Introduction

SO Structure
SO consists of the following seven main sections:

- **Tool Settings** – storing the reference to any file containing the tool settings of a performed task.
- **Raw results** – placing references to original output files, both data and graphics, produced by any target tool.
- **Task Information** – holding the information about the modelling step execution.
- **Estimation** – storing typical output of interest resulting from an estimation task.
- **Model Diagnostic** – designed for storing information resulting from typical model diagnostic plots.
- **Simulation** – storing typical results produced in a simulation task.
- **Optimal Design** – storing results coming from a evaluation or optimization step.

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Example 1: Population estimates
Typical output for parameter estimation. First the columns – here the names of population parameters – are specified. Then two options exist: either the results are stored inline or in an external data file.

Example 2: Optimal design
In an optimal design task, e.g., evaluation, relevant results such as the Fisher Information Matrix (FIM) and the covariance matrix are captured.

Model Definition

- **Variability Model** – allows to define any number of variability levels as a nested hierarchy.
- **Covariate Model** – describes the covariates, both continuous and discrete, their distribution, transformation and interpolation.
- **Parameter Model** – offers flexible structure to encode structured and equation type parameter models with any number of variability levels and covariates.
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- **Structural Model** – prediction PK, PD or disease models can be formulated here as ODE, DDE or algebraic equations.
- **Observation Model** – model for continuous or discrete data models.

Trial Design

Specifies explicitly the structure of a clinical study, used for optimal design and simulations, as an alternative to a design sourced from a database.

Modeling Steps

The specification of how a mathematical model and the associated trial design can be used, e.g., for simulation, estimation or optimal design tasks.

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