### Open Systems Pharmacology Suite - 11 Folder Comparison

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#### Chapter 1

## Folder Comparison Results

Overall Comparison Result: Valid Number of Compared Files: 155

#### 1.1 Comparison Results

Overall Comparison Result

Valid

Old Folder

D:\Outputs\_11.0

New Folder

D:\Outputs\_11.1

#### 1.1.1 Valid Simulations (155/155)

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

Result of the validation: Valid

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

 $\mathbf{5}$ 

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

Result of the validation: Valid

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

 $Simulation: \ DDI\_Multiple Combinations - 03\_MM\_Noncompetitive\_Noncompetitive$ 

Result of the validation: Valid

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

Result of the validation: Valid

 $Simulation: DDI\_MultipleCombinations-05\_MM\_Mechanismbased\_Mechanismbased$ 

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

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

Mechanismbased

Result of the validation: Valid

 $Simulation: \ DDI\_Multiple Combinations-09\_MM\_Noncompetitive\_Noncompetitive\_Mechanism based\_-incompetitive\_No$ 

Mechanismbased

Result of the validation: Valid

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

Result of the validation: Valid

 $Simulation: \ DDI\_Multiple Combinations - 11\_MM\_Mechanism based\_Mechanism based\_Induction\_- 11\_MM\_Mechanism based\_Mechanism based\_Mechanism$ 

Induction

Result of the validation: Valid

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

Result of the validation: Valid

 $Simulation: \ DDI\_Multiple Combinations \textbf{-} 21\_1st\_Competitive\_Competitive$ 

Result of the validation: Valid

Simulation: DDI\_MultipleCombinations-23\_1st\_Noncompetitive\_Noncompetitive

Result of the validation: Valid

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

 $Simulation: \ DDI\_Multiple Combinations \textbf{-} 25\_1 st\_Mechanism based\_Mechanism based$ 

Result of the validation: Valid

 $Simulation: \ DDI\_Multiple Combinations - 26\_1st\_Induction\_Induction$ 

Result of the validation: Valid

Simulation: DDI\_MultipleCombinations-27\_1st\_Competitive\_Competitive\_Mechanismbased\_Mechanismbased

Result of the validation: Valid

 $Simulation: DDI\_Multiple Combinations - 28\_1st\_Uncompetitive\_Uncompetitive\_Mechanism based\_-1st\_Uncompetitive\_Mechanism based\_-1st\_Uncompetitive\_Uncompetitive\_Mechanism based\_-1st\_Uncompetitive\_Uncompeti$ 

Mechanismbased

Result of the validation: Valid

Simulation: DDI\_MultipleCombinations-29\_1st\_Noncompetitive\_Noncompetitive\_Mechanismbased\_-

Mechanismbased

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\_MultipleCombinations-32\_1st\_All\_DDI\_Types

Result of the validation: Valid

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

Result of the validation: Valid

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

Result of the validation: Valid

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

Result of the validation: Valid

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

Result of the validation: Valid

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

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 <code>ICRP\_AGP-03\_ICRP\_0.18y\_Male</code>

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

Result of the validation: Valid

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

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

 $Simulation: Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved\_EHC\_continuous\_fraction\_0.5$ 

Result of the validation: Valid

 $Simulation: \ Human\_MultiORAL\_6\_12\_12\_Dissolved-Human\_MultiORAL\_6\_12\_12\_Dissolved\_EHC\_-IVAL\_6\_12\_Dissolved\_EHC\_-IVAL_6\_12\_Dissolved\_EHC\_-IVAL_6\_12\_Dissolved\_EHC\_-IVAL_6\_12\_Dissolved\_EHC\_-IVAL_6\_12\_Dissolved\_EHC\_-IVAL_6\_12\_Dissolved\_EHC\_-IVAL_6\_12\_Dissolved\_EHC\_-IVAL_6\_12\_Dissolved\_EHC\_-IVAL_6\_12\_Dissolved\_EHC\_-IVAL_6\_12\_Dissolved\_EHC\_-IVAL_6\_12\_Dissolved\_EHC\_-IVAL_6\_12\_Dissolved\_EHC_6\_12\_Disso$ 

 $continuous\_fraction\_1$ 

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

 $Simulation: \ Human\_MultipleIV\_EffluxBasolateral-Human\_MultipleIV\_EffluxBasolateral$ 

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

 $Simulation: \ Human\_Multiple IV\_Influx-Human\_Multiple IV\_Active Influx$ 

Result of the validation: Valid

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

Result of the validation: Valid

 ${\bf Simulation: \ Human\_Multiple IV\_Metabolizm-Human\_Multiple IV\_Metabolizm}$ 

Result of the validation: Valid

 $Simulation: \ Human\_Multiple IV\_PGPB a solateral-Human\_Multiple IV\_PGPB a solateral-$ 

Result of the validation: Valid

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

 $Simulation: \ Human\_NonCompetitiveInhibition-Human\_NonCompetitiveInhibition$ 

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

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

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

Result of the validation: Valid

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

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

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

5

Result of the validation: Valid

 $Simulation: Human\_SingleORAL\_Dissolved\_Human\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL_Dissolved\_MW_800\_fu\_0.6\_LogP\_-RAL_Dissolved\_MW_800$ 

-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

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

**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\_-

MW\_800\_fu\_0.6\_LogP\_-5

Result of the validation: Valid

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

Result of the validation: Valid

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

Result of the validation: Valid

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

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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

 $Simulation: Minipig\_SingleORAL\_Dissolved\_Minipig\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Installation: Minipig\_SingleORAL\_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Installation: Minipig\_SingleORAL_Dissolved\_MW\_200\_fu\_0.2\_LogP\_-Installation: Minipig\_SingleORAL_Dissolved\_MW\_200\_Fu\_0.2\_LogP\_-Installation: Minipig\_SingleORAL_Dissolved\_MW\_200\_Fu\_0.2\_LogP\_-I$ 

5

Result of the validation: Valid

 $Simulation: Minipig\_SingleORAL\_Dissolved\_Minipig\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL\_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL_Dissolved\_MW_800\_fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL_Dissolved\_MW_800\_Fu\_0.6\_LogP\_-Installation: Minipig\_SingleORAL_Dissolved\_MW_800\_Fu\_0.6\_LogP\_-I$ 

-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\_-

5

Result of the validation: Valid

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

-5

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

Result of the validation: Valid

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

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

Result of the validation: Valid

Result of the validation: Valid

 $Simulation: Preterm\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_Age\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA\_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA_32\_CYP3A4-PreterM\_SingleIV\_AGe\_15\_GA_32\_CYP3$ 

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

 $Simulation: Rabbit\_SingleORAL\_Dissolved\_Rabbit\_SingleORAL\_Dissolved\_MW\_800\_fu\_0.6\_LogP\_-Incomplete the control of the contro$ 

-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

Result of the validation: Valid

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

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

Result of the validation: Valid

Simulation: SingleIV\_2Pores\_Human\_SingleIV\_2Pores\_Human\_SimulationC

Result of the validation: Valid

Simulation: SingleIV\_2Pores\_Human\_SingleIV\_2Pores\_Human\_SimulationD

Result of the validation: Valid

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

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

 $Simulation: Single IV\_2 Pores\_Monkey\_Single IV\_2 Pores\_Monkey\_Simulation H$ 

Result of the validation: Valid

Simulation: SingleIV\_2Pores\_Mouse-SingleIV\_2Pores\_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

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

standard

Result of the validation: Valid

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

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

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

Result of the validation: Valid

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

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

Result of the validation: Valid

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

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

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

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

 $Simulation: Single IV\_C5\_2 Pores\_RR\_schmitt\_standard-Single IV\_S-2 Pores\_S-2 Pores\_S-2 Pores\_S-2 Pores\_S-2 Pores\_S-2 Pores\_S-2 Pores\_S-2 Pores\_S-2 Pores\_S-2 Pores\_S$ 

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

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

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

 $Simulation: Single IV\_C8\_2 Pores\_standard\_schmittnormalized\_standard-Single IV\_C8\_2 Pores\_standard\_schmittnormalized\_standard$ 

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

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

Result of the validation: Valid

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

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

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

Result of the validation: Valid

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

Result of the validation: Valid

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

Result of the validation: Valid

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

Result of the validation: Valid

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

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

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

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

Result of the validation: Valid

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

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

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

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