

The R packages Ecosystem of the Open Systems Pharmacology

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Introduction

The Open Systems Pharmacology (OSP) platform is supported by an ecosystem of R packages that combine into a framework for reproducible, quality-controlled, and standardized PBPK/QSP modeling and simulation (M&S) projects, while minimizing error probability coming from maintaining complex R code.

Methods

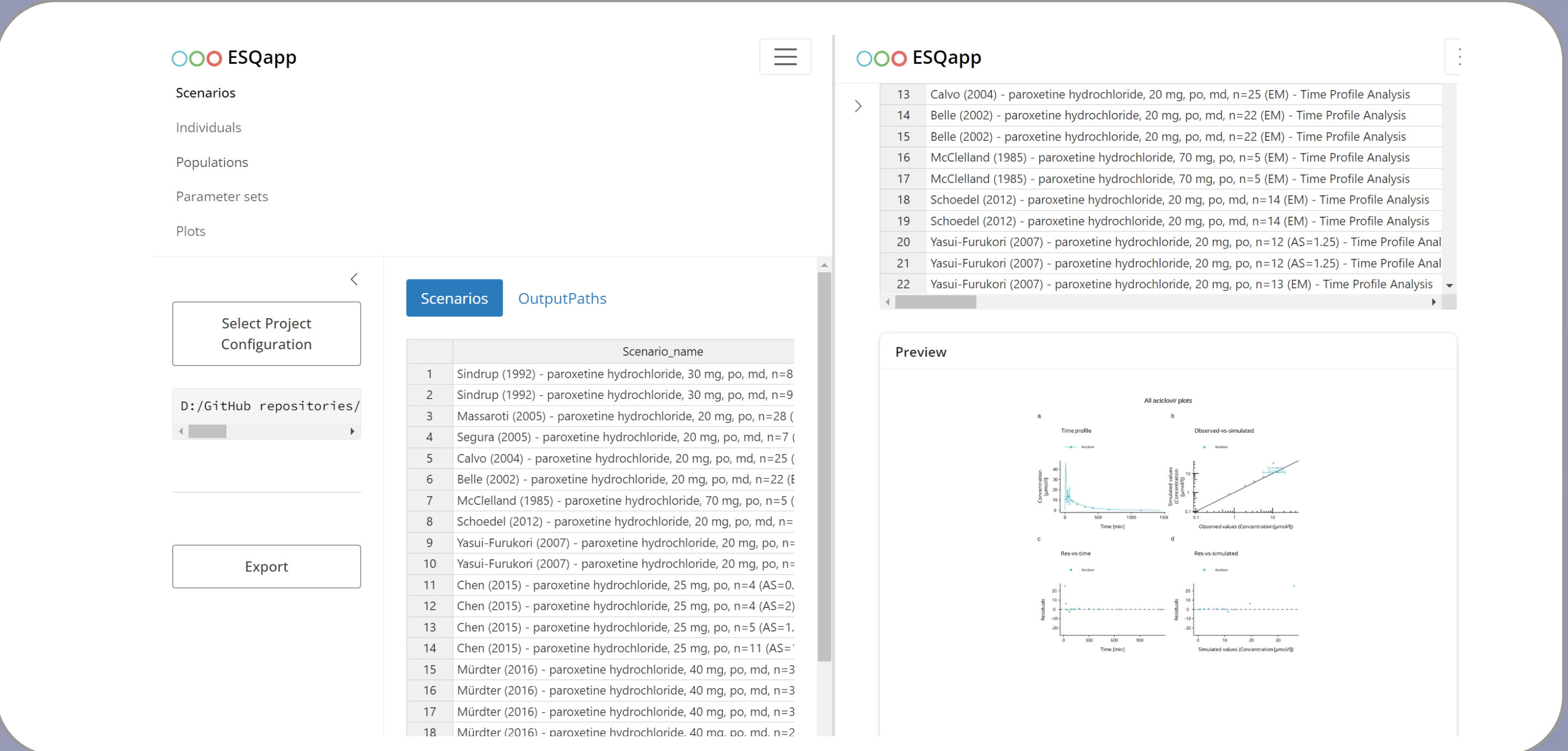
All packages are being developed according to the established best practices for software development. These include automated **testing**, thorough **code reviews**, continuous integration and deployment (CI/CD), and **documentation**. All packages are freely available on GitHub, and contributions by community members are highly encouraged. Comprehensive **Collaboration Guideline** and **Coding Standards** have been written to support new contributors and ensure high quality of the developed products.

Collaboration Guide

Coding Standards

OSP Packages

- {ospsuite}** - loading, manipulating, and running the simulations created in the tools PK-Sim and MoBi, calculating PK-Parameters, Sensitivity Analysis, and Plotting
- {ospsuite.parameteridentification}** - estimation of model parameter values by fitting the OSP simulations to observed data
- {esqlabsR}** – framework for standardized M&S workflows, with advanced scenario definition, sensitivity analysis, and report generation
- {ESQapp}** – GUI for {esqlabsR} projects
- {ospsuite.reportingframework}** – advanced report generation using {esqlabsR}
- {ospsuite.globalsensitivity}** – Global Sensitivity Analysis for OSP models
- {ospsuite.vbe-toolbox}** – set of tools for Virtual Bioequivalence
- {ospsuite.BMLM}** - Bayesian Multi-Level Modeling parameter identification



Graphical user interface of the **ESQapp** – a ShinyApp for setting up simulation scenarios, figures, and interactive plot preview.

Outlook

Version 12 of the OSP Software brings a modularization concept to the development of complex PBPK-QSP models. In version 13, the functionalities of the OSP R packages will be extended to load MoBi projects and create simulations from combinations of modules. This will further unlock the benefits of the modularization concept and allow an automated re-qualification process for MoBi projects. The new functionalities will be fully supported by {esqlabsR}, enabling more flexible and performance-oriented workflows.

User-friendly and Quality-Controlled PBPK/QSP M&S workflows for Regulatory Submissions

MIDD Ecosystem Management

The R frameworks play a central role in developing a comprehensive Ecosystem for Model-Informed Drug Development (MIDD).

Supporting R packages

A number of supporting R packages are used by the core user-oriented packages:

- {rSharp}** – Interface between R and .NET
- {ospsuite.plots}** – standard figure generation used in {ospsuite} and the reporting workflows
- {ospsuite.reportingengine}** – framework for automated generation of validation and qualification reports for the OSP Model Database

Modeling

Coding

Supporting the open-source development of:
 OPEN SYSTEMS PHARMACOLOGY Software Suite
www.Open-Systems-Pharmacology.org