

Open Systems Pharmacology Suite - 12

Folder Comparison

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Chapter 1

Folder Comparison Results

Overall Comparison Result: **Invalid**
Number of Compared Files: 155

1.1 Comparison Results

Overall Comparison Result
Invalid

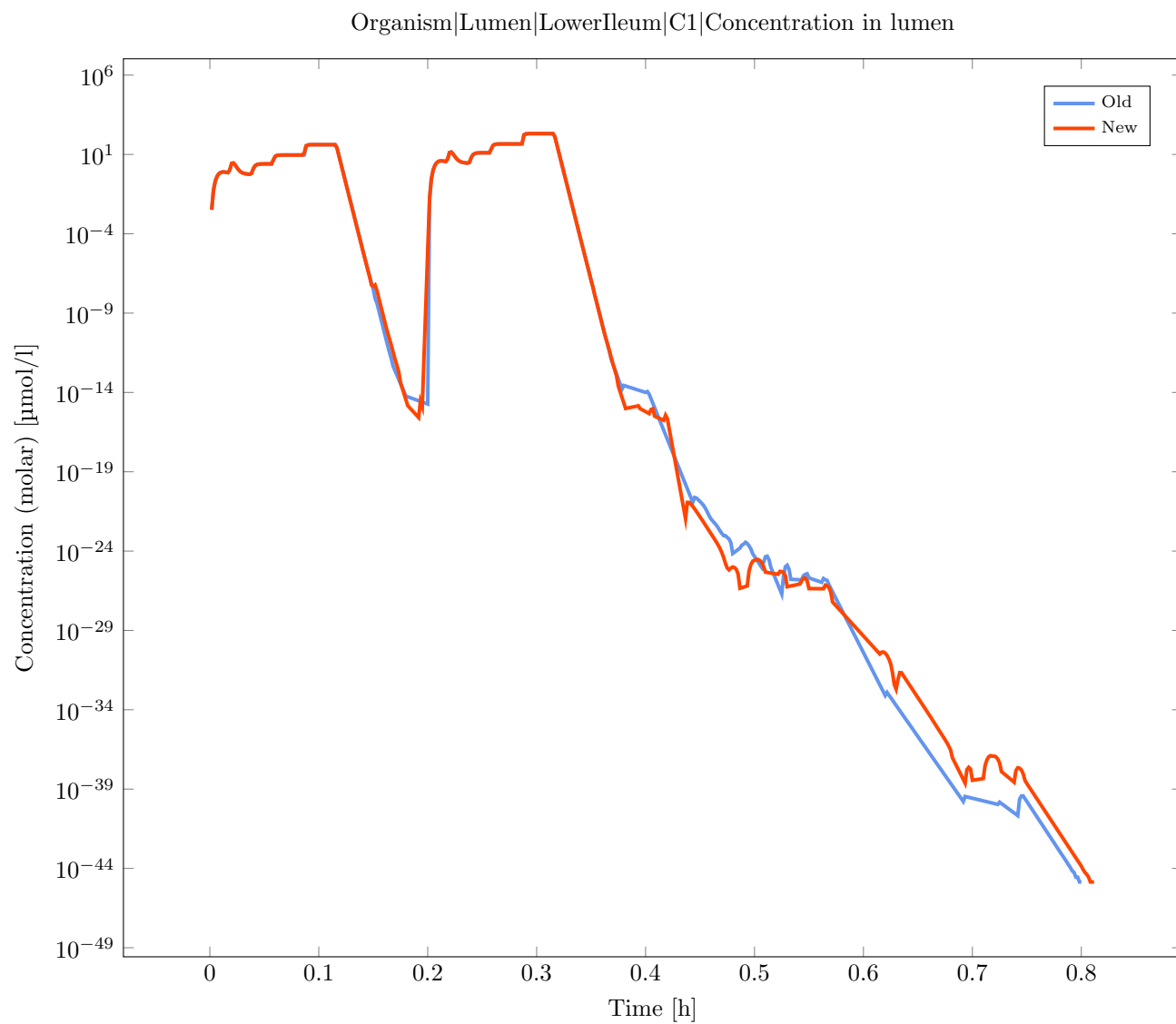
Old Folder
D:\Outputs_11.3

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 allowed max. tolerance of 3.00%
Deviation: 0.34

**Figure 1.1**

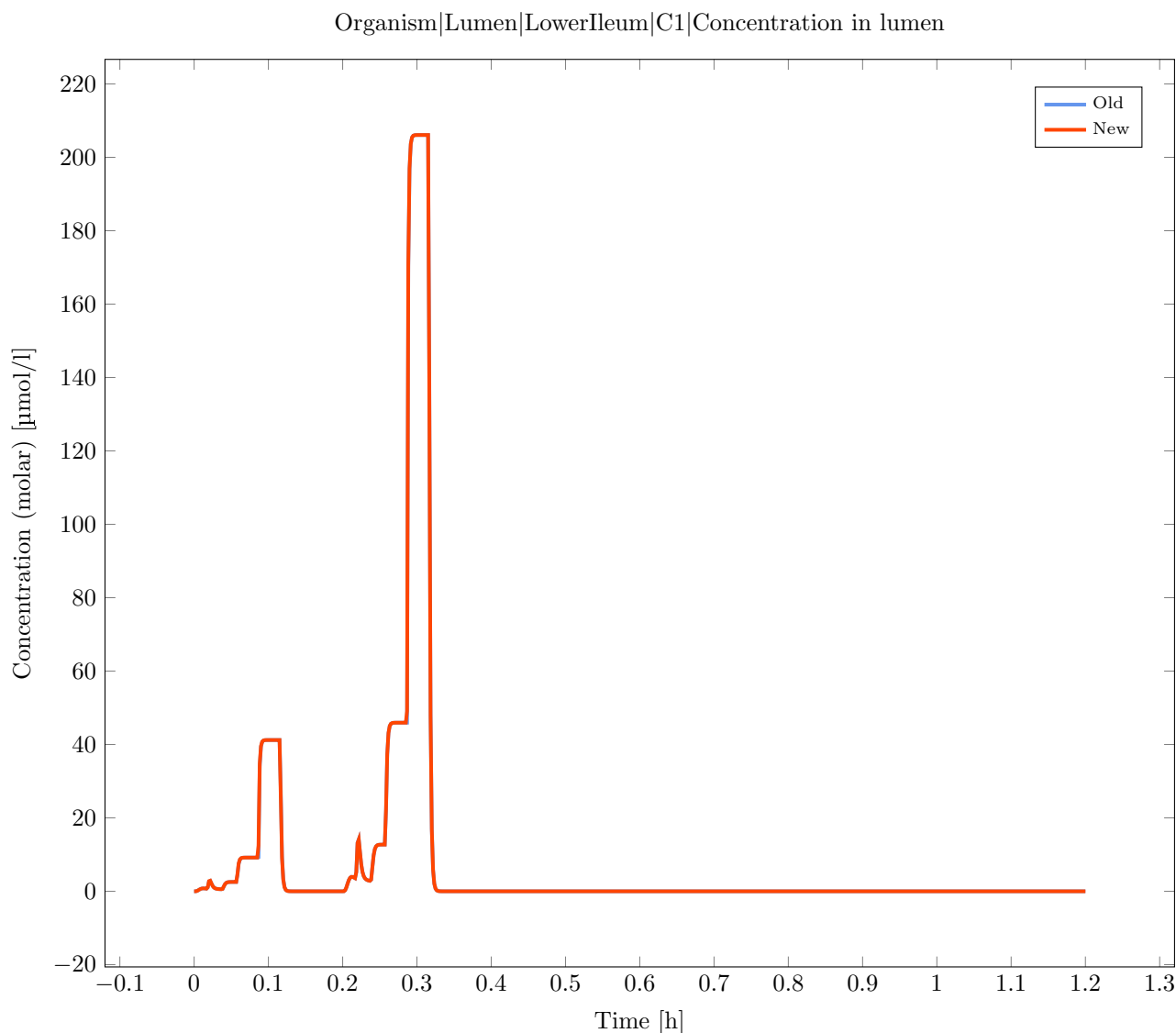


Figure 1.2

Simulation: Human_SingleORAL_Weibull-Human_SingleORAL_Weibull_MW_200_fu_0.2_LogP_5

Result of the validation: **Invalid**

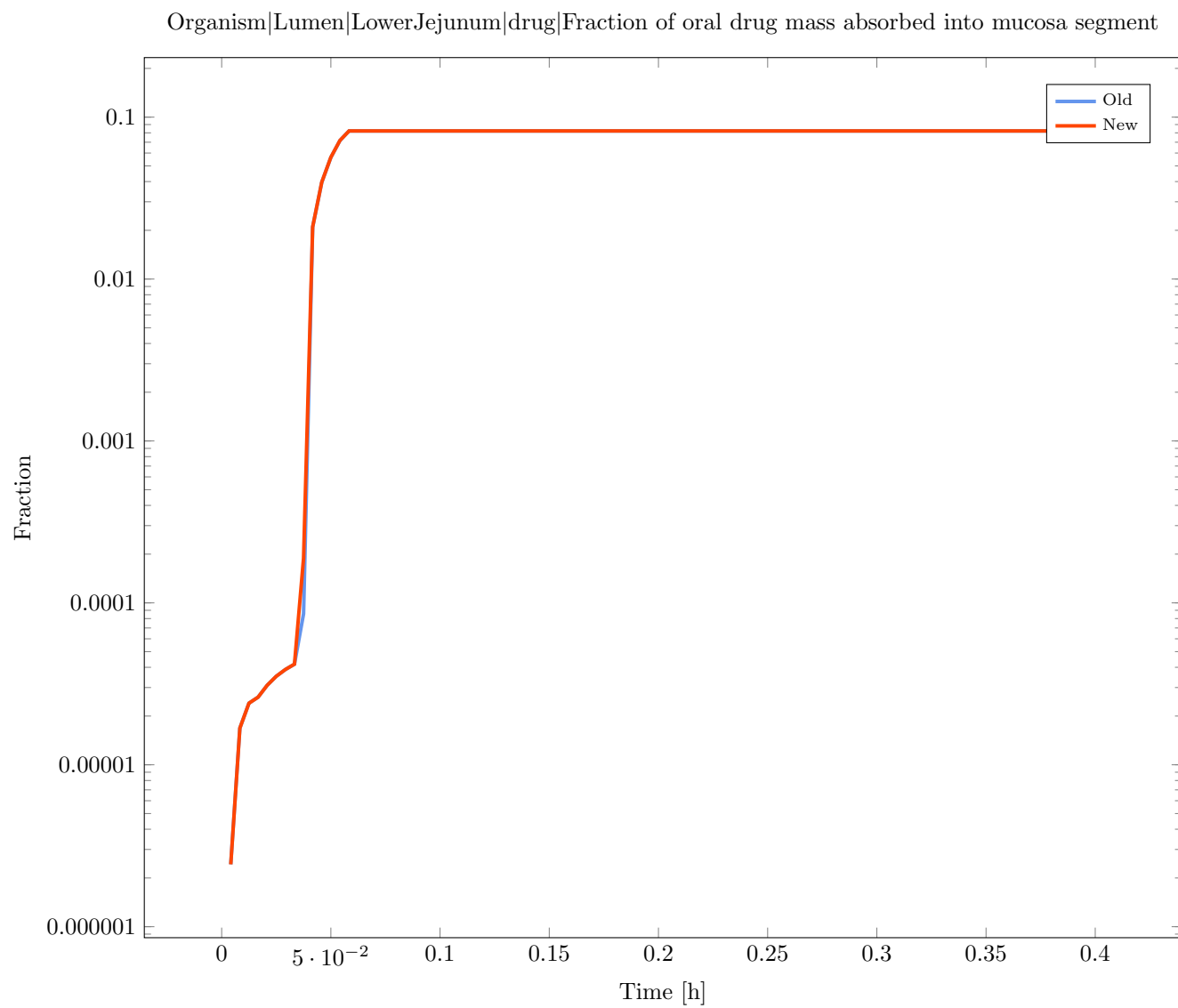
Absolute Tolerance: 1.00E-10

Relative Tolerance: 1.00E-5

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

Deviation for 'Organism|Lumen|LowerJejunum|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

**Figure 1.3**

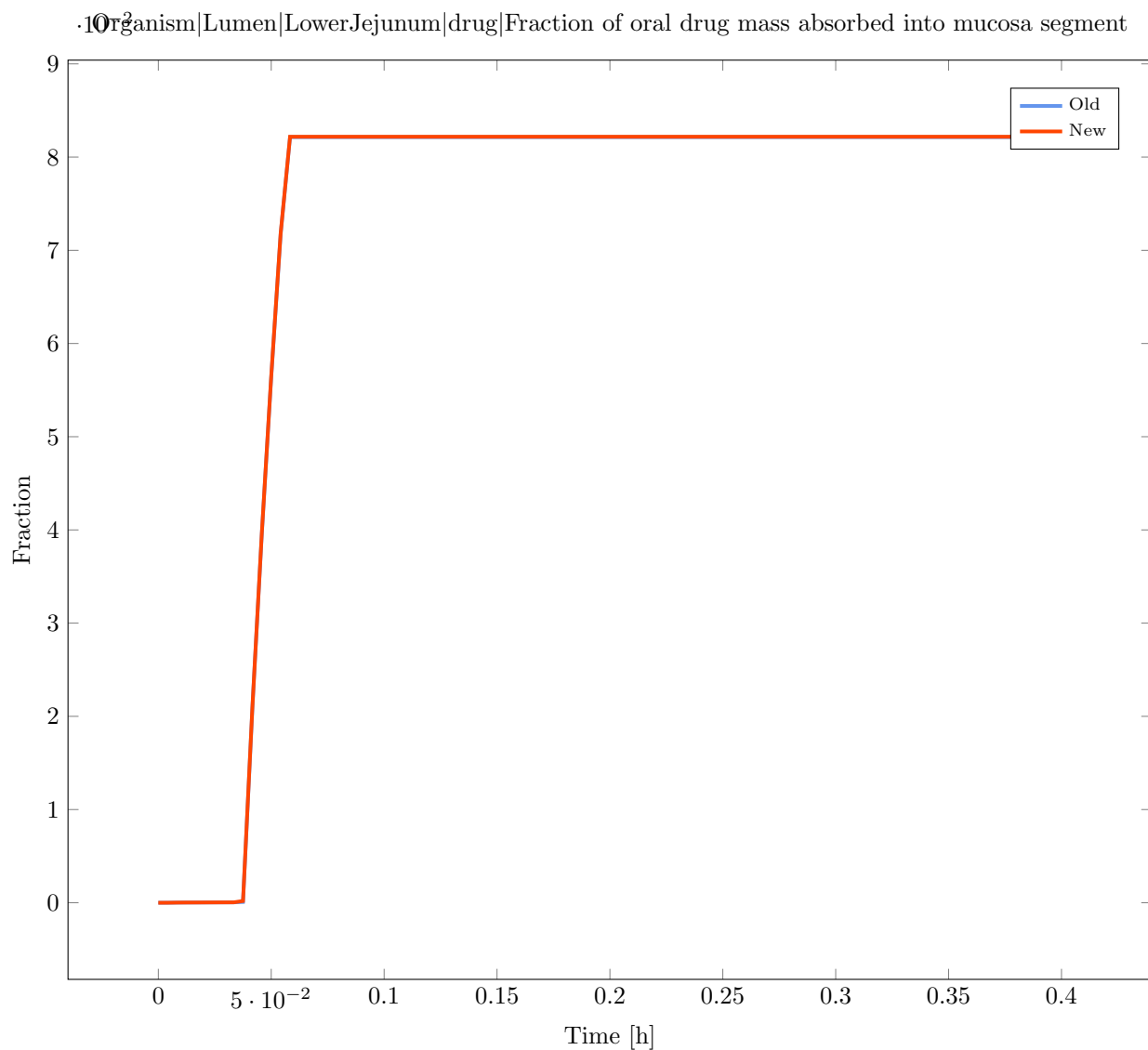


Figure 1.4

1.1.2 Valid Simulations (153/155)

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_-5

Result of the validation: Valid

Simulation: Beagle_SingleORAL_Dissolved-Beagle_SingleORAL_Dissolved_MW_800_fu_0.6_LogP_-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

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_MultipleCombinations-05_MM_Mechanismbased_Mechanismbased

Result of the validation: Valid

Simulation: DDI_MultipleCombinations-06_MM_Induction_Induction

Result of the validation: Valid

Simulation: DDI_MultipleCombinations-07_MM_Competitive_Competitive_Mechanismbased_Mechanismbased

Result of the validation: Valid

**Simulation: DDI_MultipleCombinations-08_MM_Uncompetitive_Uncompetitive_Mechanismbased_-
Mechanismbased**

Result of the validation: Valid

**Simulation: DDI_MultipleCombinations-09_MM_Noncompetitive_Noncompetitive_Mechanismbased_-
Mechanismbased**

Result of the validation: Valid

Simulation: DDI_MultipleCombinations-10_MM_Mixed_Mixed_Mechanismbased_Mechanismbased

Result of the validation: Valid

**Simulation: DDI_MultipleCombinations-11_MM_Mechanismbased_Mechanismbased_Induction_-
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

Result of the validation: Valid

Simulation: DDI_MultipleCombinations-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_MultipleCombinations-27_1st_Competitive_Competitive_Mechanismbased_Mechanismbased

Result of the validation: Valid

Simulation: DDI_MultipleCombinations-28_1st_Uncompetitive_Uncompetitive_Mechanismbased_-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_MultipleCombinations-31_1st_Mechanismbased_Mechanismbased_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

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

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**

Simulation: Human_IrreversibleInhibition-Human_IrreversibleInhibition

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

Result of the validation: **Valid**

Simulation: Human_MultiORAL_6_12_12_Dissolved-Human_MultiORAL_6_12_12_Dissolved_absorption_-sink_conditions

Result of the validation: **Valid**

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_-continuous_fraction_1

Result of the validation: **Valid**

Simulation: Human_MultiORAL_6_12_12_Dissolved-Human_MultiORAL_6_12_12_Dissolved_pKa-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_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

Result of the validation: **Valid**

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-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

Result of the validation: Valid

Simulation: Human_SingleORAL_Dissolved_PlasmaClearance-Human_SingleORAL_Dissolved_PlasmaClearance
MW_200_fu_0.2_LogP_5

Result of the validation: Valid

Simulation: Human_SingleORAL_Dissolved_PlasmaClearance-Human_SingleORAL_Dissolved_PlasmaClearance_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_-5

Result of the validation: Valid

Simulation: Human_SingleORAL_Dissolved-Human_SingleORAL_Dissolved_MW_800_fu_0.6_LogP_-5

Result of the validation: Valid

Simulation: Human_SingleORAL_Lint80_AsSuspension-Human_SingleORAL_Lint80_AsSuspension

Result of the validation: Valid

Simulation: Human_SingleORAL_Lint80-Human_SingleORAL_Lint80

Result of the validation: Valid

Simulation: Human_SingleORAL_MonoParticles_AsSuspension-Human_SingleORAL_MonoParticles_AsSuspension

Result of the validation: Valid

Simulation: Human_SingleORAL_PolyParticlesLogNormal_AsSuspension-Human_SingleORAL_PolyParticlesLogNormal_AsSuspension

Result of the validation: Valid

Simulation: Human_SingleORAL_PolyParticlesNormal_AsSuspension-Human_SingleORAL_PolyParticlesNormal_AsSuspension

Result of the validation: Valid

Simulation: Human_SingleORAL_PolyParticlesNormal_AsSuspension-Human_SingleORAL_PolyParticlesNormal_AsSuspension_dissolved_radius

Result of the validation: Valid

Simulation: Human_SingleORAL_PolyParticlesNormal_AsSuspension-Human_SingleORAL_PolyParticlesNormal_AsSuspension_treat_precipitated_drug_as_soluble

Result of the validation: Valid

Simulation: Human_SingleORAL_Weibull_AsSuspension-Human_SingleORAL_Weibull_AsSuspension

Result of the validation: Valid

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_800_fu_0.6_LogP_-5

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_-5

Result of the validation: Valid

Simulation: Minipig_SingleORAL_Dissolved-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_-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

Result of the validation: Valid

Simulation: Mouse_SingleORAL_Dissolved-Mouse_SingleORAL_Dissolved_MW_200_fu_0.2_LogP_-5

Result of the validation: Valid

Simulation: Mouse_SingleORAL_Dissolved-Mouse_SingleORAL_Dissolved_MW_800_fu_0.6_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

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

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_-5

Result of the validation: Valid

Simulation: Rabbit_SingleORAL_Dissolved-Rabbit_SingleORAL_Dissolved_MW_800_fu_0.6_LogP_-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_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

Result of the validation: Valid

Simulation: SingleIV_2Pores_Human-SingleIV_2Pores_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: 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: SingleIV_2Pores_Mouse-SingleIV_2Pores_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: SingleIV_2Pores_Mouse-SingleIV_2Pores_Mouse_SimulationE

Result of the validation: Valid

Simulation: SingleIV_C1_4Comp_standard_standard_standard-SingleIV_C1_4Comp_standard_standard_standard

Result of the validation: Valid

Simulation: SingleIV_C2_4Comp_PT_standard_standard-SingleIV_C2_4Comp_PT_standard_standard

Result of the validation: Valid

Simulation: SingleIV_C2_4Comp_RR_standard_standard-SingleIV_C2_4Comp_RR_standard_standard

Result of the validation: Valid

Simulation: SingleIV_C2_4Comp_standard_schmitt_standard-SingleIV_C2_4Comp_standard_schmitt_standard

Result of the validation: Valid

Simulation: SingleIV_C3_4Comp_RR_schmitt_standard-SingleIV_C3_4Comp_RR_schmitt_standard

Result of the validation: Valid

Simulation: SingleIV_C3_4Comp_standard_schmittnormalized_standard-SingleIV_C3_4Comp_standard_schmittnormalized_standard

Result of the validation: Valid

Simulation: SingleIV_C4_2Pores_RR_standard_standard-SingleIV_C4_2Pores_RR_standard_standard

Result of the validation: Valid

Simulation: SingleIV_C4_4Comp_Ber_standard_standard-SingleIV_C4_4Comp_Ber_standard_standard

Result of the validation: Valid

Simulation: SingleIV_C5_2Pores_Ber_standard_standard-SingleIV_C5_2Pores_Ber_standard_standard

Result of the validation: Valid

Simulation: SingleIV_C5_2Pores_PT_standard_standard-SingleIV_C5_2Pores_PT_standard_standard

Result of the validation: Valid

Simulation: SingleIV_C5_2Pores_RR_schmitt_standard-SingleIV_C5_2Pores_RR_schmitt_standard

Result of the validation: Valid

Simulation: SingleIV_C6_2Pores_standard_standard_standard-SingleIV_C6_2Pores_standard_standard_standard

Result of the validation: Valid

Simulation: SingleIV_C7_2Pores_standard_schmitt_standard-SingleIV_C7_2Pores_standard_schmitt_standard

Result of the validation: Valid

Simulation: SingleIV_C7_4Comp_schmitt_standard_standard-SingleIV_C7_4Comp_schmitt_standard_standard

Result of the validation: Valid

Simulation: SingleIV_C8_2Pores_standard_schmittnormalized_standard-SingleIV_C8_2Pores_standard_schmittnormalized_standard

Result of the validation: Valid

Simulation: SingleIV_C9_2Pores_schmitt_standard_standard-SingleIV_C9_2Pores_schmitt_standard_standard

Result of the validation: Valid

Simulation: SingleORAL_C10_4Comp_PT_standard_standard-SingleORAL_C10_4Comp_PT_standard_standard

Result of the validation: Valid

Simulation: SingleORAL_C11_4Comp_schmitt_standard_standard-SingleORAL_C11_4Comp_schmitt_standard_standard

Result of the validation: Valid

Simulation: SingleORAL_C11_4Comp_standard_standard_standard-SingleORAL_C11_4Comp_standard_standard_standard

Result of the validation: Valid

Simulation: SingleORAL_C12_4Comp_standard_schmitt_standard-SingleORAL_C12_4Comp_standard_schmitt_standard

Result of the validation: Valid

Simulation: SingleORAL_C13_2Pores_schmitt_standard_standard-SingleORAL_C13_2Pores_schmitt_standard_standard

Result of the validation: Valid

Simulation: SingleORAL_C13_4Comp_standard_schmittnormalized_standard-SingleORAL_C13_4Comp_standard_schmittnormalized_standard

Result of the validation: Valid

Simulation: SingleORAL_C14_2Pores_PT_standard_standard-SingleORAL_C14_2Pores_PT_standard_standard

Result of the validation: Valid

Simulation: SingleORAL_C2_2Pores_standard_standard_standard-SingleORAL_C2_2Pores_standard_standard_standard

Result of the validation: Valid

Simulation: SingleORAL_C3_2Pores_standard_schmitt_standard-SingleORAL_C3_2Pores_standard_schmitt_standard

Result of the validation: Valid

Simulation: SingleORAL_C4_2Pores_standard_schmittnormalized_standard-SingleORAL_C4_2Pores_standard_schmittnormalized_standard

Result of the validation: Valid

Simulation: SingleORAL_C6_4Comp_Ber_standard_standard-SingleORAL_C6_4Comp_Ber_standard_standard

Result of the validation: Valid

Simulation: SingleORAL_C6_4Comp_RR_standard_standard-SingleORAL_C6_4Comp_RR_standard_standard

Result of the validation: Valid

Simulation: SingleORAL_C7_2Pores_Ber_standard_standard-SingleORAL_C7_2Pores_Ber_standard_standard

Result of the validation: Valid

Simulation: SingleORAL_C7_4Comp_RR_schmitt_standard-SingleORAL_C7_4Comp_RR_schmitt_standard

Result of the validation: Valid

Simulation: SingleORAL_C8_2Pores_RR_standard_standard-SingleORAL_C8_2Pores_RR_standard_standard

Result of the validation: Valid

Simulation: SingleORAL_C9_2Pores_RR_schmitt_standard-SingleORAL_C9_2Pores_RR_schmitt_standard

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

Result of the validation: Valid