### Open Systems Pharmacology Suite - 9 Folder Comparison

 ${\rm gibpk}$ 

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### Chapter 1

# Folder Comparison Results

Overall Comparison Result: Valid Number of Compared Files: 125

#### 1.1 Comparison Results

**Overall Comparison Result** 

Valid

Old Folder

D:\Outputs\_9.0

New Folder

D:\Outputs\_9.1

#### 1.1.1 Valid Simulations (125/125)

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

Result of the validation: Valid

 $Simulation: Beagle\_SingleORAL\_Dissolved\_Beagle\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Included to the control of the contr$ 

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Result of the validation: Valid

 $Simulation: Beagle\_SingleORAL\_Dissolved\_Beagle\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-Included to the property of the prop$ 

-5

Result of the validation: Valid

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

Result of the validation: Valid

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

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

Result of the validation: Valid

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

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

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

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

Result of the validation: Valid

 $Simulation: \ Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_13\_13\_Dissolved-Human\_MultiORAL\_6\_13\_Dissolved-Human\_MultiORAL\_6\_13\_Dissolved-Human_6\_13\_Dissolved-Human_6\_13\_Dissolved-Human_6\_13\_Dissolved-Human_6\_13\_Dissolved-Human_6\_13\_Dissolved-Human_6\_13\_Dissolved-Human_6\_13\_Dissolved-Human_6\_13\_Dissolved-Human_6\_13\_Disso$ 

Result of the validation: Valid

 $Simulation: Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved\_absorption\_-tolder and the control of the co$ 

 $sink\_conditions$ 

Result of the validation: Valid

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

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

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

continuous\_fraction\_1

Result of the validation: Valid

 $Simulation: \ Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved\_pKandler (A.C.) \\$ 

**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

 $Simulation: \ Human\_MultipleIV\_AllActive Processes-Human\_MultipleIV\_AllActive Processes$ 

Result of the validation: Valid

 $Simulation: \ Human\_Multiple IV\_transporters-Human\_Multiple IV\_transporters$ 

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\_Oral\_BiDaily\_TableFormulation-S2\_NoSuspension

Result of the validation: Valid

Simulation: Human\_pH\_SolubilityTable-S1\_Table

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-S4\_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

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

MW\_200\_fu\_0.2\_LogP\_5
Result of the validation: Valid

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

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

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

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_Dissolved\_Human\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-INFIGURE AND SINGLE AN$ 

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Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_Dissolved\_Human\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-INFIGURE AND SINGLE AN$ 

-5

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

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$ 

 ${\bf PolyParticlesLogNormal\_AsSuspention}$ 

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

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

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

Result of the validation: Valid

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

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

Result of the validation: Valid

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

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_Weibull\_AsSuspention-Human\_SingleORAL\_Weibull\_AsSuspention\_-Income and the property of the prop$ 

 $MW_200_fu_0.2_LogP_5$ 

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_Weibull\_AsSuspention-Human\_SingleORAL\_Weibull\_AsSuspention\_-Institute and the state of the$ 

 $MW_800_fu_0.6_LogP_-5$ 

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\_200\_fu\_0.2\_LogP\_5

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

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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

 $Simulation: Minipig\_SingleORAL\_Dissolved\_Minipig\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Included to the control of the con$ 

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Result of the validation: Valid

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

-5

Result of the validation: Valid

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

Result of the validation: Valid

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

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Result of the validation: Valid

 $Simulation: Monkey\_SingleORAL\_Dissolved\_Monkey\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-Installation: Monkey\_SingleORAL\_Dissolved\_Monkey\_Sin$ 

-5

Result of the validation: Valid

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

Result of the validation: Valid

 $Simulation: Mouse\_SingleORAL\_Dissolved\_Mouse\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-INFIGURE AND SINGLE AN$ 

5

Result of the validation: Valid

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

-5

Result of the validation: Valid

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

 $Simulation: \ Preterm\_SingleIV\_Age\_0\_GA\_32\_GFR-Preterm\_SingleIV\_Age\_0\_GA\_32\_GFR$ 

Result of the validation: Valid

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

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

 $Simulation: Rabbit\_SingleORAL\_Dissolved\_Rabbit\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-INFIGURE AND SINGLE AND SINGLE$ 

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Result of the validation: Valid

 $Simulation: Rabbit\_SingleORAL\_Dissolved\_Rabbit\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-Rabbit\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW_800\_fu\_0.6\_LogP\_-Rabbit\_MW$ 

-5

Result of the validation: Valid

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

Result of the validation: Valid

Simulation: Rat\_MultiORAL\_6\_6\_6\_Dissolved-Rat\_MultiORAL\_6\_6\_6\_6\_Dissolved

Result of the validation: Valid

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

Result of the validation: Valid

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

Result of the validation: Valid

 $Simulation: Single IV\_2 Pores\_Human\_Single IV\_2 Pores\_Human\_Simulation C$ 

Result of the validation: Valid

 $Simulation: Single IV\_2 Pores\_Human\_Single IV\_2 Pores\_Human\_Simulation D$ 

Result of the validation: Valid

 $Simulation: Single IV\_2 Pores\_Human\_Single IV\_2 Pores\_Human\_Simulation F$ 

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

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

Result of the validation: Valid

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

Result of the validation: Valid

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

Result of the validation: Valid

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

 $\operatorname{standard}$ 

Result of the validation: Valid

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

Result of the validation: Valid

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

Result of the validation: Valid

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

standard

Result of the validation: Valid

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

Result of the validation: Valid

 $Simulation: Single IV\_C3\_4 Comp\_standard\_schmittnormlized\_standard\_Single IV\_C3\_4 Comp\_standard\_schmittnormlized\_standard\_Single IV\_C3\_4 Comp\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_standard\_schmittnormlized\_schmittn$ 

 $schmittnormlized\_standard$ 

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

 $Simulation: Single IV\_C4\_4 Comp\_Ber\_standard\_standard\_standard\_Single IV\_C4\_4 Comp\_Ber\_standard\_stan$ 

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

 $Simulation: Single IV\_C5\_2 Pores\_PT\_standard\_s$ 

 $Simulation: Single IV\_C5\_2 Pores\_RR\_schmitt\_standard-Single IV\_SChmitt\_standard-Single IV\_SChmitt\_standard-Single IV\_SChmitt\_standard-Single IV\_SChmitt\_standard-Single IV\_SChmitt\_standard-Single IV\_SChmitt\_standard-Single IV\_SChmitt\_standard-Single IV\_SChmitt\_Schmitt\_Standard-Single IV\_SChmitt\_Schmitt\_Standard-Single IV\_SChmitt\_Schmit$ 

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

Result of the validation: Valid

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

Result of the validation: Valid

 $Simulation: Single IV\_C7\_4 Comp\_schmitt\_standard\_standa$ 

Result of the validation: Valid

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

Result of the validation: Valid

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

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

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

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

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

 $Simulation: Single ORAL\_C13\_2 Pores\_schmitt\_standard\_st$ 

Result of the validation: Valid

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

Result of the validation: Valid

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

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

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

Result of the validation: Valid

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

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

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

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

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

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

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