# Open Systems Pharmacology Suite - 12 Folder Comparison

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# Contents

1	Folder Comparison Results	2
	1.1 Comparison Results	2
	1.1.1 Invalid Simulations $(2/155)$	2
	1.1.2 Valid Simulations (153/155)	6

## Chapter 1

# Folder Comparison Results

Overall Comparison Result: Invalid Number of Compared Files: 155

### 1.1 Comparison Results

Overall Comparison Result

Invalid

Old Folder

 $D: \backslash Outputs\_11.3$ 

New Folder

D:\Outputs\_12.0

### 1.1.1 Invalid Simulations (2/155)

 $Simulation: \ Human\_Oral\_BiDaily\_TableFormulation-S2\_NoSuspension$ 

Result of the validation: Invalid Absolute Tolerance: 1.00E-10 Relative Tolerance: 1.00E-5

### Output Path: Organism|Lumen|LowerIleum|C1|Concentration in lumen

Deviation for 'Organism|Lumen|LowerIleum|C1|Concentration in lumen' is 33.86% and is greater than the al-

lowed max. tolerance of 3.00%

Deviation: 0.34

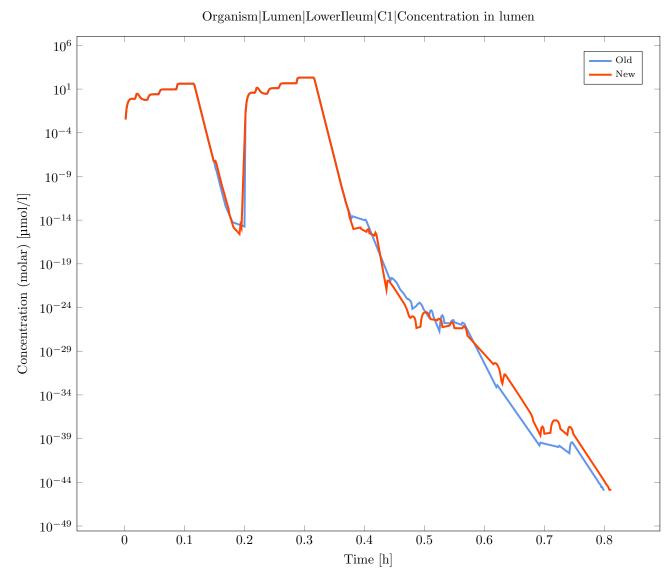


Figure 1.1

## Organism|Lumen|LowerIleum|C1|Concentration in lumen 220 OldNew 200 180 160 Concentration (molar) [µmol/l] 140 120 100 80 6040 20 0 0.1 0.2 0.3 0.4 0.50.6 0.7 0.8 0.9 1.1 1.2 1.3 -0.1Time [h]

### Figure 1.2

 $Simulation: \ Human\_SingleORAL\_Weibull-Human\_SingleORAL\_Weibull\_MW\_200\_fu\_0.2\_LogP\_5$ 

Result of the validation: Invalid Absolute Tolerance: 1.00E-10 Relative Tolerance: 1.00E-5

#### Output Path: Organism |Lumen |LowerJejunum |drug |Fraction of oral drug mass absorbed into mucosa segment

Deviation for 'Organism | Lumen | Lower Jejunum | drug | Fraction of oral drug mass absorbed into mucosa segment' is 120.45% and is greater than the allowed max. tolerance of 3.00%

Deviation: 1.20

 $Organism | Lumen | Lower Jejunum | drug | Fraction \ of \ oral \ drug \ mass \ absorbed \ into \ mucosa \ segment$ 

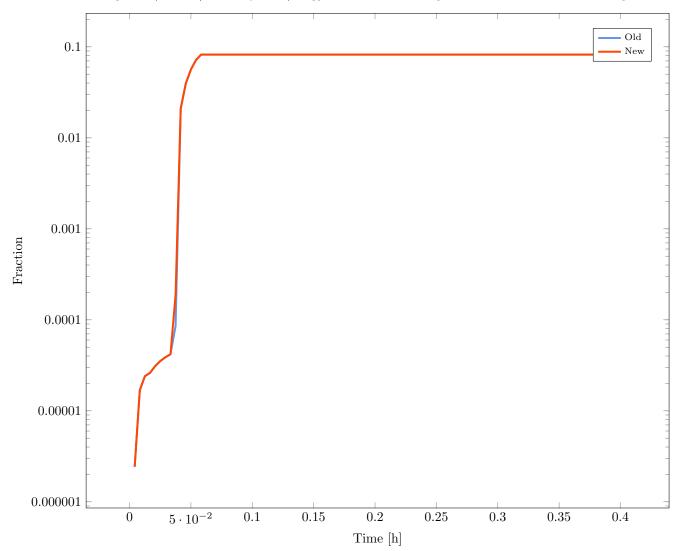
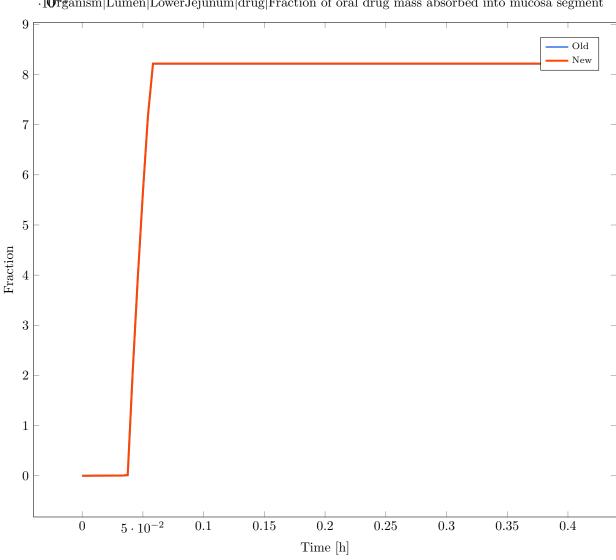


Figure 1.3



·10rganism|Lumen|LowerJejunum|drug|Fraction of oral drug mass absorbed into mucosa segment

Figure 1.4

#### Valid Simulations (153/155) 1.1.2

 $Simulation: \ Beagle\_SingleORAL\_Dissolved-Beagle\_SingleORAL\_Dissolved$ 

Result of the validation: Valid

 $Simulation: Beagle\_SingleORAL\_Dissolved\_Beagle\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-INFIGURE AND SIMULATION FOR SIMULATI$ 

Result of the validation: Valid

 $Simulation: Beagle\_SingleORAL\_Dissolved\_Beagle\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-fu\_0.6$ 

Simulation: DDI\_MultipleCombinations-01\_MM\_Competitive\_Competitive

Result of the validation: Valid

Simulation: DDI\_MultipleCombinations-02\_MM\_Uncompetitive\_Uncompetitive

Result of the validation: Valid

Simulation: DDI\_MultipleCombinations-03\_MM\_Noncompetitive\_Noncompetitive

Result of the validation: Valid

Simulation: DDI\_MultipleCombinations-04\_MM\_Mixed\_Mixed

Result of the validation: Valid

 $Simulation: \ DDI\_Multiple Combinations-05\_MM\_Mechanism based\_Mechanism based$ 

Result of the validation: Valid

 $Simulation: \ DDI\_Multiple Combinations-06\_MM\_Induction\_Induction$ 

Result of the validation: Valid

 $Simulation: DDI\_MultipleCombinations-07\_MM\_Competitive\_Competitive\_Mechanism based\_Mechanism based\_Mechanism$ 

Result of the validation: Valid

 $Simulation: \ DDI\_Multiple Combinations - 08\_MM\_Uncompetitive\_Uncompetitive\_Mechanism based\_-incompetitive\_Mechanism based\_-incompetitive\_-incom$ 

 ${\bf Mechanism based}$ 

Result of the validation: Valid

 $Simulation: \ DDI\_Multiple Combinations - 09\_MM\_Noncompetitive\_Noncompetitive\_Mechanism based\_-like and the property of the$ 

Mechanismbased

Result of the validation: Valid

 $Simulation: DDI\_MultipleCombinations-10\_MM\_Mixed\_Mechanismbased\_Mechanismbased$ 

Result of the validation: Valid

Induction

Result of the validation: Valid

Simulation: DDI\_MultipleCombinations-12\_MM\_All\_DDI\_Types

Result of the validation: Valid

Simulation: DDI\_MultipleCombinations-21\_1st\_Competitive\_Competitive

 $Simulation: \ DDI\_Multiple Combinations \textbf{-23\_1st\_Noncompetitive\_Noncompetitive}$ 

Result of the validation: Valid

 $Simulation: \ DDI\_MultipleCombinations-24\_1st\_Mixed\_Mixed$ 

Result of the validation: Valid

Simulation: DDI\_MultipleCombinations-25\_1st\_Mechanismbased\_Mechanismbased

Result of the validation: Valid

 $Simulation: \ DDI\_MultipleCombinations-26\_1st\_Induction\_Induction$ 

Result of the validation: Valid

 $Simulation: DDI\_Multiple Combinations \textbf{-} 27\_1 st\_Competitive\_Competitive\_Mechanism based\_Mechanism based\_M$ 

Result of the validation: Valid

 $Simulation: DDI\_Multiple Combinations - 28\_1st\_Uncompetitive\_Uncompetitive\_Mechanism based\_-like the competitive of the compe$ 

Mechanismbased

Result of the validation: Valid

 $Simulation: DDI\_Multiple Combinations - 29\_1st\_Noncompetitive\_Noncompetitive\_Mechanism based\_-1st\_Noncompetitive\_Noncompetit$ 

 ${\bf Mechanism based}$ 

Result of the validation: Valid

Simulation: DDI\_MultipleCombinations-30\_1st\_Mixed\_Mixed\_Mechanismbased\_Mechanismbased

Result of the validation: Valid

 $Simulation: \ DDI\_Multiple Combinations - 31\_1st\_Mechanism based\_Mechanism based\_Induction\_Induction$ 

Result of the validation: Valid

 $Simulation: \ DDI\_Multiple Combinations - 32\_1st\_All\_DDI\_Types$ 

Result of the validation: Valid

 $Simulation: \ Dog\_MultiORAL\_12\_12\_Dissolved-Dog\_MultiORAL\_12\_Dissolved-Dog\_MultiORAL_12\_Dissolved-Dog\_MultiORAL_12\_Dissolved-Dog\_MultiORAL_12\_Dissolved-Dog\_MultiORAL_12\_Dissolved-Dog\_MultiORAL_12\_Dissolved-Dog\_MultiORAL_12\_Dissolved-Dog\_MultiORAL_12\_Dissolved-Dog\_MultiORAL_12\_Dissol$ 

Result of the validation: Valid

 $Simulation: \ Dog\_MultiORAL\_24\_Dissolved-Dog\_MultiORAL\_24\_Dissolved$ 

Result of the validation: Valid

 $Simulation: European\_SingleORAL\_Age\_0\_CYP3A4-European\_SingleORAL_Age\_0\_CYP3A4-European\_SingleORAL_Age\_0\_CYP3A4-European\_SingleORAL_Age\_0\_CYP3A4-European\_SingleORAL_Age\_0\_CYP3A4-European\_SingleORAL_Age\_0\_CYP3A4-European\_SingleORAL$ 

Simulation: European\_SingleORAL\_Age\_0\_GFR-European\_SingleORAL\_Age\_0\_GFR

Result of the validation: Valid

 $Simulation: European\_SingleORAL\_Age\_1\_CYP3A4-European\_SingleORAL\_Age\_1\_CYP3A4$ 

Result of the validation: Valid

 $Simulation: European\_SingleORAL\_Age\_1\_GFR-European\_SingleORAL\_Age\_1\_GFR$ 

Result of the validation: Valid

Simulation: Human\_CompetitiveInhibition-Human\_CompetitiveInhibition

Result of the validation: Valid

 $Simulation: \ Human\_ICRP\_AGP-01\_ICRP\_0y\_Male$ 

Result of the validation: Valid

Simulation: Human\_ICRP\_AGP-02\_ICRP\_0.05y\_Female

Result of the validation: Valid

 $Simulation: \ Human\_ICRP\_AGP-03\_ICRP\_0.18y\_Male$ 

Result of the validation: Valid

 $Simulation: \ Human\_ICRP\_AGP-04\_ICRP\_1y\_Female$ 

Result of the validation: Valid

Simulation: Human\_ICRP\_AGP-05\_ICRP\_12y\_Male

Result of the validation: Valid

Simulation: Human\_ICRP\_AGP-06\_ICRP\_30y\_Female

Result of the validation: Valid

 $Simulation: \ Human\_ICRP\_AGP-07\_ICRP\_100y\_Male$ 

Result of the validation: Valid

 ${\bf Simulation: \ Human\_Irreversible Inhibition-Human\_Irreversible Inhibition}$ 

Result of the validation: Valid

 $Simulation: \ Human\_MixedInhibition-Human\_MixedInhibition$ 

Result of the validation: Valid

 $Simulation: \ Human\_MultiIV\_6\_6\_12-Human\_MultiIV\_6\_6\_12$ 

Simulation: Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved

Result of the validation: Valid

 $Simulation: Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved\_absorption\_-touching the control of the cont$ 

 $sink\_conditions$ 

Result of the validation: Valid

 $Simulation: Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved\_EHC\_-IVAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_Dissolved-Human\_MultiORAL\_6\_12\_Dissolved-Human\_MultiORAL\_6\_12\_Dissolved-Human\_MultiORAL\_6\_12\_Dissolved-Human\_MultiORAL\_6\_12\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_MultiORAL\_6\_Dissolved-Human\_6\_Dissolv$ 

continuous\_fraction\_0.5
Result of the validation: Valid

 $Simulation: \ Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved\_EHC\_-12\_1$ 

 $continuous\_fraction\_1$ 

Result of the validation: Valid

 $Simulation: Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved\_pKandle (Application) and the property of th$ 

**dependent penalty factor**Result of the validation: Valid

 $Simulation: Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved\_solubility$ 

Result of the validation: Valid

Simulation: Human\_MultipleIV\_Binding-Human\_MultipleIV\_Binding

Result of the validation: Valid

 $Simulation: \ Human\_Multiple IV\_Efflux Basolateral-Human\_Multiple IV\_Efflux Basolat$ 

Result of the validation: Valid

 $Simulation: \ Human\_MultipleIV\_Efflux-Human\_MultipleIV\_Efflux$ 

Result of the validation: Valid

 $Simulation: \ Human\_MultipleIV\_InfluxBasolateral-Human\_MultipleIV\_InfluxBasolateral$ 

Result of the validation: Valid

 $Simulation: \ Human\_MultipleIV\_Influx-Human\_MultipleIV\_ActiveInflux$ 

Result of the validation: Valid

Simulation: Human\_MultipleIV\_MetabolizmBinding-Human\_MultipleIV\_MetabolizmBinding

Result of the validation: Valid

Simulation: Human\_MultipleIV\_Metabolizm-Human\_MultipleIV\_Metabolizm

Simulation: Human\_MultipleIV\_PGPBasolateral-Human\_MultipleIV\_PGPBasolateral

Result of the validation: Valid

Simulation: Human\_MultipleIV\_PGP-Human\_MultipleIV\_PGP

Result of the validation: Valid

Simulation: Human\_NonCompetitiveInhibition-Human\_NonCompetitiveInhibition

Result of the validation: Valid

Simulation: Human\_Oral\_BiDaily\_TableFormulation-S1\_suspension

Result of the validation: Valid

Simulation: Human\_pH\_SolubilityTable-S1\_Table

Result of the validation: Valid

 $Simulation: \ Human\_pH\_SolubilityTable-S2\_Measurement$ 

Result of the validation: Valid

Simulation: Human\_pH\_SolubilityTable-S3\_Table\_SolubilityChanged

Result of the validation: Valid

 $Simulation: \ Human\_pH\_SolubilityTable\_Sd\_Table\_SolubilityTableChanged$ 

Result of the validation: Valid

Simulation: Human\_SingleIV\_Configuration-Human\_SingleIV\_Configuration

Result of the validation: Valid

Simulation: Human\_SingleIV-Human\_SingleIV

Result of the validation: Valid

Simulation: Human\_SingleIV-Human\_SingleIV\_MW\_200\_fu\_0.2\_LogP\_5

Result of the validation: Valid

 $Simulation: \ Human\_SingleIV-Human\_SingleIV\_MW\_800\_fu\_0.6\_LogP\_-5$ 

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_Singl$ 

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_Singl$ 

 $MW_200_fu_0.2_LogP_5$ Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_SingleORAL_Dissolved\_PlasmaClearance-Human\_Singl$ 

Result of the validation: Valid

Simulation: Human\_SingleORAL\_Dissolved-Human\_SingleORAL\_Dissolved

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_Dissolved\_Human\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Installation: SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Installation: SingleORAL_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Installation: SingleORAL_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Installation: SingleORAL_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Installation: SingleORAL_Dissolve$ 

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Result of the validation: Valid

 $Simulation: \ Human\_SingleORAL\_Dissolved\_Human\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-logP\_-$ 

-5

Result of the validation: Valid

Simulation: Human\_SingleORAL\_Lint80\_AsSuspention-Human\_SingleORAL\_Lint80\_AsSuspention

Result of the validation: Valid

Simulation: Human\_SingleORAL\_Lint80-Human\_SingleORAL\_Lint80

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_MonoParticles\_AsSuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_SingleORAL\_MonoParticles\_Assuspention-Human\_Si$ 

AsSuspention

Result of the validation: Valid

 $Simulation: \ Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesLogNormal\_Assuspention-Human\_SingleORAL$ 

 $PolyParticlesLogNormal\_AsSuspention$ 

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesNormal\_SingleORAL\_PolyParticlesNormal\_SingleORAL\_PolyParticlesNormal\_SingleORAL\_PolyParticlesNormal\_SingleORAL\_PolyParticlesNormal\_SingleORAL\_PolyParticlesNormal\_SingleORAL\_PolyParticlesNormal\_SingleORAL\_PolyParticlesNormal\_SingleORAL\_Single$ 

**AsSuspention** 

Result of the validation: Valid

Simulation: Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesNorm

 ${\bf As Suspention\_dissolved\_radius}$ 

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_AsSuspention-Human\_SingleORAL\_PolyParticlesNormal\_Assuspention-Human\_SingleORAL\_PolyParticlesNo$ 

 $As Suspention\_treat\_precipated\_drug\_as\_soluble$ 

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_Weibull\_AsSuspention-Human\_SingleORAL\_Weibull\_AsSuspention$ 

 $Simulation: Human\_SingleORAL\_Weibull\_AsSuspention-Human\_SingleORAL\_Weibull\_AsSuspention\_MW\_200\_fu\_0.2\_LogP\_5$ 

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_Weibull\_AsSuspention-Human\_SingleORAL\_Weibull\_AsSuspention\_-Incomplete the control of the contr$ 

MW\_800\_fu\_0.6\_LogP\_-5
Result of the validation: Valid

Simulation: Human\_SingleORAL\_Weibull-Human\_SingleORAL\_Weibull

Result of the validation: Valid

 $Simulation: \ Human\_SingleORAL\_Weibull-Human\_SingleORAL\_Weibull\_MW\_800\_fu\_0.6\_LogP\_-logP$ 

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Result of the validation: Valid

Simulation: Human\_UncompetitiveInhibition-Human\_UncompetitiveInhibition

Result of the validation: Valid

Simulation: Minipig\_SingleORAL\_Dissolved-Minipig\_SingleORAL\_Dissolved

Result of the validation: Valid

Simulation: Minipig\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-

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Result of the validation: Valid

Simulation: Minipig\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-

-5

Result of the validation: Valid

Simulation: Monkey\_SingleORAL\_Dissolved-Monkey\_SingleORAL\_Dissolved

Result of the validation: Valid

 $Simulation: Monkey\_SingleORAL\_Dissolved\_Monkey\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-logP\_-$ 

 $\mathbf{5}$ 

Result of the validation: Valid

Simulation: Monkey\_SingleORAL\_Dissolved-Monkey\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-

-5

Result of the validation: Valid

 $Simulation: \ Mouse\_SingleORAL\_Dissolved-Mouse\_SingleORAL\_Dissolved$ 

 $Simulation: Mouse\_SingleORAL\_Dissolved\_Mouse\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Lo$ 

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Result of the validation: Valid

 $Simulation: Mouse\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-logP\_$ 

-5

Result of the validation: Valid

Simulation: Preterm\_SingleIV\_Age\_0\_GA\_32\_CYP3A4-Preterm\_SingleIV\_Age\_0\_GA\_32\_CYP3A4

Result of the validation: Valid

Result of the validation: Valid

 $Simulation: Preterm\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGA\_32\_CYP3A4-PreterM\_SingleIV\_AGA\_32\_CYP3A4-PreterM\_SingleIV\_AGA\_32\_CYP3A4-PreterM\_SingleIV\_AGA\_32\_CYP3A4-PreterM\_SingleIV\_AGA\_32\_CYP3A4-PreterM\_SingleIV\_AGA\_32\_CYP3A4-PreterM\_SingleIV\_AGA_32\_CYP3A4-PreterM\_SingleIV\_AGA_32\_CYP3A4-PreterM\_SingleIV\_AGA_32\_CYP3A4-PreterM\_Single$ 

Result of the validation: Valid

 $Simulation: \ Preterm\_SingleIV\_Age\_15\_GA\_32\_GFR-Preterm\_SingleIV\_Age\_15\_GA\_32\_GFR$ 

Result of the validation: Valid

 $Simulation: Rabbit\_SingleORAL\_Dissolved-Rabbit\_SingleORAL\_Dissolved$ 

Result of the validation: Valid

 $Simulation: Rabbit\_SingleORAL\_Dissolved\_Rabbit\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Incomplete the control of the contro$ 

 $\mathbf{5}$ 

Result of the validation: Valid

 $Simulation: Rabbit\_SingleORAL\_Dissolved\_Rabbit\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-Rabbit\_SingleORAL\_Dissolved\_Rabbit\_SingleORALDissolved\_Rabbit\_SingleORALDissolved\_Rabbit\_SingleORALDissolved\_Rabbit\_SingleORALDissolved\_Rabbit\_SingleORALDissolved\_Rabbit\_SingleORALDissolved\_Rabbit\_SingleORALDissolved\_Rabbit\_SingleORALDissolved\_Rabb$ 

-5

Result of the validation: Valid

Result of the validation: Valid

 $Simulation: \ Rat\_MultiORAL\_6\_6\_6\_6\_Dissolved-Rat\_MultiORAL\_6\_6\_6\_6\_Dissolved-Rat\_MultiORAL\_6\_6\_6\_6\_Dissolved-Rat\_MultiORAL\_6\_6\_6\_0.$ 

Result of the validation: Valid

Simulation: Rat\_MultiORAL\_8\_8\_8\_Dissolved-Rat\_MultiORAL\_8\_8\_8\_Dissolved

Result of the validation: Valid

Simulation: SingleIV\_2Pores\_Human-SingleIV\_2Pores\_Human

Simulation: SingleIV\_2Pores\_Human-SingleIV\_2Pores\_Human\_SimulationC

Result of the validation: Valid

Simulation: SingleIV\_2Pores\_Human\_SimulationD

Result of the validation: Valid

Simulation: SingleIV\_2Pores\_Human-SingleIV\_2Pores\_Human\_SimulationF

Result of the validation: Valid

Simulation: SingleIV\_2Pores\_Monkey-SingleIV\_2Pores\_Monkey

Result of the validation: Valid

Simulation: SingleIV\_2Pores\_Monkey\_SingleIV\_2Pores\_Monkey\_SimulationG

Result of the validation: Valid

Simulation: SingleIV\_2Pores\_Monkey\_SingleIV\_2Pores\_Monkey\_SimulationH

Result of the validation: Valid

 $Simulation: Single IV\_2 Pores\_Mouse-Single IV\_2 Pores\_Mouse$ 

Result of the validation: Valid

Simulation: SingleIV\_2Pores\_Mouse\_SingleIV\_2Pores\_Mouse\_SimulationA

Result of the validation: Valid

Simulation: SingleIV\_2Pores\_Mouse-SingleIV\_2Pores\_Mouse\_SimulationB

Result of the validation: Valid

 $Simulation: Single IV\_2 Pores\_Mouse\_Single IV\_2 Pores\_Mouse\_Simulation E$ 

Result of the validation: Valid

 $Simulation: Single IV\_C1\_4 Comp\_standard\_stand$ 

standard

Result of the validation: Valid

 $Simulation: Single IV\_C2\_4 Comp\_PT\_standard\_st$ 

Result of the validation: Valid

 $Simulation: Single IV\_C2\_4 Comp\_RR\_standard\_st$ 

 $Simulation: Single IV\_C2\_4 Comp\_standard\_schmitt\_standard-Single IV\_C2\_4 Comp\_standard-Single IV\_C2\_4 Comp\_$ 

Result of the validation: Valid

 $Simulation: Single IV\_C3\_4 Comp\_RR\_schmitt\_standard-Single IV\_C3\_schmitt\_standard-Single IV\_schmitt\_standard-Single IV\_schmitt\_standard-Single$ 

Result of the validation: Valid

 $Simulation: Single IV\_C3\_4 Comp\_standard\_schmittnorm lized\_standard\_Single IV\_C3\_4 Comp\_standard\_schmittnorm lized\_standard\_schmittnorm lized\_schmittnorm lized\_schmittnorm$ 

 ${\bf schmittnormlized\_standard}$ 

Result of the validation: Valid

 $Simulation: Single IV\_C4\_2 Pores\_RR\_standard\_s$ 

Result of the validation: Valid

 $Simulation: Single IV\_C4\_4 Comp\_Ber\_standard\_s$ 

Result of the validation: Valid

 $Simulation: Single IV\_C5\_2 Pores\_Ber\_standard\_$ 

Result of the validation: Valid

 $Simulation: Single IV\_C5\_2 Pores\_PT\_standard\_standard\_Single IV\_C5\_2 Pores\_PT\_standard\_stan$ 

Result of the validation: Valid

 $Simulation: Single IV\_C5\_2 Pores\_RR\_schmitt\_standard-Single IV\_C5\_2 Pores\_schmitt\_standard-Single IV\_C5\_2 Pores\_schmitt\_schmitt_standard-Single IV\_C5\_2 Pores\_schmitt\_schmitt_schm$ 

Result of the validation: Valid

 $Simulation: Single IV\_C6\_2 Pores\_standard\_stan$ 

standard

Result of the validation: Valid

 $Simulation: Single IV\_C7\_2 Pores\_standard\_schmitt\_standard\_Single IV\_C7\_2 Pores\_standard\_schmitt\_schmitt_schmitt_schmittt\_schmitt_schmitt_schmitt_schmitt_schmittt_schmitt_schmitt_schmitt_schmitt_schmitt_schmitt_schmitt_schmitt_schmitt_schmitt_$ 

standard

Result of the validation: Valid

 $Simulation: Single IV\_C7\_4 Comp\_schmitt\_standard\_standard\_Single IV\_C7\_4 Comp\_schmitt\_standard\_stand$ 

 $\operatorname{standard}$ 

Result of the validation: Valid

 $Simulation: Single IV\_C8\_2 Pores\_standard\_schmittnormalized\_standard\_Single IV\_C8\_2 Pores\_standard\_schmittnormalized\_standard\_Single IV\_C8\_2 Pores\_standard\_schmittnormalized\_standard\_schmittnormalized\_standard\_schmittnormalized\_standard\_schmittnormalized\_standard\_schmittnormalized\_standard\_schmittnormalized\_standard\_schmittnormalize$ 

 $schmittnormalized\_standard$ 

 $Simulation: Single IV\_C9\_2 Pores\_schmitt\_standard\_standard\_Single IV\_C9\_2 Pores\_schmitt\_standard\_sta$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C10\_4 Comp\_PT\_standard\_standard\_Single ORAL\_C10\_4 Comp\_PT\_standard\_$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C11\_4 Comp\_schmitt\_standard\_standard\_Single ORAL\_C11\_4 Comp\_schmitt\_standard$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C11\_4 Comp\_standard\_st$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C12\_4 Comp\_standard\_schmitt\_standard-Single ORAL\_C12\_4 Comp\_standard\_schmitt\_standard\\$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C13\_2 Pores\_schmitt\_standard\_standard\_Single ORAL\_C13\_2 Pores\_schmitt\_standard\_standa$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C13\_4 Comp\_standard\_schmittnormalized\_standard\_Single ORAL\_C13\_4 Comp\_standard\_schmittnormalized\_standard$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C14\_2 Pores\_PT\_standard\_standard-Single ORAL\_C14\_2 Pores\_PT\_standard-Single ORAL\_C14\_2 Pores\_SINGARD-Single ORAL\_C14\_2 Pores\_SINGARD-SINGARD-Single ORAL\_C14\_2 Pores\_SINGARD-Single ORAL\_C14\_2 Pores\_SI$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C2\_2 Pores\_standard\_st$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C3\_2 Pores\_standard\_schmitt\_standard-Single ORAL\_C3\_2 Pores\_standard\_schmitt\_standard$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C4\_2 Pores\_standard\_schmittnormalized\_standard\_Single ORAL\_C4\_2 Pores\_standard\_schmittnormalized\_standard$ 

 $Simulation: Single ORAL\_C6\_4 Comp\_Ber\_standard\_standard\_Single ORAL\_C6\_4 Comp\_Ber\_standard\_$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C6\_4 Comp\_RR\_standard\_standard\_Single ORAL\_C6\_4 Comp\_RR\_standard\_st$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C7\_2 Pores\_Ber\_standard\_standard\_Single ORAL\_C7\_2 Pores\_Ber\_standard\_standar$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C7\_4 Comp\_RR\_schmitt\_standard-Single ORAL\_C7\_standard-Single ORAL\_C7\_standard-Sing$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C8\_2 Pores\_RR\_standard\_standard\_Single ORAL\_C8\_2 Pores\_RR\_standard\_$ 

Result of the validation: Valid

 $Simulation: Single ORAL\_C9\_2 Pores\_RR\_schmitt\_standard-Single ORAL\_C9\_2 Pores\_S_RR\_schmitt\_standard-Single ORAL\_C9\_2 Pores\_S_RR\_schmitt\_standard-Single$ 

Result of the validation: Valid

Simulation: Test  $18.1\_I1\_C1\_A1\_Config1$ -Test  $18.1\_I1\_C1\_A1\_Config1$ 

Result of the validation: Valid

Simulation: Test  $18.1\_I2\_C1\_A1\_Config2$ -Test  $18.1\_I2\_C1\_A1\_Config2$ 

Result of the validation: Valid

Simulation: Test 18.1\_I2\_C3\_A1\_Config2-Test 18.1\_I2\_C3\_A1\_Config2

Result of the validation: Valid

Simulation: Test 18.1\_I3\_C3\_A3\_Config2-Test 18.1\_I3\_C3\_A3\_Config2