plot_lowlevel(plot_spec, ax, conditions, ms, ...)</code>	Plotting routine / preparations: set properties of figure and plot the data with given specifications (lineplot with errorbars, or barplot)
<code>square_plot_equal_ranges(ax, lim, Tuple, ...)</code>	Square plot with equal range for scatter plots

`petab.visualize.plotting_config.plot_lowlevel` (*plot_spec: pandas.core.series.Series, ax: matplotlib.pyplot.Axes, conditions: pandas.core.series.Series, ms: pandas.core.frame.DataFrame, plot_sim: bool*) → *matplotlib.pyplot.Axes*

Plotting routine / preparations: set properties of figure and plot the data with given specifications (lineplot with errorbars, or barplot)

Parameters

- **plot_spec** – contains defined data format (visualization file)
- **ax** – axes to which to plot
- **conditions** – Values on x-axis
- **ms** – contains measurement data which should be plotted
- **plot_sim** – tells whether or not simulated data should be plotted as well

Returns Updated axis object.

`petab.visualize.plotting_config.square_plot_equal_ranges` (*ax: matplotlib.pyplot.Axes, lim: Union[List[T], Tuple, None] = None*) → *matplotlib.pyplot.Axes*

Square plot with equal range for scatter plots

Returns Updated axis object.

8.3 PEtch changelog

8.3.1 0.1 series

0.1.11

- Function for generating synthetic data (#472)
- Minor documentation updates (#470)

0.1.10

Fixed deployment setup, no further changes.

0.1.9

Library:

- Allow URL as filenames for YAML files and SBML models (Closes #187) (#459)
- Allow model time in observable formulas (#445)
- Make float parsing from CSV round-trip (#444)
- Validator: Error message for missing IDs, with line numbers. (#467)
- Validator: Detect duplicated observable IDs (#446)
- Some documentation and CI fixes / updates
- Visualization: Add option to save visualization specification (#457)
- Visualization: Column XValue not mandatory anymore (#429)
- Visualization: Add sorting of indices of dataframes for the correct sorting of x-values (#430)
- Visualization: Default value for the column x_label in vis_spec (#431)

0.1.8

Library:

- Use `core.is_empty` to check for empty values (#434)
- Move tests to python 3.8 (#435)
- Update to libcombine 0.2.6 (#437)
- Make float parsing from CSV round-trip (#444)
- Lint: Allow model time in observable formulas (#445)
- Lint: Detect duplicated observable ids (#446)
- Fix likelihood calculation with missing values (#451)

Documentation:

- Move format documentation to restructuredtext format (#452)
- Document all noise distributions and observable scales (#452)
- Fix documentation for prior distribution (#449)

Visualization:

- Make XValue column non-mandatory (#429)

- Apply correct condition sorting (#430)
- Apply correct default x label (#431)

0.1.7

Documentation:

- Update coverage and links of supporting tools
- Update explanatory figure

0.1.6

Library:

- Fix handling of empty columns for residual calculation (#392)
- Allow optional fixing of fixed parameters in parameter mapping (#399)
- Fix function to flatten out time-point specific overrides (#404)
- Add function to create a problem yaml file (#398)
- Allow merging of multiple parameter files (#407)

Documentation:

- In README, add to the overview table the coverage for the supporting tools, and links and usage examples (various commits)
- Show REAMDE on readthedocs documentation front page (#400)
- Correct description of observable and noise formulas (#401)
- Update documentation on optional visualization values (#405, #419)

Visualization:

- Fix sorting problem (#396)
- More generously handle optional values (#405, #419)
- Create dataset id also for simulation dataframe (#408)
- Extend test suite for visualization (#418)

0.1.5

Library:

- New create empty observable function (issue 386) (#387)
- Deprecate `petab.sbml.globalize_parameters` (#381)
- Fix computing log10 likelihood (#380)
- Documentation update and typehints for visualization (#372)
- Ordered result of `petab.get_output_parameters`
- Fix missing argument to `parameters.create_parameter_df`

Documentation:

- Add overview of supported PEtac feature in toolboxes
- Add contribution guide
- Fix optional values in documentation (#378)

0.1.4

Library:

- Fixes / updates in functions for computing llh and chi2
- Allow and require output parameters defined in observable table to be defined in parameter table
- Fix merge_preeq_and_sim_pars_condition which incorrectly assumed lists instead of dicts
- Update parameter mapping to deal with species and compartments in condition table
- Removed petab.migrations.sbml_observables_to_table
For converting older PEtac files to observable table format, use one of the previous releases
- Visualization:
 - Fix various issues with get_data_to_plot
 - Fixed various issues with expected presence of optional columns

0.1.3

File format:

- Updated documentation
- Observables table in YAML file now mandatory in schema (was implicitly mandatory before, as observable table was required already)

Library:

- petablnt:
 - Fix: allow specifying observables file via CLI (Closes #302)
 - Fix: nominalValue is optional unless estimated!=1 anywhere (Fixes #303)
 - Fix: handle undefined observables more gracefully (Closes #300) (#351)
- Parameter mapping:
 - Fix / refactor parameter mapping (breaking change) (#344) (now performing parameter value and scale mapping together)
 - check optional measurement cols in mapping (#350)
- allow calculating llhs (#349), chi2 values (#348) and residuals (#345)
- Visualization
 - Basic Scatterplots & lot of bar plot fixes (#270)
 - Fix incorrect length of bool bool_preequ when subsetting with ind_meas (Closes #322)
- make libcombine optional (#338)

0.1.2

Library:

- Extensions and fixes for the visualization functions (#255, #262)
- Allow to extract fixed/free and scaled/non-scaled parameters (#256, #268, #273)
- Various fixes (esp. #264)
- Add function to get observable ids (#269)
- Improve documentation (esp. #289)
- Set default column for simulation results to 'simulation'
- Add support for COMBINE archives (#271)
- Fix sbml observables to table
- Improve prior and dataframe tests (#285, #286, #297)
- Add function to get parameter table with all default values (#288)
- Move tests to github actions (#281)
- Check for valid identifiers
- Fix handling of empty values in dataframes
- Allow to get numeric values in parameter mappings in scaled form (#308)

0.1.1

Library:

- Fix parameter mapping: include output parameters not present in SBML model
- Fix missing `petab/petab_schema.yaml` in source distribution
- Let `get_placeholders` return an (ordered) list of placeholders
- Deprecate `petab.problem.from_folder` and related functions (obsolete after introducing more flexible YAML files for grouping tables and models)

0.1.0

Data format:

- Introduce observables table instead of SBML assignment rules for defining observation model (#244) (moves `observableTransformation` and `noiseModel` from the measurement table to the observables table)
- Allow initial concentrations / sizes in condition table (#238)
- Fixes and clarifications in the format documentation
- Changes in prior columns of the parameter table (#222)
- Introduced separate version number of file format, this release being version 1

Library:

- Adaptations to new file formats
- Various bugfixes and clean-up, especially in visualization and validator

- Parameter mapping changed to include all model parameters and not only those differing from the ones defined inside the SBML model
- Introduced constants for all field names and string options, replacing most string literals in the code (#228)
- Added unit tests and additional format validation steps
- Optional parallelization of parameter mapping (#205)
- Extended documentation (in-source and example Jupyter notebooks)

0.0.2

Bugfix release

- Fix `petablint` error
- Fix minor issues in `petab.visualize`

0.0.1

Data format:

- Update format and documentation with respect to data and parameter scales (#169)
- Define YAML schema for grouping PEPetab files, also allowing for more complex combinations of files (#183)

Library:

- Refactor library. Reorganize `petab.core` functions.
- Fix visualization w/o condition names #142
- Extend validator
- Removed deprecated functions `petab.Problem.get_constant_parameters` and `petab.sbml.constant_species_to_parameters`
- Minor fixes and extensions

8.3.2 0.0 series

0.0.0a17

Data format: *No changes*

Library:

- Extended visualization support
- Add helper function and test case to deal with timepoint-specific parameters `flatten_timepoint_specific_output_overrides` (#128) (Closes #125)
- Fix `get_noise_distributions`: so far we got 'normal' everywhere due to wrong grouping (#147)
- Fix `create_parameter_df`: Exclude rule targets (#149)
- Verify condition table column names occur as model parameters (Closes #150) (#151)
- More informative error messages in case of wrongly set observable and noise parameters (Closes #118) (#155)
- Update doc for copasi import and github installation (#158)

- Extend validator to check if all required parameters are present in parameter table (Closes #43) (#159)
- Setup documentation for RTD (#161)
- Handle None in `petab.core.split_parameter_replacement_list` (Closes #121)
- Fix(lint) correct handling of optional columns. Check before access.
- Remove obsolete `generate_experiment_id.py` (Closes #111) #166

0.0.0a16 and earlier

See git history

8.4 How to cite

Help us to promote PEOtab: When using PEOtab, please cite our [preprint](#):

```
@misc{schmiester2020petab,
  title={PEtab -- interoperable specification of parameter estimation problems in
↪systems biology},
  author={Leonard Schmiester and Yannik Schälte and Frank T. Bergmann and Tacio
↪Camba and Erika Dudkin and Janine Egert and Fabian Fröhlich and Lara Fuhrmann and
↪Adrian L. Hauber and Svenja Kemmer and Polina Lakrisenko and Carolin Loos and Simon
↪Merkt and Wolfgang Müller and Dilan Pathirana and Elba Raimúndez and Lukas Refisch
↪and Marcus Rosenblatt and Paul L. Stapor and Philipp Städter and Dantong Wang and
↪Franz-Georg Wieland and Julio R. Banga and Jens Timmer and Alejandro F. Villaverde
↪and Sven Sahle and Clemens Kreutz and Jan Hasenauer and Daniel Weindl},
  year={2020},
  eprint={2004.01154},
  archivePrefix={arXiv},
  primaryClass={q-bio.QM}
}
```

8.5 License

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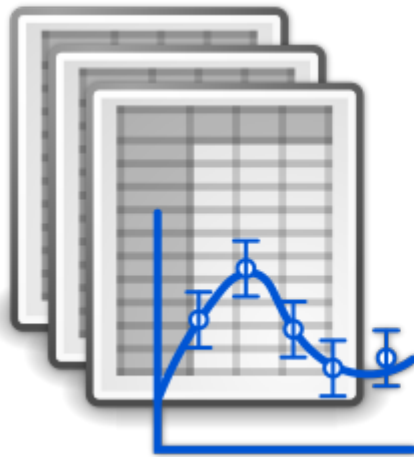
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8.6 PEtap logo license

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PEtap

8.7 Examples

The following examples should help to get a better idea of how to use the PEtap library.

8.7.1 Using petablint

petablint is a tool to validate a model against the PEtap standard. When you have installed PEtap, you can simply call it from the command line. It takes the following arguments:

```
[1]: !petablint -h
usage: petablint [-h] [-v] [-s SBML_FILE_NAME] [-m MEASUREMENT_FILE_NAME]
                [-c CONDITION_FILE_NAME] [-p PARAMETER_FILE_NAME]
                [-y YAML_FILE_NAME | -n MODEL_NAME] [-d DIRECTORY]

Check if a set of files adheres to the PEtap format.

optional arguments:
  -h, --help            show this help message and exit
  -v, --verbose          More verbose output
  -s SBML_FILE_NAME, --sbml SBML_FILE_NAME
                        SBML model filename
  -m MEASUREMENT_FILE_NAME, --measurements MEASUREMENT_FILE_NAME
                        Measurement table
```

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```
-c CONDITION_FILE_NAME, --conditions CONDITION_FILE_NAME
    Conditions table
-p PARAMETER_FILE_NAME, --parameters PARAMETER_FILE_NAME
    Parameter table
-y YAML_FILE_NAME, --yaml YAML_FILE_NAME
    PEtAb YAML problem filename
-n MODEL_NAME, --model-name MODEL_NAME
    Model name where all files are in the working
    directory and follow PEtAb naming convention.
    Specifying -[smcp] will override defaults
-d DIRECTORY, --directory DIRECTORY
```

Let's look at an example: In the `example_Fujita` folder, we have a PEtAb configuration file `Fujita.yaml` telling which files belong to the Fujita model:

```
[2]: !cat example_Fujita/Fujita.yaml

parameter_file: Fujita_parameters.tsv
petab_version: 0.0.0a17
problems:
- condition_files:
  - Fujita_experimentalCondition.tsv
  measurement_files:
  - Fujita_measurementData.tsv
  sbml_files:
  - Fujita_model.xml
```

To verify everything is ok, we can just call:

```
[3]: !petablint -y example_Fujita/Fujita.yaml
```

If there were some inconsistency or error, we would see that here. `petablint` can be called in different ways. You can e.g. also pass SBML, measurement, condition, and parameter file directly, or, if the files follow PEtAb naming conventions, you can just pass the model name.

8.7.2 Visualization of data and simulations

In this notebook, we illustrate the visualization functions of petab.

```
[1]: from petab.visualize import plot_data_and_simulation
import matplotlib.pyplot as plt

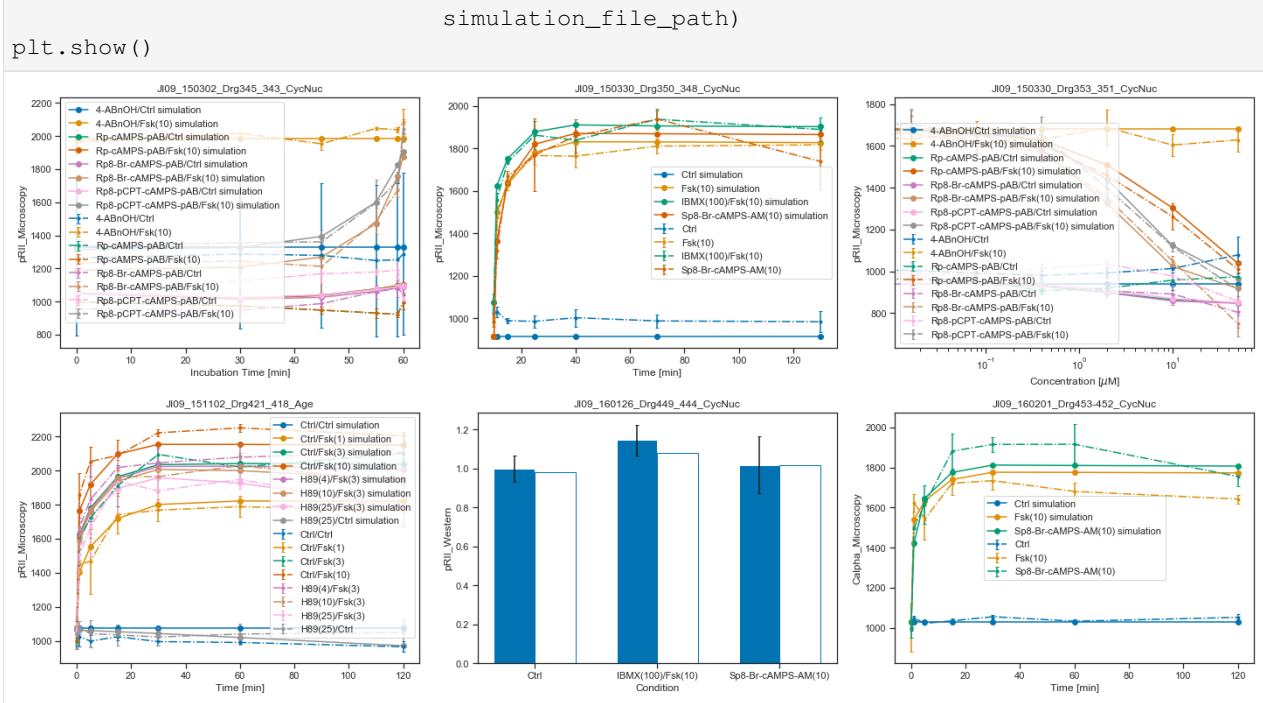
[2]: folder = "example_Isensee/"

data_file_path = folder + "Isensee_measurementData.tsv"
condition_file_path = folder + "Isensee_experimentalCondition.tsv"
visualization_file_path = folder + "Isensee_visualizationSpecification.tsv"
simulation_file_path = folder + "Isensee_simulationData.tsv"

# function to call, to plot data and simulations
ax = plot_data_and_simulation(data_file_path,
                             condition_file_path,
                             visualization_file_path,
```

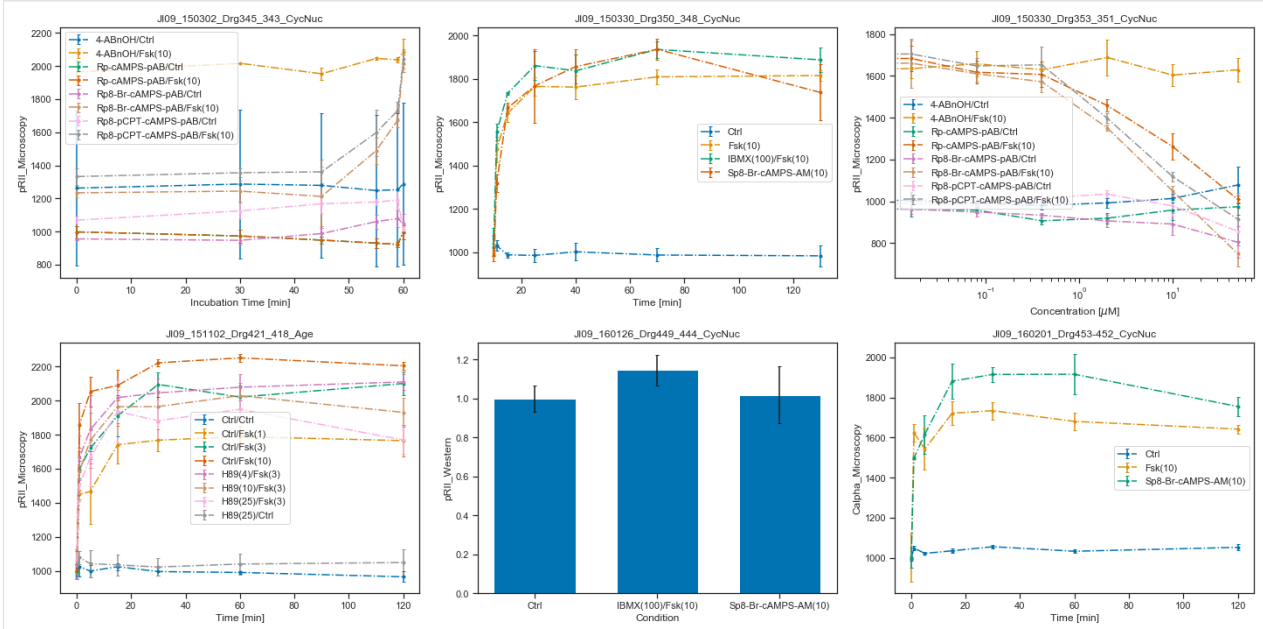
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Now, we want to call the plotting routines without using the simulated data, only the visualization specification file.

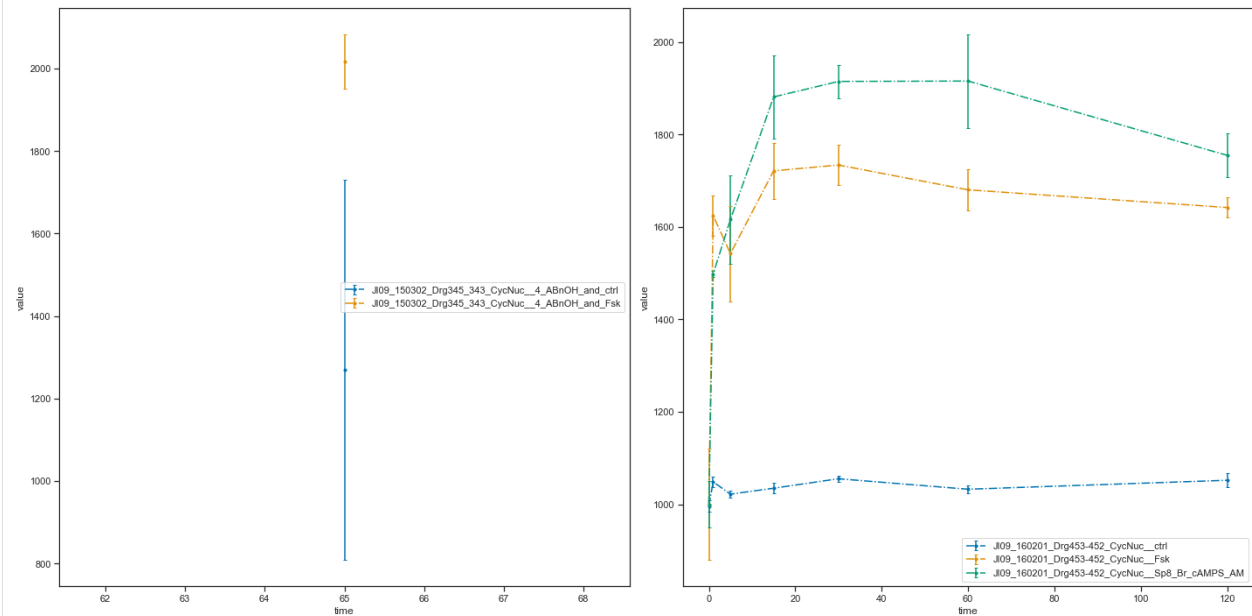
```
[3]: ax_without_sim = plot_data_and_simulation(
    data_file_path,
    condition_file_path,
    visualization_file_path)
plt.show()
```



We can also call the plotting routine without the visualization specification file, but by passing a list of lists as `dataset_id_list`. Each sublist corresponds to a plot, and contains the datasetIds which should be plotted. In this simply structured plotting routine, the independent variable will always be time.

```
[4]: ax_without_sim = plot_data_and_simulation(
    data_file_path,
    condition_file_path,
    dataset_id_list = [['JI09_150302_Drg345_343_CycNuc__4_ABnOH_and_ctrl',
                        'JI09_150302_Drg345_343_CycNuc__4_ABnOH_and_Fsk'],
                       ['JI09_160201_Drg453-452_CycNuc__ctrl',
                        'JI09_160201_Drg453-452_CycNuc__Fsk',
                        'JI09_160201_Drg453-452_CycNuc__Sp8_Br_cAMPS_AM']])

plt.show()
```



Let's look more closely at the plotting routines, if no visualization specification file is provided. If such a file is missing, PETab needs to know how to group the data points. For this, five options can be used: `* dataset_id_list *` `sim_cond_id_list *` `sim_cond_num_list *` `observable_id_list *` `observable_num_list *`

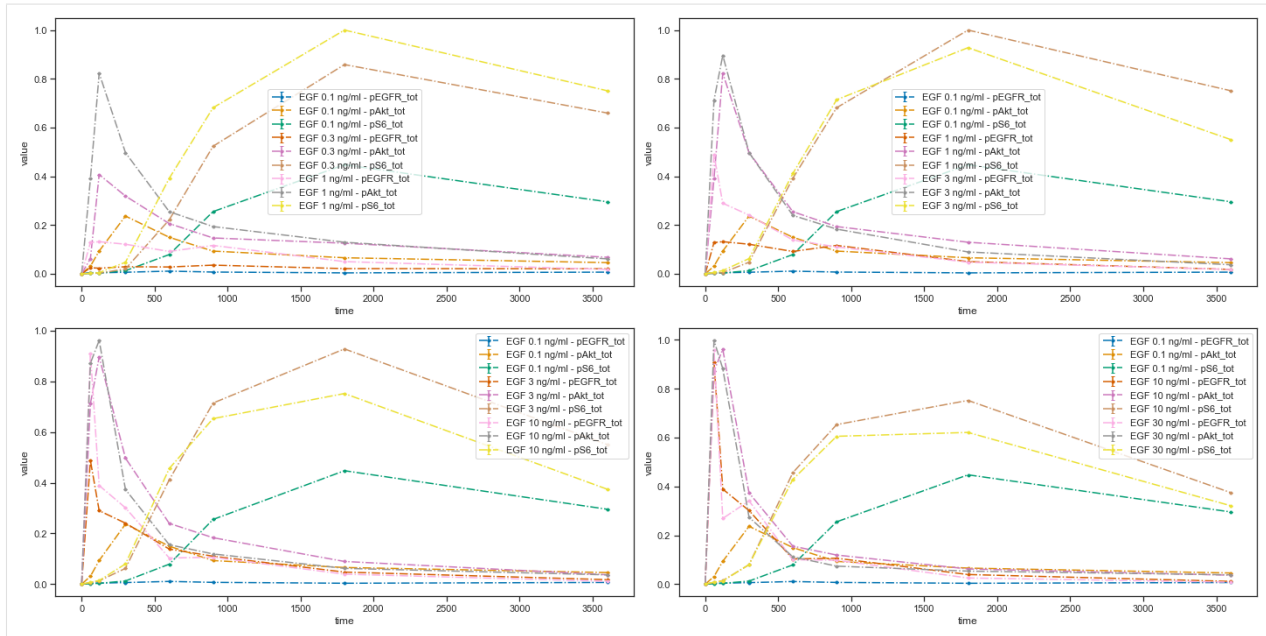
Each of them is a list of lists. Again, each sublist is a plot and its content are either simulation condition IDs or observable IDs (or their corresponding number when being enumerated) or the dataset IDs.

We want to illustrate this functionality by using a simpler example, a model published in 2010 by Fujita et al.

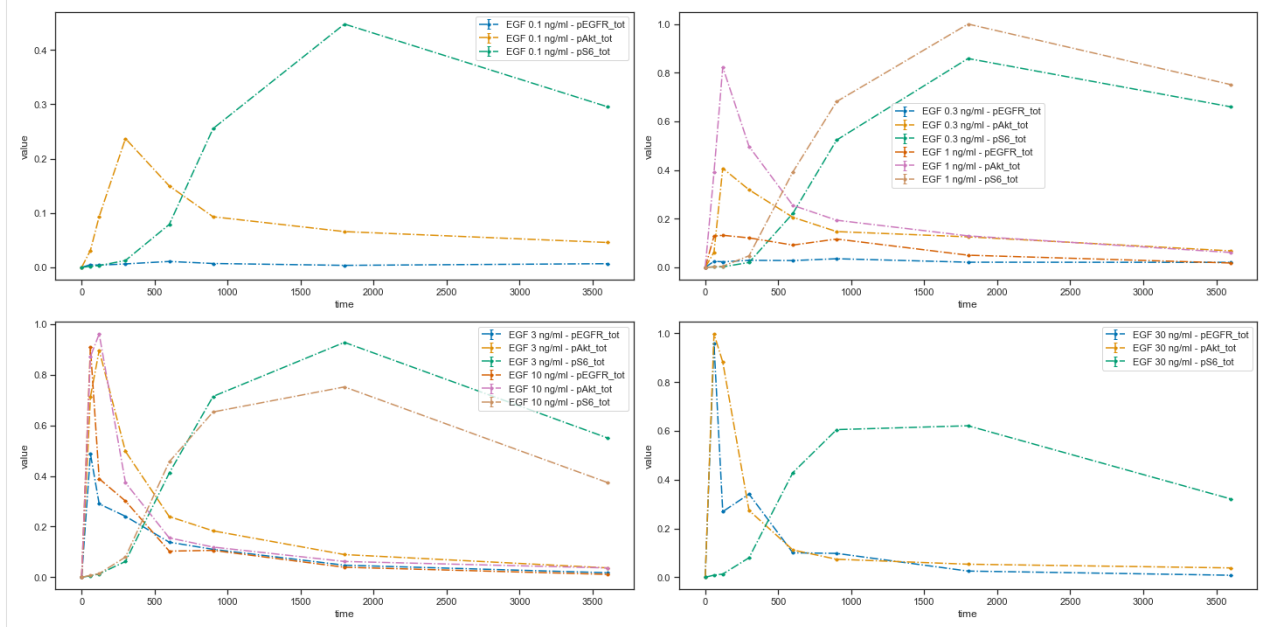
```
[5]: data_file_path = "example_Fujita/Fujita_measurementData.tsv"
    condition_file_path = "example_Fujita/Fujita_experimentalCondition.tsv"

    # Plot 4 axes objects, plotting
    # - in the first window all observables of the 1st, 2nd, and 3rd simulation condition
    # - in the second window all observables of the 1st, 3rd, and 4th simulation condition
    # - in the third window all observables of the 1st, 4th, and 5th simulation condition
    # - in the fourth window all observables of the 1st, 5th, and 6th simulation condition
    plot_data_and_simulation(data_file_path, condition_file_path,
                            sim_cond_num_list = [[0, 1, 2], [0, 2, 3], [0, 3, 4], [0, 4, 5]])
    plt.show()

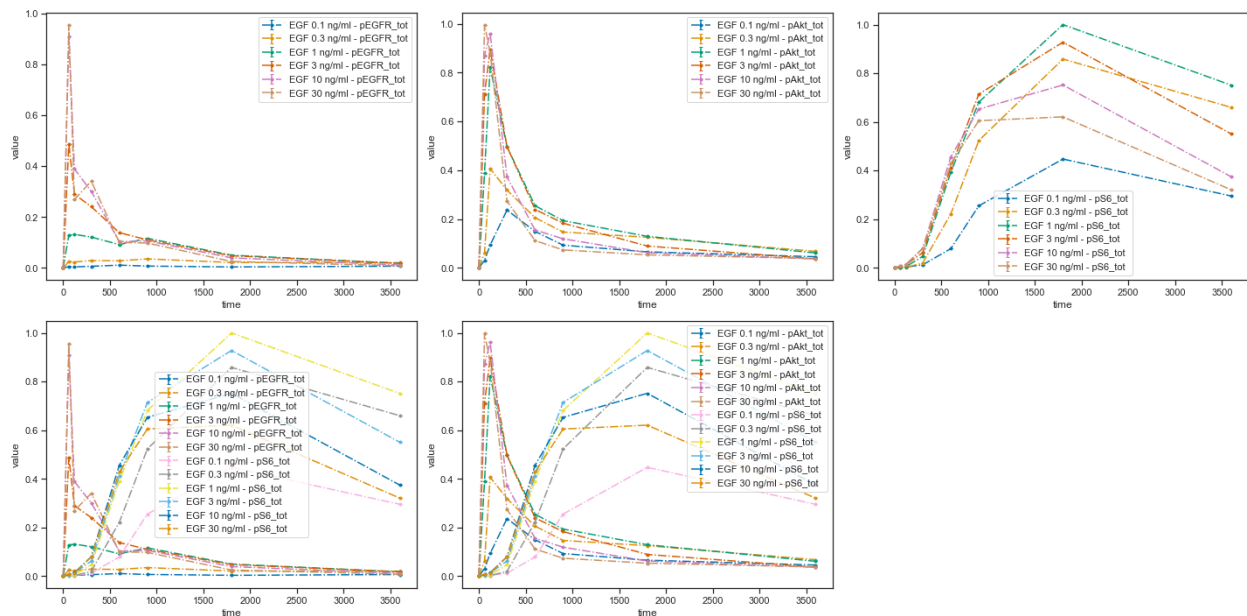
/home/polina/Documents/Development/PETab/petab/visualize/helper_functions.py:157:
↳ UserWarning: DatasetIds would have been available, but other grouping was requested.
↳ Consider using datasetId.
    warnings.warn("DatasetIds would have been available, but other "
```



```
[6]: # Plot 4 axes objects, plotting
# - in the first window all observables of the simulation condition 'modell_data1'
# - in the second window all observables of the simulation conditions 'modell_data2',
#   'modell_data3'
# - in the third window all observables of the simulation conditions 'modell_data4',
#   'modell_data5'
# - in the fourth window all observables of the simulation condition 'modell_data6'
plot_data_and_simulation(
    data_file_path, condition_file_path,
    sim_cond_id_list = [['modell_data1'], ['modell_data2', 'modell_data3'],
                       ['modell_data4', 'modell_data5'], ['modell_data6']])
plt.show()
```

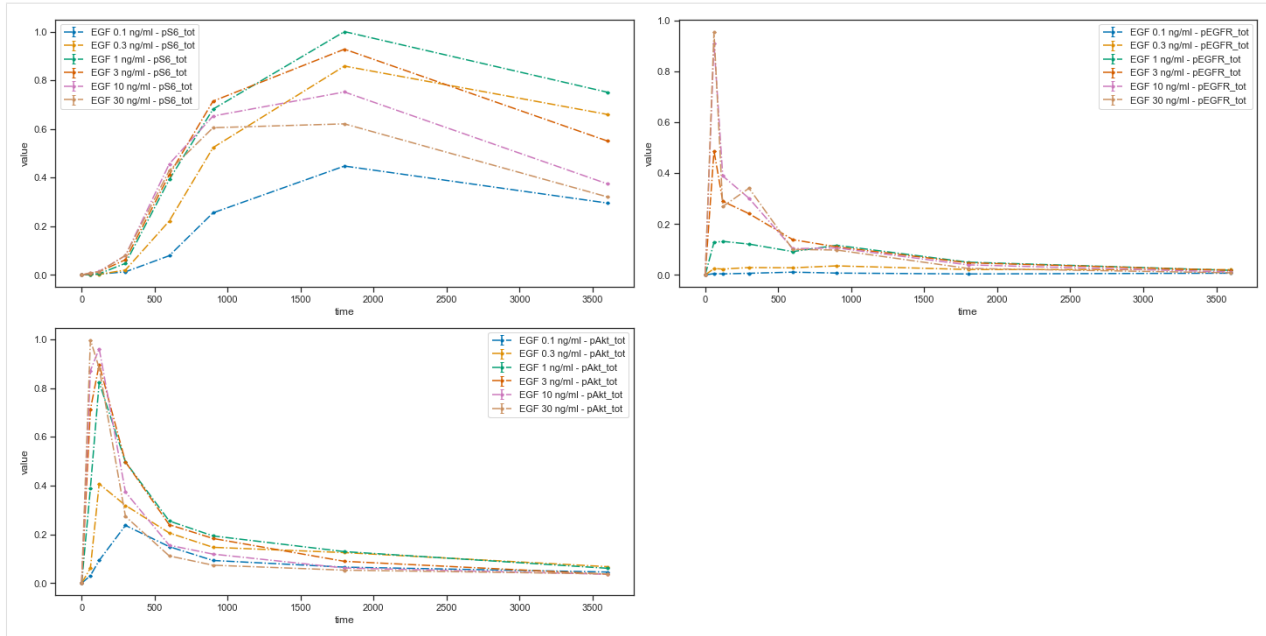


```
[7]: # Plot 5 axes objects, plotting
# - in the first window the 1st observable for all simulation conditions
# - in the second window the 2nd observable for all simulation conditions
# - in the third window the 3rd observable for all simulation conditions
# - in the fourth window the 1st and 3rd observable for all simulation conditions
# - in the fifth window the 2nd and 3rd observable for all simulation conditions
plot_data_and_simulation(
    data_file_path, condition_file_path,
    observable_num_list = [[0], [1], [2], [0, 2], [1, 2]])
plt.show()
```



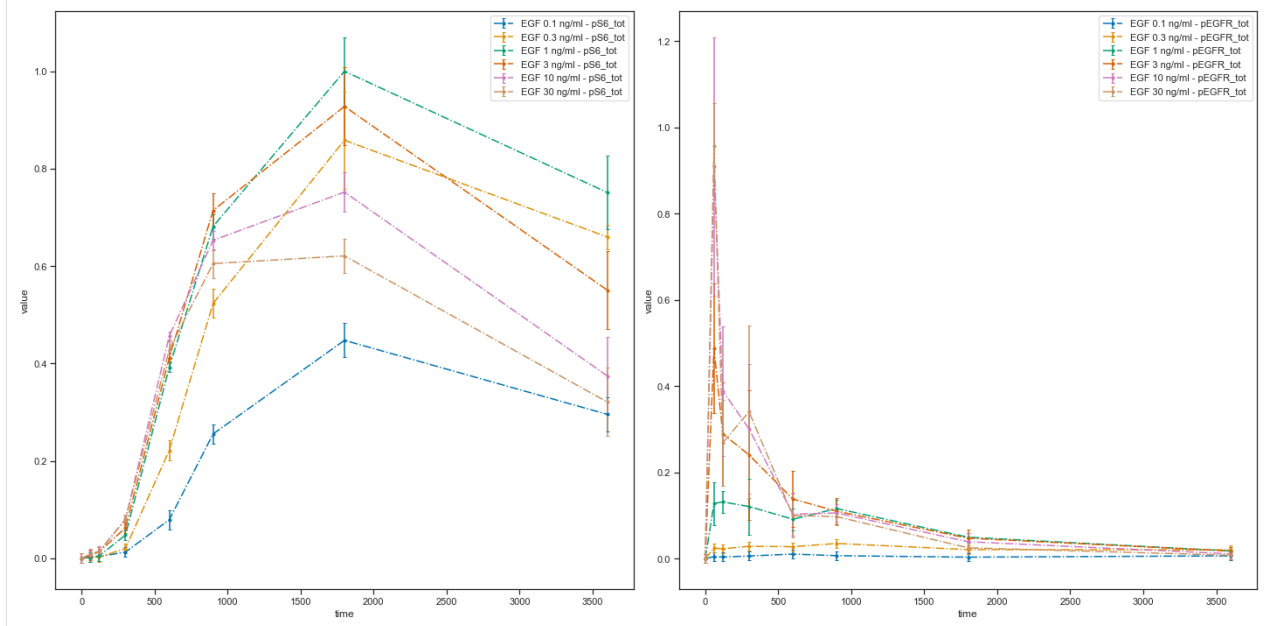
```
[8]: # Plot 3 axes objects, plotting
# - in the first window the observable 'pS6_tot' for all simulation conditions
# - in the second window the observable 'pEGFR_tot' for all simulation conditions
# - in the third window the observable 'pAkt_tot' for all simulation conditions

plot_data_and_simulation(
    data_file_path, condition_file_path,
    observable_id_list = [['pS6_tot'], ['pEGFR_tot'], ['pAkt_tot']])
plt.show()
```



```
[9]: # Plot 2 axes objects, plotting
# - in the first window the observable 'pS6_tot' for all simulation conditions
# - in the second window the observable 'pEGFR_tot' for all simulation conditions
# - in the third window the observable 'pAkt_tot' for all simulation conditions
# while using the noise values which are saved in the PTEtab files
```

```
plot_data_and_simulation(
    data_file_path, condition_file_path,
    observable_id_list = [['pS6_tot'], ['pEGFR_tot']],
    plotted_noise='provided')
plt.show()
```



Examples of systems biology parameter estimation problems specified in PTEtab can be found in the [systems biology benchmark model collection](#).

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