esqlabsR.report.template

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1 Notes

> ℹ️ **Note**
>
> This report has been created by running the simulations.

> ⚠️ **Warning**
>
> `setTestParameters` is set to `TRUE` !

2 Introduction

This document describes the qualification of a published paroxetine physiologically-based pharmacokinetics (PBPK) model for use with the Open Systems Pharmacology Software (OSPS) Version 11.2.

The PBPK model has been developed with OSPS version 10 and published by [@rudesheimPhysiologicallyBasedPharmacokinetic2022]. Model snapshot was downloaded on 21.07.2023 from the model repository. As of 21.07.2023, no model version qualified for OSP version 11.2 is publicly available.

3 Methods

3.1 Software

The qualification is performed with OSPS version 11.2.142.

3.2 Qualification process

1. Import project snapshot "paroxetine-model.json" in PK-Sim v11.2.

2. The snapshot contains 33 simulations. All simulations were exported to `*.pkml` for simulation in R.

3. All observed data from the project created with version 11.2 were exported `*.pkml` for loading in R.

4. Simulations were simulated in R and the results visually compared to the results reported in the original publication.

3.3 Data

3.4 Model consolidation

During conversion of projects created with versions before 11, a separate expression profile is created for each individual. To ensure that all individuals are using the same expression, expression profiles of the same protein were compared. All expression profiles for the same protein were equal. Therefore, the same expression profile was set in every individual, and the remaining profiles were removed.

4 Results

Comparison of time-concentration profiles with observed data are presented in the following:

5 Conclusion

All simulations that are available in the snapshot produced the same results as in the original publication (by visual comparison). Not all reported simulations are implemented in the snapshot, their comparison was not possible. It is, however, assumed that the model behaves exactly as described in the original publication.