OSP 2026
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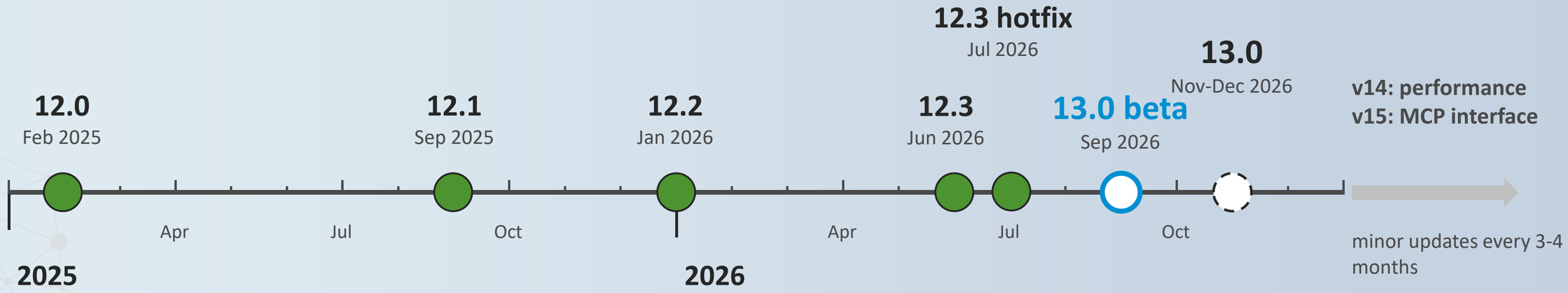
OSP Software Roadmap

Pavel Balazki
ESQlabs GmbH



Release history

Where we stand



Public beta at this conference
Final release 1-2 months later

OPEN SYSTEMS PHARMACOLOGY

Since Paris

Everything we announced for v13 is in v13

Announced here last year, and in the v13 beta today

- Automated **re-qualification** of MoBi projects, via the MoBi CLI and QualificationRunner
- **MoBi.R** - MoBi workflows scripted from R
- Refined **oral absorption** model, including a refined intestinal solubility model
- **Modularization**: "Extend" now genuinely differs from "Overwrite" across building blocks
- **Events** inside PK-Sim administration protocols
- Compound **Overwrite Parameter Sets** - announced last year as the Simulation Parameters building block

One thing slipped: the date.

Announced for H1 2026. Public beta September 2026, final release one to two months later.

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OSP Release strategy

One major release per year

- Major improvements
- New model features and components
- Structural model changes

Minor updates every 3-4 months

- Usability improvements
- Bug fixes
- No changes to model behavior

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V13

Latest major release

V13

Public beta today - five highlights

1. Refined oral absorption model - the PBBM workflow inside PK-Sim
2. Compound Overwrite Parameter Sets
3. Events in administration protocols
4. MoBi command-line interface and R interface
5. Refined module merge behavior - and the main breaking change

Public beta for testing from today. Final release follows in one to two months.

Documentation is live: docs.open-systems-pharmacology.org/v13 What is new: .../v13/news

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Oral absorption

PK-Sim upgrade featuring an updated human GI tract and the new dissolution model for enhanced PBBK capabilities

- Physiological bile salt concentrations in the intestinal lumen
- Population variability in luminal pH across all GI tract segments
- Stomach pH as a function of hydrogen dilution due to water intake
- Integration of micellar solubilization
- Differentiation between the release kinetics of free and micelle-bound drug
- Refined particles dissolution model

Continues in 13.1 or 14: stomach emptying, further release kinetics, reusable administrations.

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V13

Modules, compounds, protocols

"Extend" and "Overwrite" now genuinely differ

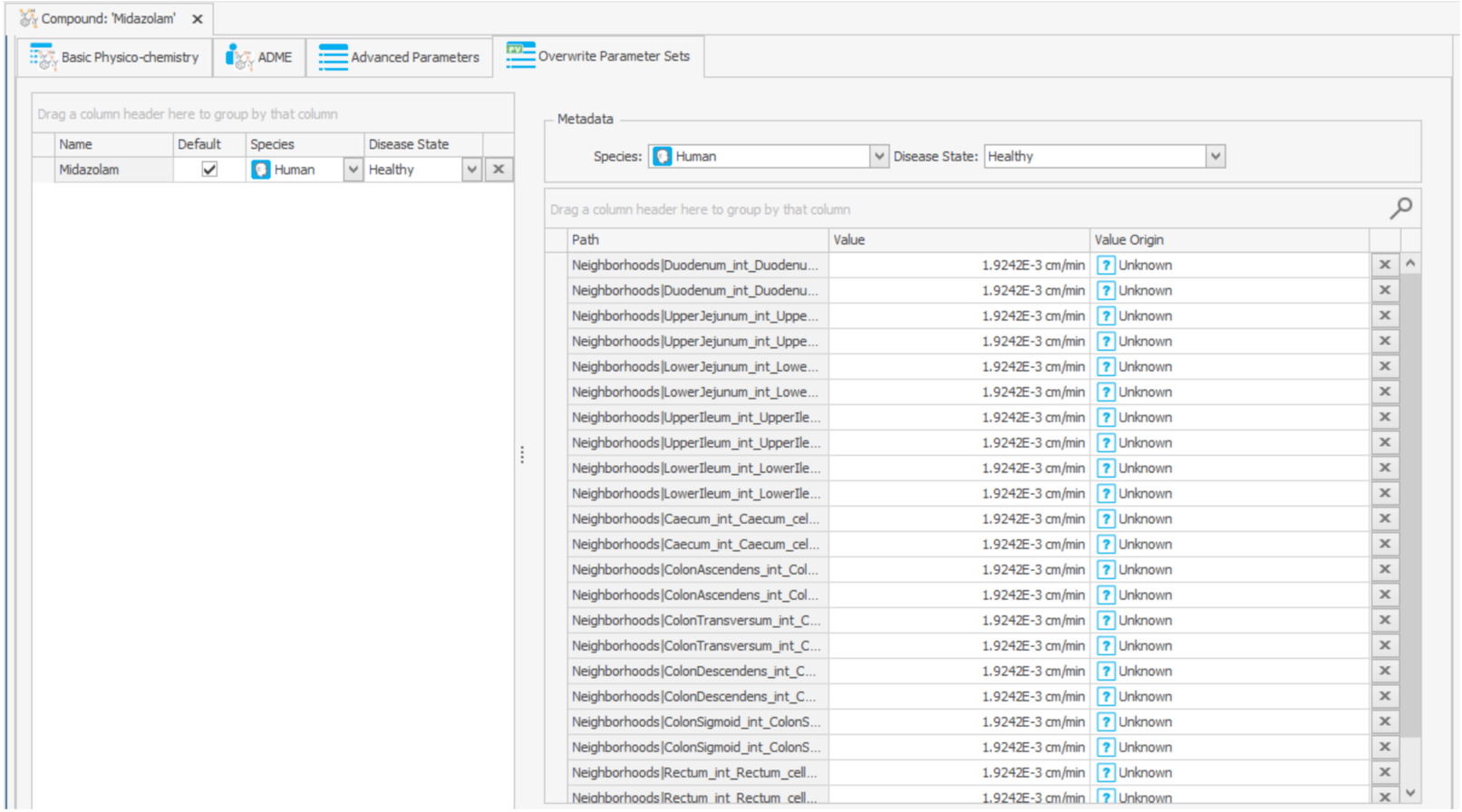
- Molecules, Reactions, Passive Transports, Observers, Events and MoleculeProperties
- New v13 modules default to "Extend"; modules from v12 keep "Overwrite"
- A later module can remove a neighborhood by redefining it without neighbors

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V13

Compound Overwrite Parameter Sets

– Named sets of compound-dependent overrides, committed from a simulation back to the Compound and re-applied elsewhere

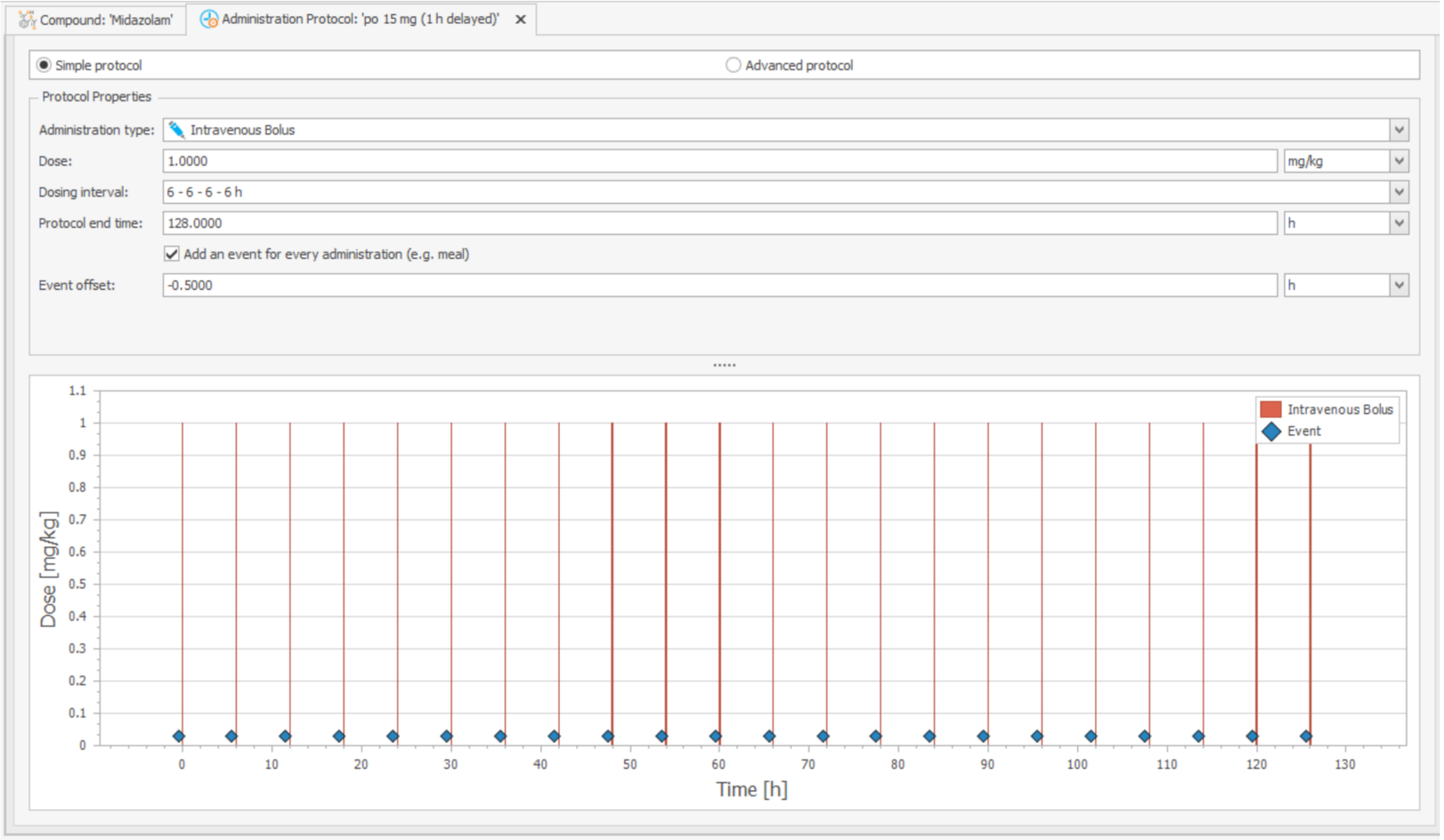


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V13

Events in administration protocols

– Defined directly in the PK-Sim protocol schema, with repetition and a timeline view



MoBi without the GUI

Command-line and R interface to MoBi, both new in v13

What you can now additionally script

- Batch conversion of snapshots
- Qualification runs without opening MoBi
- Loading MoBi projects, building simulations from modules
- Individuals, expression profiles, parameters, initial conditions

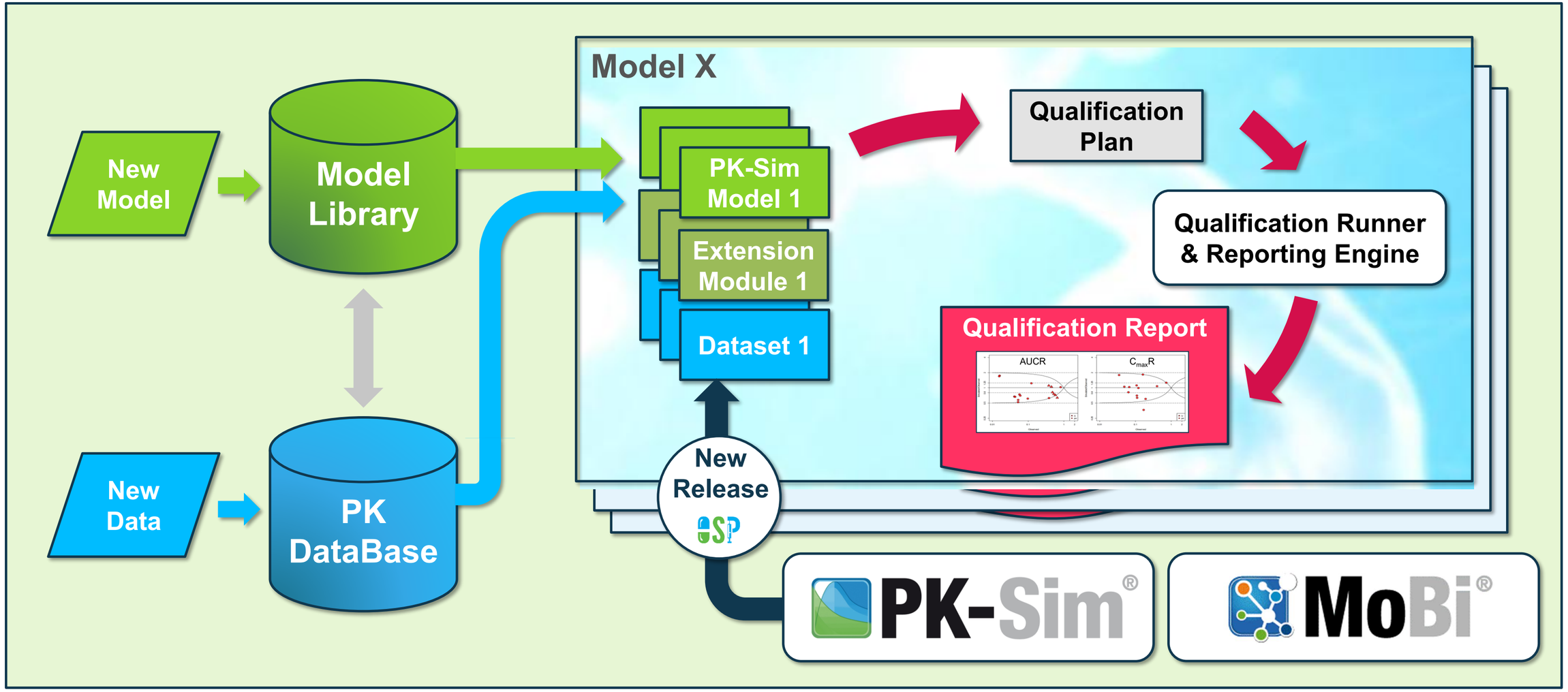




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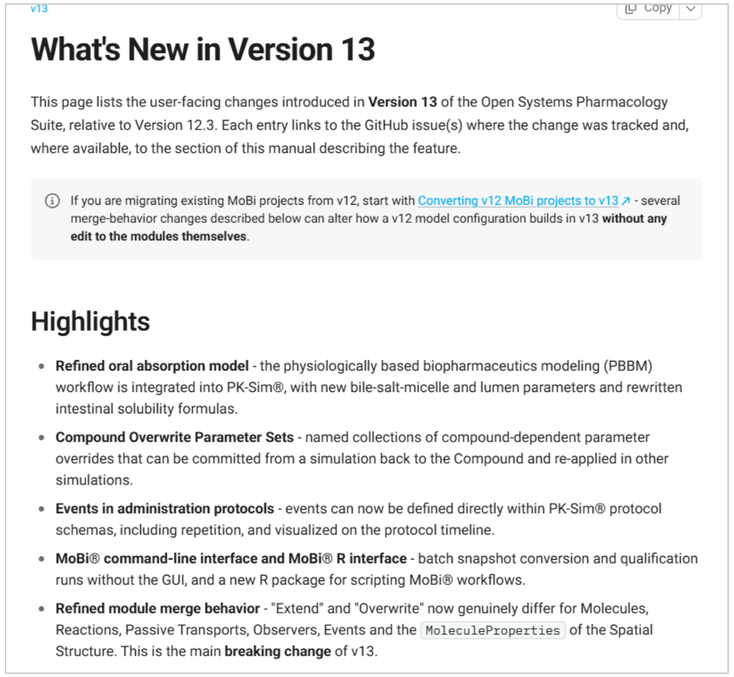
Automated re-qualification

QualificationRunner now covers MoBi projects



V13

Read this before you open a v12 project in v13



v13

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What's New in Version 13

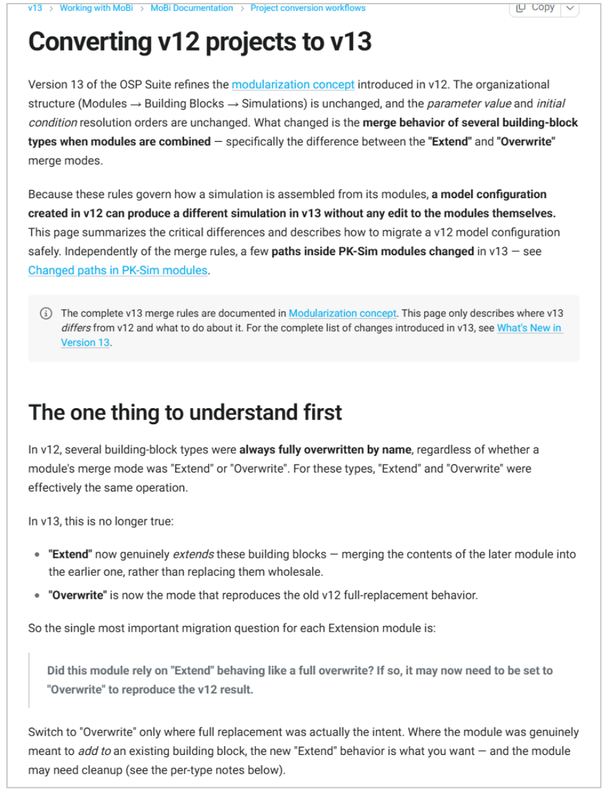
This page lists the user-facing changes introduced in **Version 13** of the Open Systems Pharmacology Suite, relative to Version 12.3. Each entry links to the GitHub issue(s) where the change was tracked and, where available, to the section of this manual describing the feature.

If you are migrating existing MoBi projects from v12, start with Converting v12 MoBi projects to v13 ↗ - several merge-behavior changes described below can alter how a v12 model configuration builds in v13 **without any edit to the modules themselves**.

Highlights

- **Refined oral absorption model** - the physiologically based biopharmaceutics modeling (PBBM) workflow is integrated into PK-Sim®, with new bile-salt-micelle and lumen parameters and rewritten intestinal solubility formulas.
- **Compound Overwrite Parameter Sets** - named collections of compound-dependent parameter overrides that can be committed from a simulation back to the Compound and re-applied in other simulations.
- **Events in administration protocols** - events can now be defined directly within PK-Sim® protocol schemas, including repetition, and visualized on the protocol timeline.
- **MoBi® command-line interface and MoBi® R interface** - batch snapshot conversion and qualification runs without the GUI, and a new R package for scripting MoBi® workflows.
- **Refined module merge behavior** - "Extend" and "Overwrite" now genuinely differ for Molecules, Reactions, Passive Transports, Observers, Events and the `MoleculeProperties` of the Spatial Structure. This is the main **breaking change** of v13.

What is new in Version 13
docs.open-systems-pharmacology.org/v13/news



v13 › Working with MoBi › MoBi Documentation › Project conversion workflows

Copy

Converting v12 projects to v13

Version 13 of the OSP Suite refines the modularization concept introduced in v12. The organizational structure (Modules → Building Blocks → Simulations) is unchanged, and the *parameter value* and *initial condition* resolution orders are unchanged. What changed is the **merge behavior of several building-block types when modules are combined** — specifically the difference between the **"Extend"** and **"Overwrite"** merge modes.

Because these rules govern how a simulation is assembled from its modules, **a model configuration created in v12 can produce a different simulation in v13 without any edit to the modules themselves.** This page summarizes the critical differences and describes how to migrate a v12 model configuration safely. Independently of the merge rules, a few **paths inside PK-Sim modules changed** in v13 — see Changed paths in PK-Sim modules.

The complete v13 merge rules are documented in Modularization concept. This page only describes where v13 *differs* from v12 and what to do about it. For the complete list of changes introduced in v13, see What's New in Version 13.

The one thing to understand first

In v12, several building-block types were **always fully overwritten by name**, regardless of whether a module's merge mode was "Extend" or "Overwrite". For these types, "Extend" and "Overwrite" were effectively the same operation.

In v13, this is no longer true:

- **"Extend"** now genuinely *extends* these building blocks — merging the contents of the later module into the earlier one, rather than replacing them wholesale.
- **"Overwrite"** is now the mode that reproduces the old v12 full-replacement behavior.

So the single most important migration question for each Extension module is:

> **Did this module rely on "Extend" behaving like a full overwrite? If so, it may now need to be set to "Overwrite" to reproduce the v12 result.**

Switch to "Overwrite" only where full replacement was actually the intent. Where the module was genuinely meant to *add to* an existing building block, the new "Extend" behavior is what you want — and the module may need cleanup (see the per-type notes below).

Converting v12 projects to v13
.../v13/working-with-mobi > project conversion workflows

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V13

Quality of life

PK-Sim

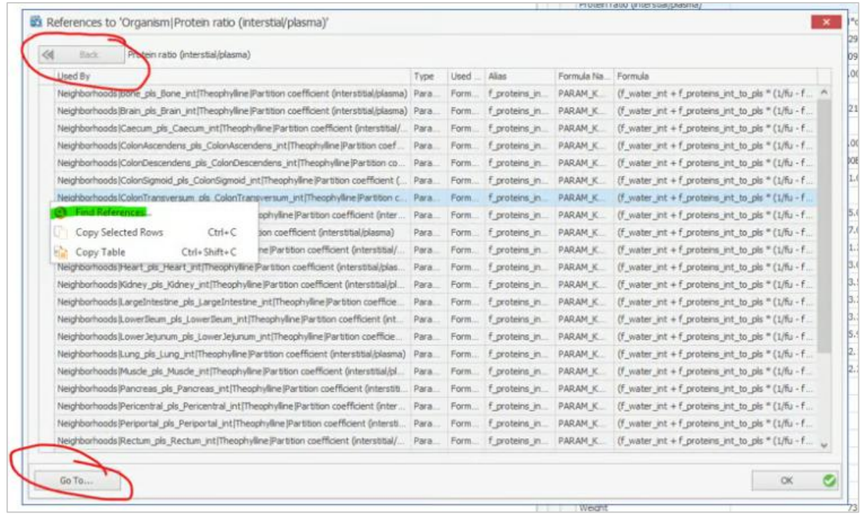
- Load building blocks from a snapshot into an existing project
- One administration protocol for several compounds
- Faster loading of snapshots (parallel simulation loading and execution)
- Subfolders for Building Blocks (UX)

MoBi

- Multiple analyses per simulation
- Find References lists every formula using a parameter
- Combined AND/OR container criteria
- Batch update of simulations from changed building blocks

Shared

- Charting: manual axis ticks, chart templates for non-time-profile curves, free line thickness
- Solver: NaN and infinity detected before the run starts
- Observed data: non-monotonic and duplicate x-values now accepted
- Option for Global Switching of CheckForNegativeValues on and off



Find References: every formula in the simulation that uses the selected parameter.

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V14 and V15

Planned releases

V14

Performance focus

Performance optimization of the simulation engine.

- **Numerics**
  - Sparse linear algebra
  - (Better) utilization of advanced ODE-Solver features
  - (Better) Event/discontinuity handling / Root finding
  - Faster sensitivity calculations
- **The structure of the model itself**
- **GPU-Utilization / Parallelization of single simulation run**
- **“Compiled models”**
  - Models translated to C++ code and compiled as native model libraries – accessible via R interface

The goal is the same results in a fraction of the runtime.

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V14

More topics

Further improvements of the Oral Absorption model (stomach emptying, further release kinetics, performance improvements)

R Interface to C++ compiled models

Flexible events and administrations in MoBi

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V15

An MCP interface for PK-Sim and MoBi

Agents are becoming how scientists drive their tools. The plan for v15: make PK-Sim and MoBi callable by them.

What an MCP interface unlocks

- An MCP-capable assistant builds, runs, and inspects a model through the same interface you use from R or any other scripting language
- Workflows ***scripted*** by agents - and therefore reproducible, reviewable, re-qualifiable

Medium priority: new populations (Chinese, obese).

Not yet scheduled. Sponsorship decides what gets built, and in which order.

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Where the roadmap is tracked

Issues, bug reports, and feature request are grouped by topics – as “Projects”

Delivery per release

v13

v13.1

v14

Intake and triage

OSP Suite Software Roadmap

Quick Gain

Modeling science

Oral absorption

IVIVE

Protein expression

PK parameters

Numerics

SBML import/export

Tooling and workflow

User Experience

MoBi: Modeling

Events Redesign in MoBi

MoBi ReQualification

Parameter Identification

Sensitivity Calculation

Data Importer

R packages

R: MoBi.R vNext

R: Observed data (mapping)

R: Plotting

R: Sensitivity Analysis

Every board carries a one-line scope description saying exactly what belongs on it.
github.com/orgs/Open-Systems-Pharmacology/projects

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BAYER

DESIGN{2}CODE

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we empower life sciences

ACKNOWLEDGMENTS

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THE COMMUNITY (YOU)

THANK YOU



Photo: Grote Markt, Antwerp, Belgium

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