Open Systems Pharmacology Suite - 9
Folder Comparison

Administrator

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Contents

Chapter 1

Folder Comparison Results

Overall Comparison Result: Invalid
Number of Compared Files: 125

1.1 Comparison Results

Overall Comparison Result
Invalid

Old Folder
C:\OSP_8.0_Outputs

New Folder
C:\OSP_9.0_Outputs

1.1.1 Invalid Simulations (4/125)

Simulation: European_SingleORAL_Age_0_CYP3A4-European_SingleORAL_Age_0_CYP3A4
Result of the validation: Invalid
Absolute Tolerance: 1.00E-13
Relative Tolerance: 1.00E-8

Output Path: Organism|LargeIntestine|Mucosa|ColonSigmoid|Intracellular|drug|Concentration in container
Deviation for 'Organism|LargeIntestine|Mucosa|ColonSigmoid|Intracellular|drug|Concentration in container' is 14.13% and is greater than the allowed max. tolerance of 2.00%
Deviation: 0.14

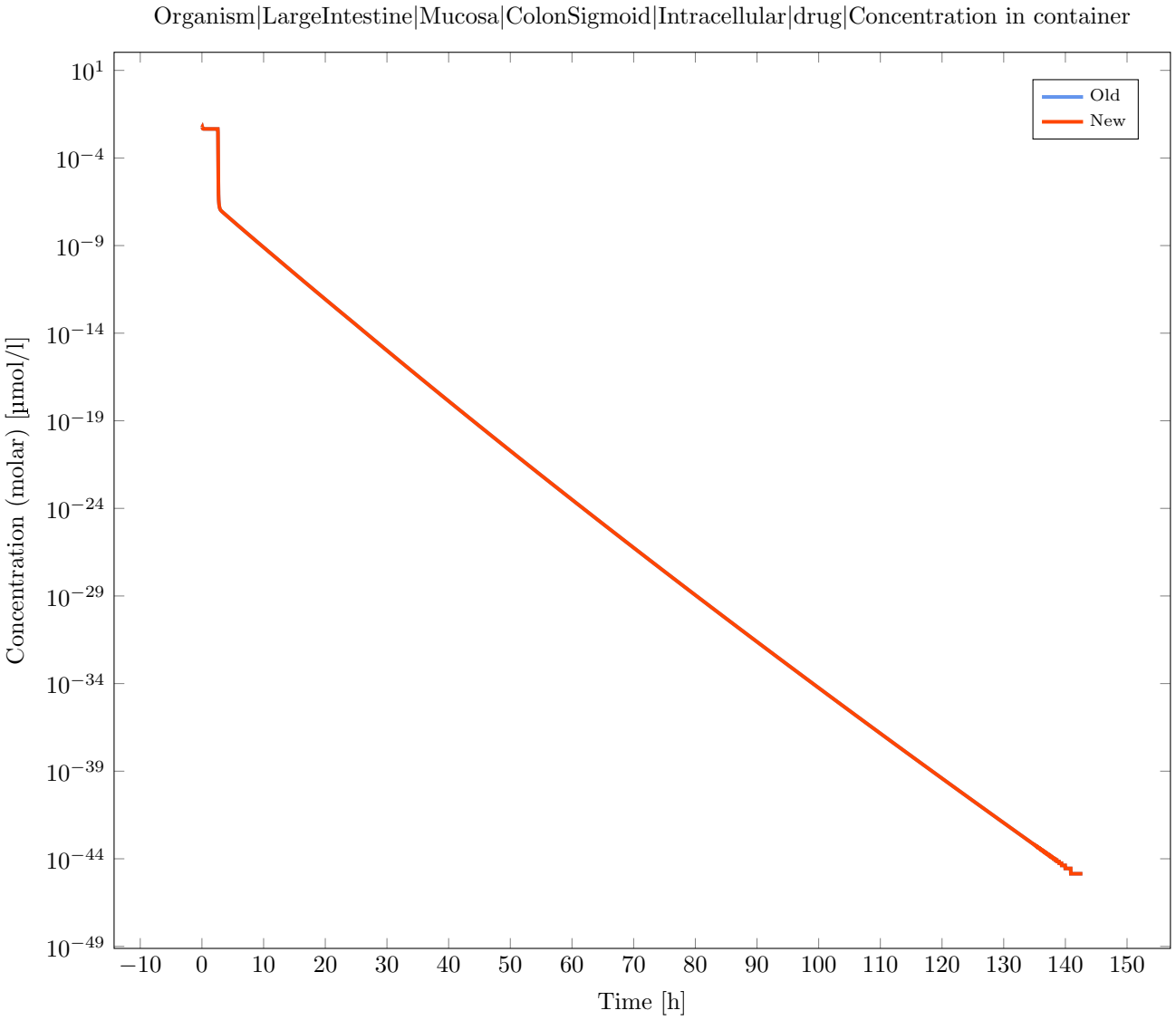
Organism|LargeIntestine|Mucosa|ColonSigmoid|Intracellular|drug|Concentration in container
Old
New
Concentration (molar) [µmol/l]
10^{1}
10^{-4}
10^{-9}
10^{-14}
10^{-19}
10^{-24}
10^{-29}
10^{-34}
10^{-39}
10^{-44}
10^{-49}
−10 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150
Time [h]

Figure 1.1

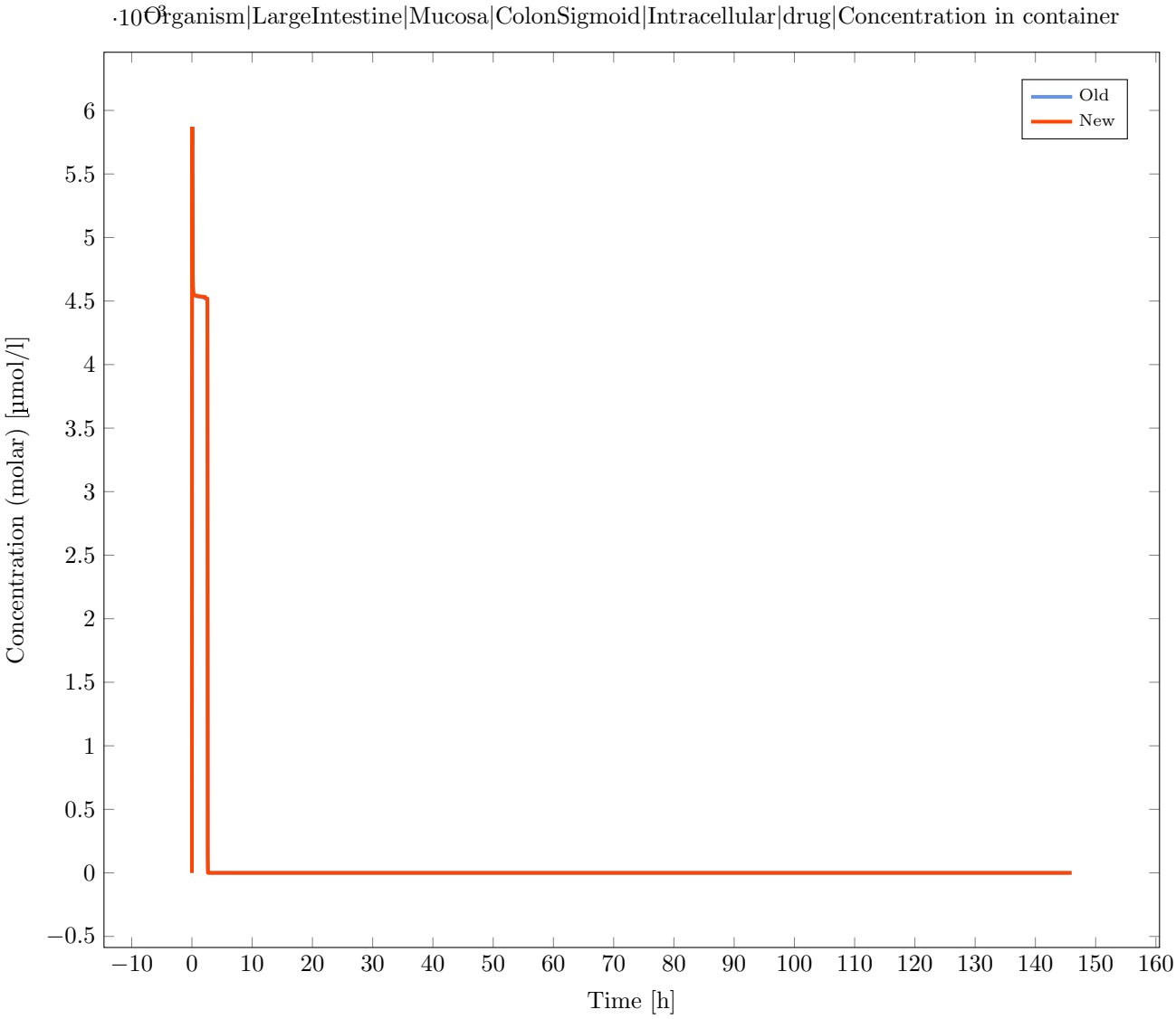

Figure 1.2

Simulation: European_SingleORAL_Age_0_GFR-European_SingleORAL_Age_0_GFR
Result of the validation: Invalid
Absolute Tolerance: 1.00E-13
Relative Tolerance: 1.00E-8

Output Path: Organism|LargeIntestine|Mucosa|ColonSigmoid|Intracellular|drug|Concentration in container
Deviation for 'Organism|LargeIntestine|Mucosa|ColonSigmoid|Intracellular|drug|Concentration in container' is 5.86% and is greater than the allowed max. tolerance of 2.00%
Deviation: 0.06

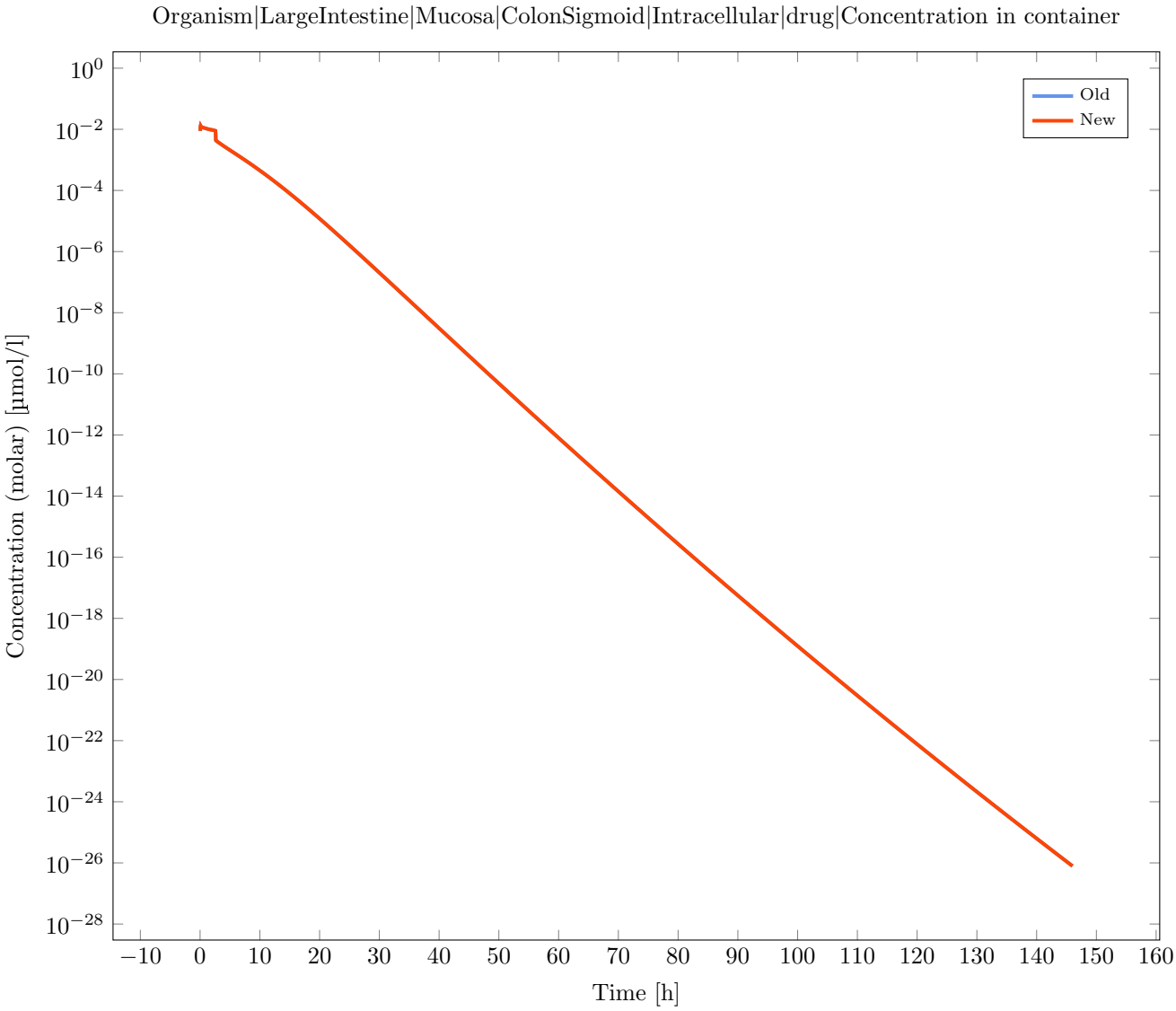
Organism|LargeIntestine|Mucosa|ColonSigmoid|Intracellular|drug|Concentration in container
Old
New
Concentration (molar) [µmol/l]
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
10^{-18}
10^{-20}
10^{-22}
10^{-24}
10^{-26}
10^{-28}
−10 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160
Time [h]

Figure 1.3

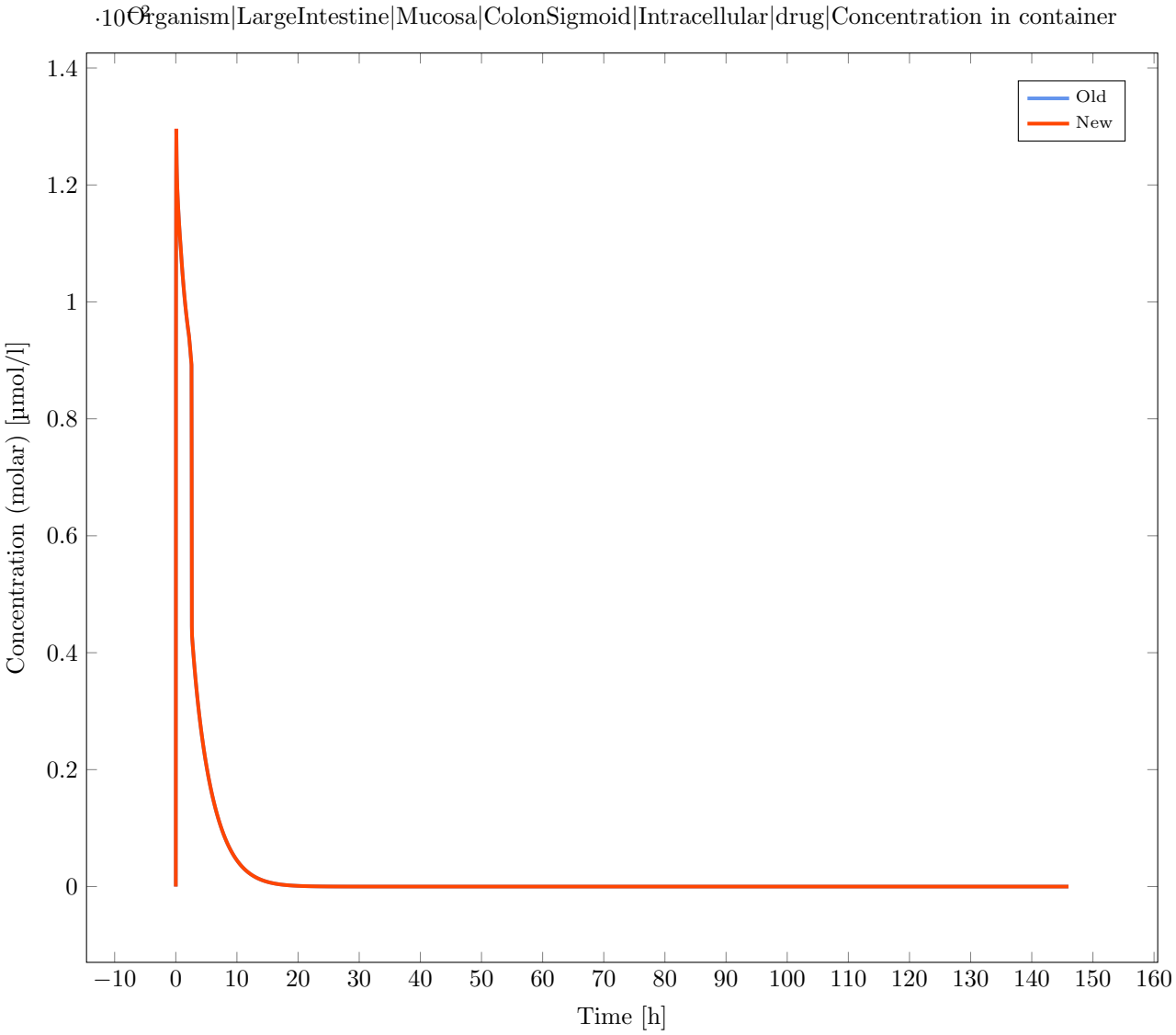

Figure 1.4

Simulation: European_SingleORAL_Age_1_CYP3A4-European_SingleORAL_Age_1_CYP3A4
Result of the validation: Invalid
Absolute Tolerance: 1.00E-13
Relative Tolerance: 1.00E-8

Output Path: Organism|LargeIntestine|Mucosa|ColonSigmoid|Intracellular|drug|Concentration in container
Deviation for 'Organism|LargeIntestine|Mucosa|ColonSigmoid|Intracellular|drug|Concentration in container' is 3.82% and is greater than the allowed max. tolerance of 2.00%
Deviation: 0.04

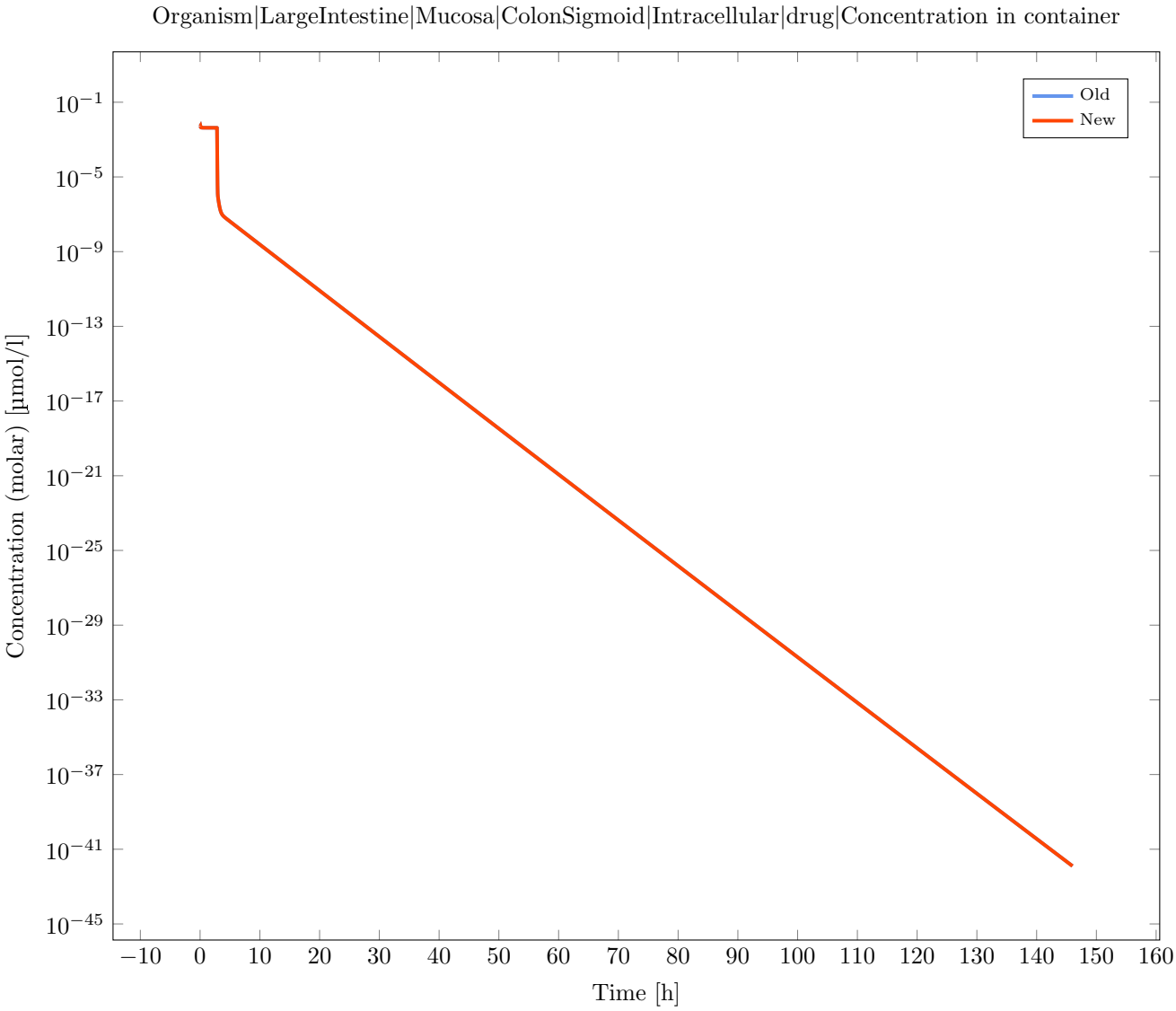
Organism|LargeIntestine|Mucosa|ColonSigmoid|Intracellular|drug|Concentration in container
Old
New
Concentration (molar) [µmol/l]
10^{-1}
10^{-5}
10^{-9}
10^{-13}
10^{-17}
10^{-21}
10^{-25}
10^{-29}
10^{-33}
10^{-37}
10^{-41}
10^{-45}
−10 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160
Time [h]

Figure 1.5

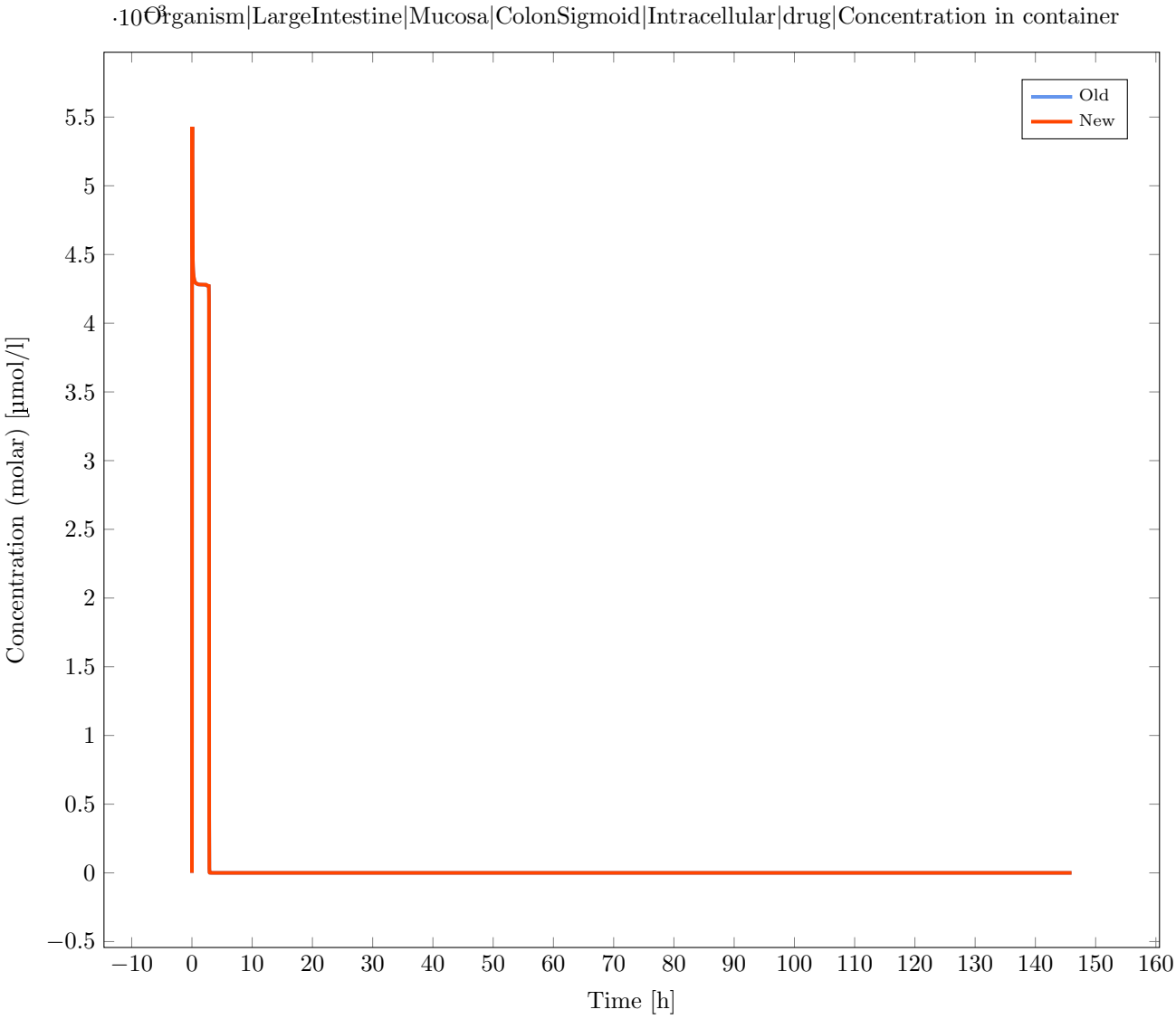

Figure 1.6

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|Rectum|C1|Concentration in lumen
Deviation for 'Organism|Lumen|Rectum|C1|Concentration in lumen' is 3.82% and is greater than the allowed max. tolerance of 2.00%
Deviation: 0.04

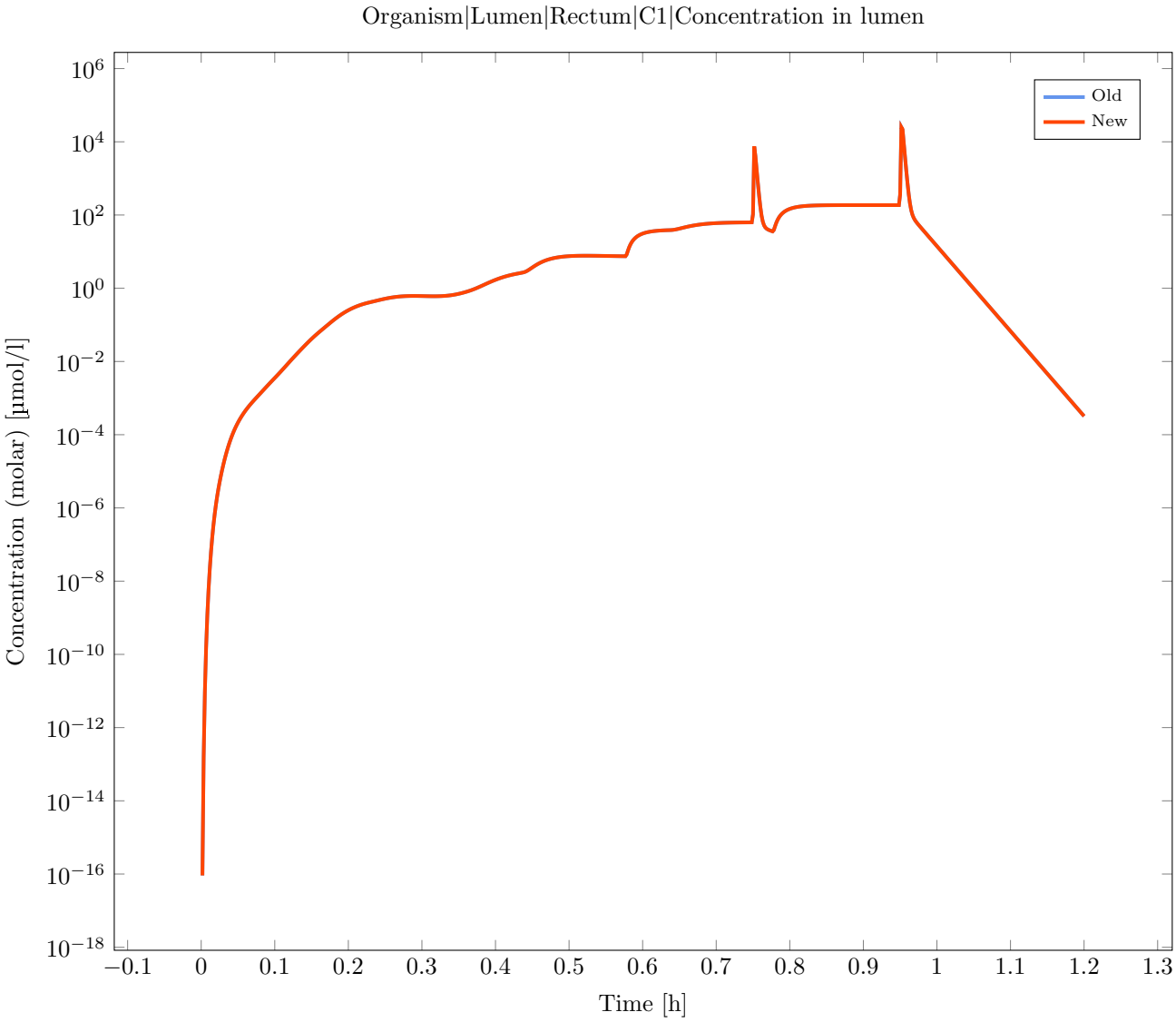
Organism|Lumen|Rectum|C1|Concentration in lumen
Old
New
Concentration (molar) [µmol/l]
10^{6}
10^{4}
10^{2}
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
10^{-18}
−0.1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
Time [h]

Figure 1.7

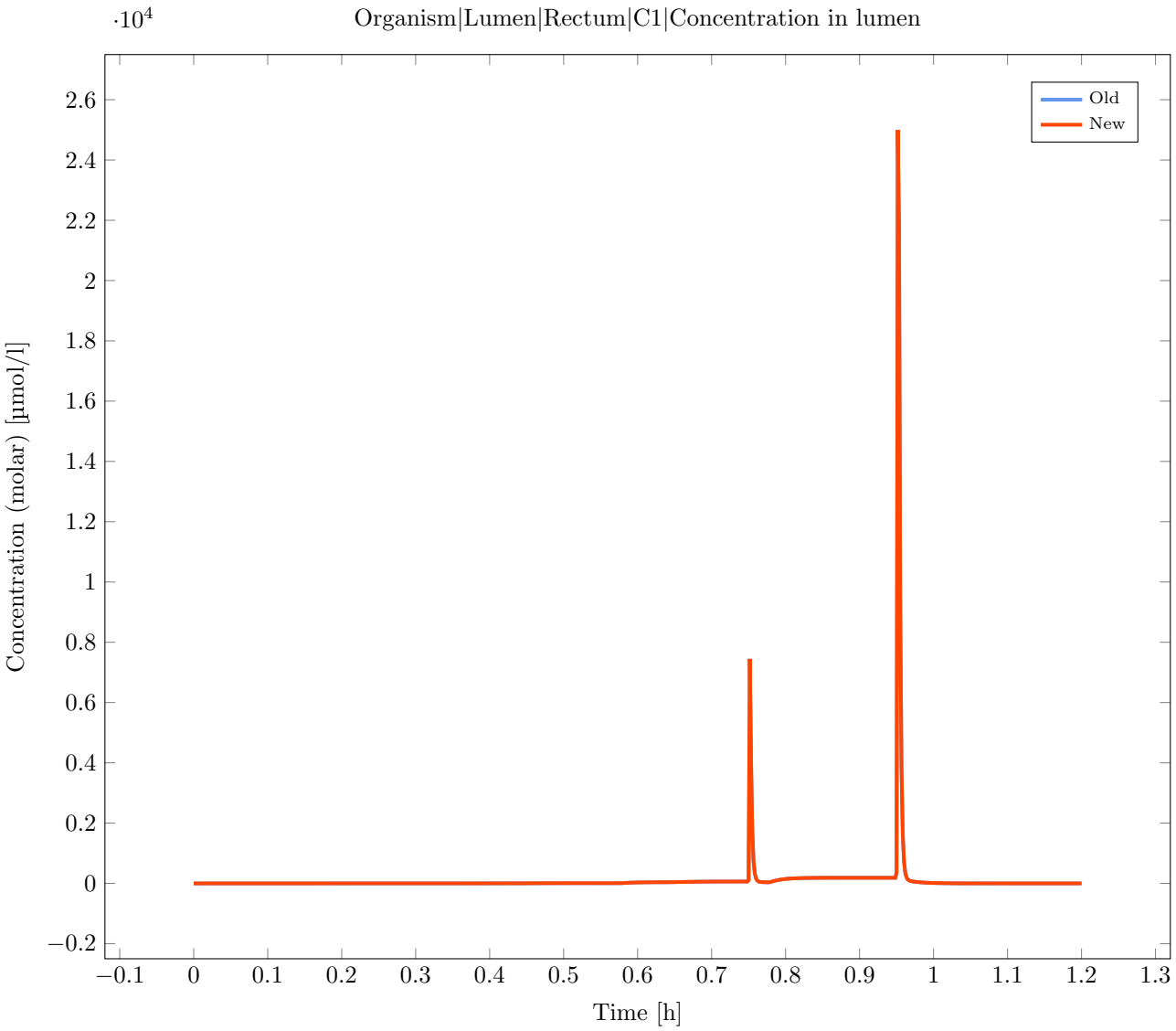

Figure 1.8

1.1.2 Valid Simulations (121/125)

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_-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: 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_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_AllActiveProcesses-Human_MultipleIV_AllActiveProcesses
Result of the validation: Valid

Simulation: Human_MultipleIV_transporters-Human_MultipleIV_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_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_PlasmaClearan
Result of the validation: Valid

Simulation: Human_SingleORAL_Dissolved_PlasmaClearance-Human_SingleORAL_Dissolved_PlasmaClearan MW_200_fu_0.2_LogP_5
Result of the validation: Valid

Simulation: Human_SingleORAL_Dissolved_PlasmaClearance-Human_SingleORAL_Dissolved_PlasmaClearan 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_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
Result of the validation: Valid

Simulation: Human_SingleORAL_PolyParticlesLogNormal_AsSuspention-Human_SingleORAL_-PolyParticlesLogNormal_AsSuspention
Result of the validation: Valid

Simulation: Human_SingleORAL_PolyParticlesNormal_AsSuspention-Human_SingleORAL_PolyParticlesNo-AsSuspention
Result of the validation: Valid

Simulation: Human_SingleORAL_PolyParticlesNormal_AsSuspention-Human_SingleORAL_PolyParticlesNo-AsSuspention_dissolved_radius
Result of the validation: Valid

Simulation: Human_SingleORAL_PolyParticlesNormal_AsSuspention-Human_SingleORAL_PolyParticlesNo-AsSuspention_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_-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_-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_schmittnormlized_standard-SingleIV_C3_4Comp_standard_schmittnormlized_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