

Open Systems Pharmacology Suite - 11 Folder Comparison

gibpk

May 20, 2022

Contents

1	Folder Comparison Results	2
1.1	Comparison Results	2
1.1.1	Invalid Simulations (13/155)	2
1.1.2	Valid Simulations (142/155)	108

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_10.0

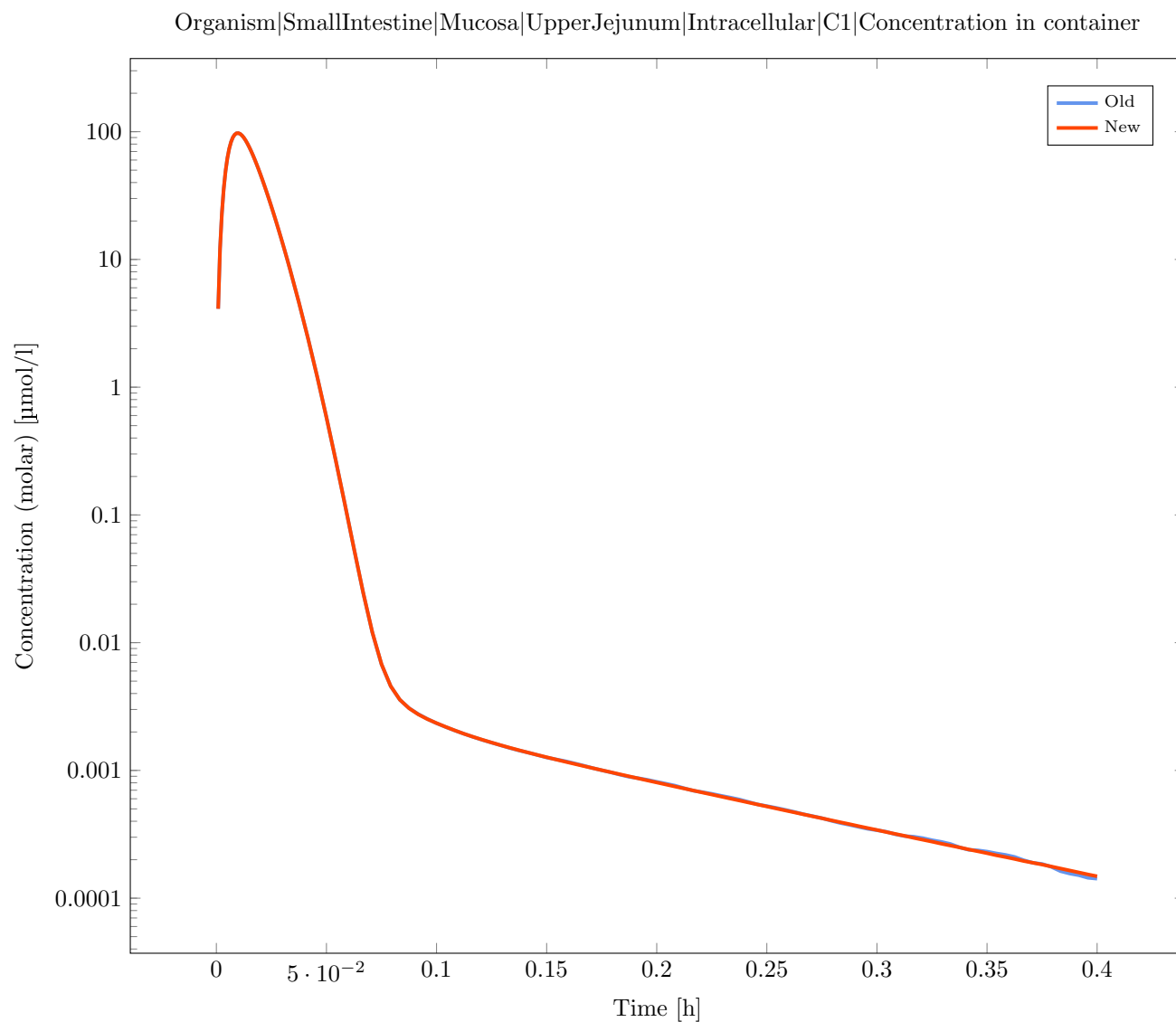
New Folder
D:\Outputs_11.0

Using exclusions
**|drug|Fraction of oral drug mass absorbed into mucosa segment
**|Receptor Occupancy-drug-BIND-Lab Complex

1.1.1 Invalid Simulations (13/155)

Simulation: DDI_MultipleCombinations-21_1st_Competitive_Competitive
Result of the validation: **Invalid**
Absolute Tolerance: 1.00E-8
Relative Tolerance: 1.00E-4

Output Path: Organism|SmallIntestine|Mucosa|UpperJejunum|Intracellular|C1|Concentration in container
Deviation for 'Organism|SmallIntestine|Mucosa|UpperJejunum|Intracellular|C1|Concentration in container' is 6.24% and is greater than the allowed max. tolerance of 3.00%
Deviation: 0.06

**Figure 1.1**

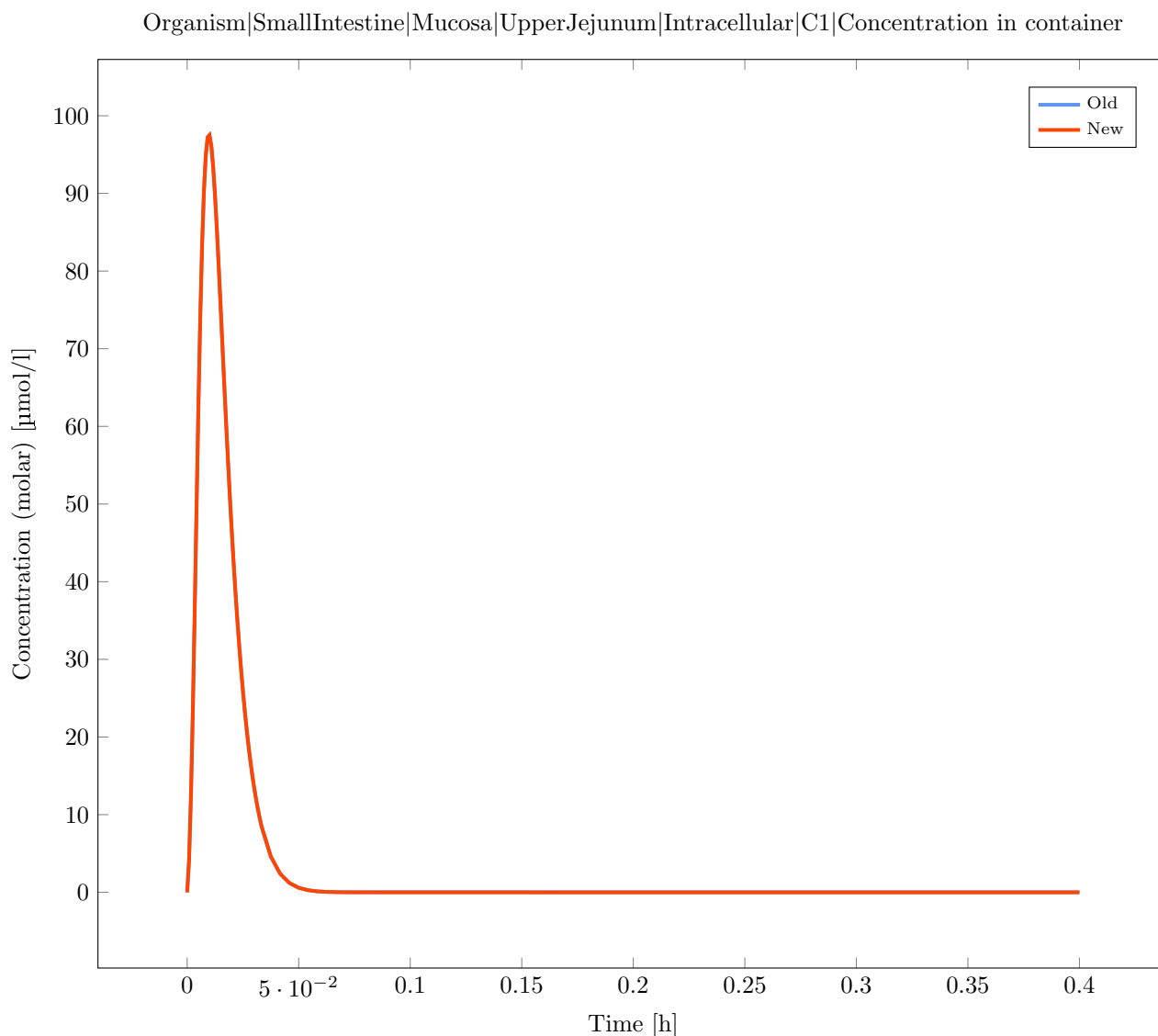


Figure 1.2

Simulation: Human_MultipleIV_PGPBasolateral-Human_MultipleIV_PGPBasolateralResult of the validation: **Invalid**

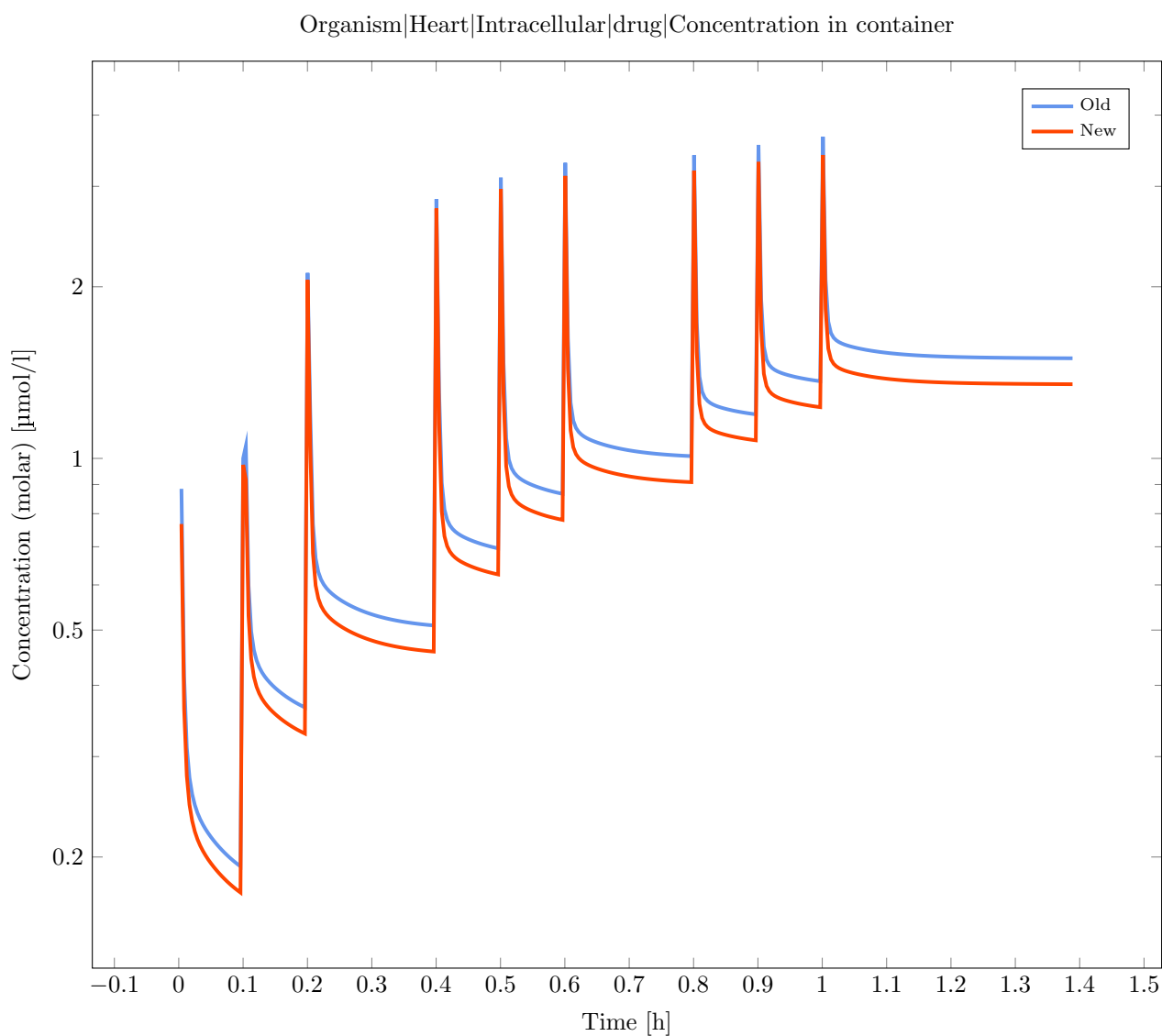
Absolute Tolerance: 1.00E-10

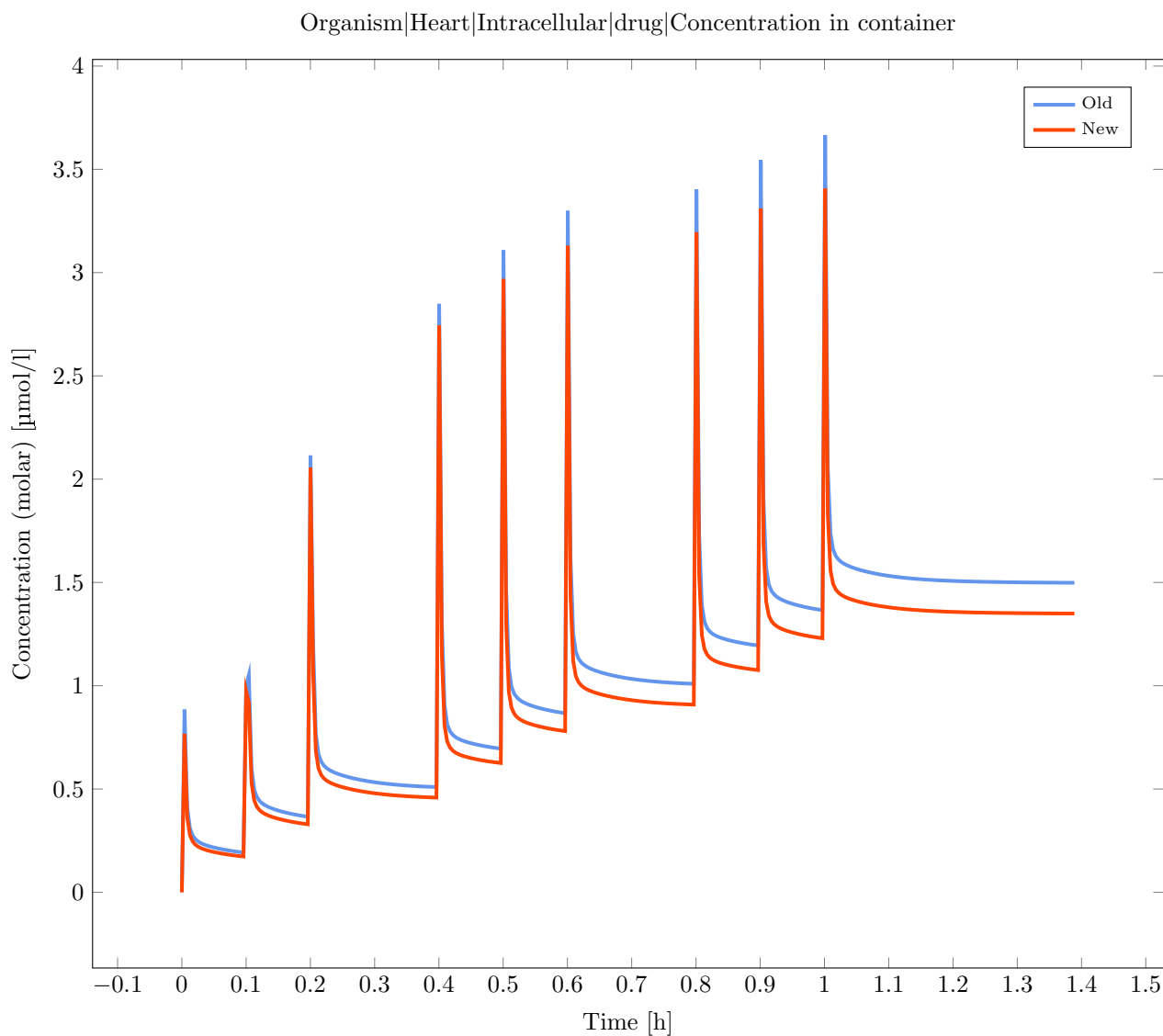
Relative Tolerance: 1.00E-5

Output Path: Organism|Heart|Intracellular|drug|Concentration in container

Deviation for 'Organism|Heart|Intracellular|drug|Concentration in container' is 13.22% and is greater than the allowed max. tolerance of 3.00%

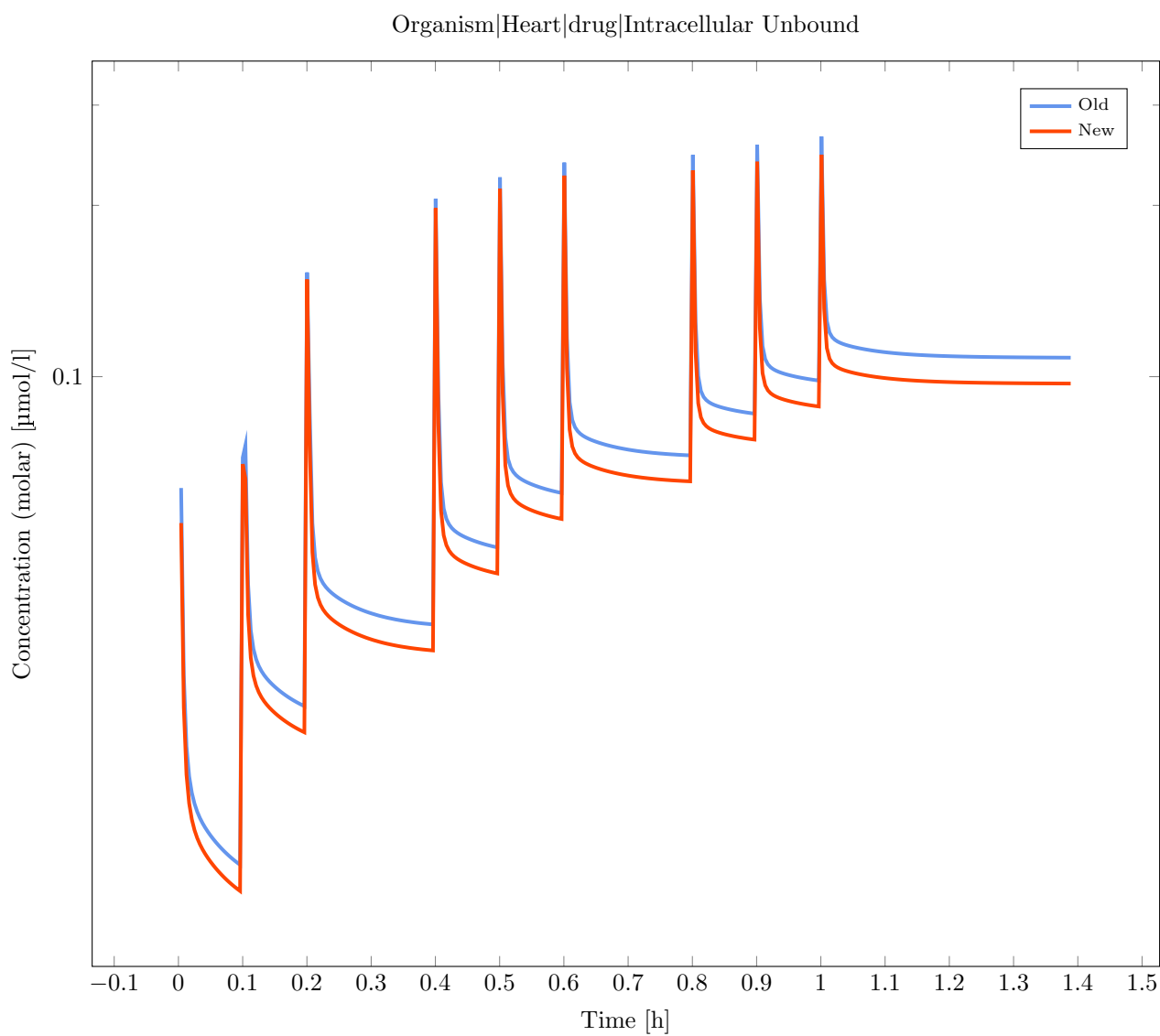
Deviation: 0.13

**Figure 1.3**

**Figure 1.4****Output Path: Organism|Heart|drug|Intracellular Unbound**

Deviation for 'Organism|Heart|drug|Intracellular Unbound' is 13.22% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.13

**Figure 1.5**

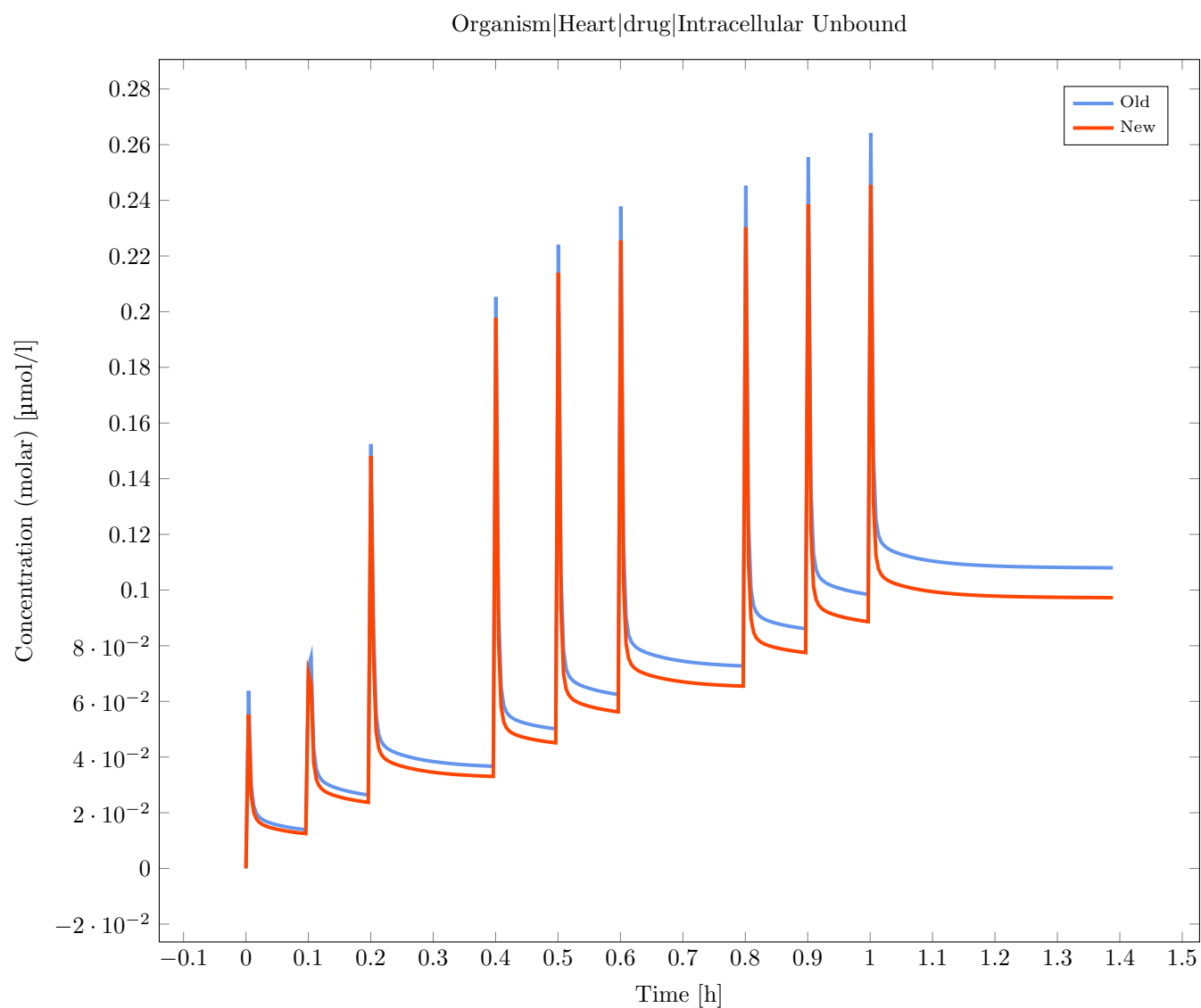
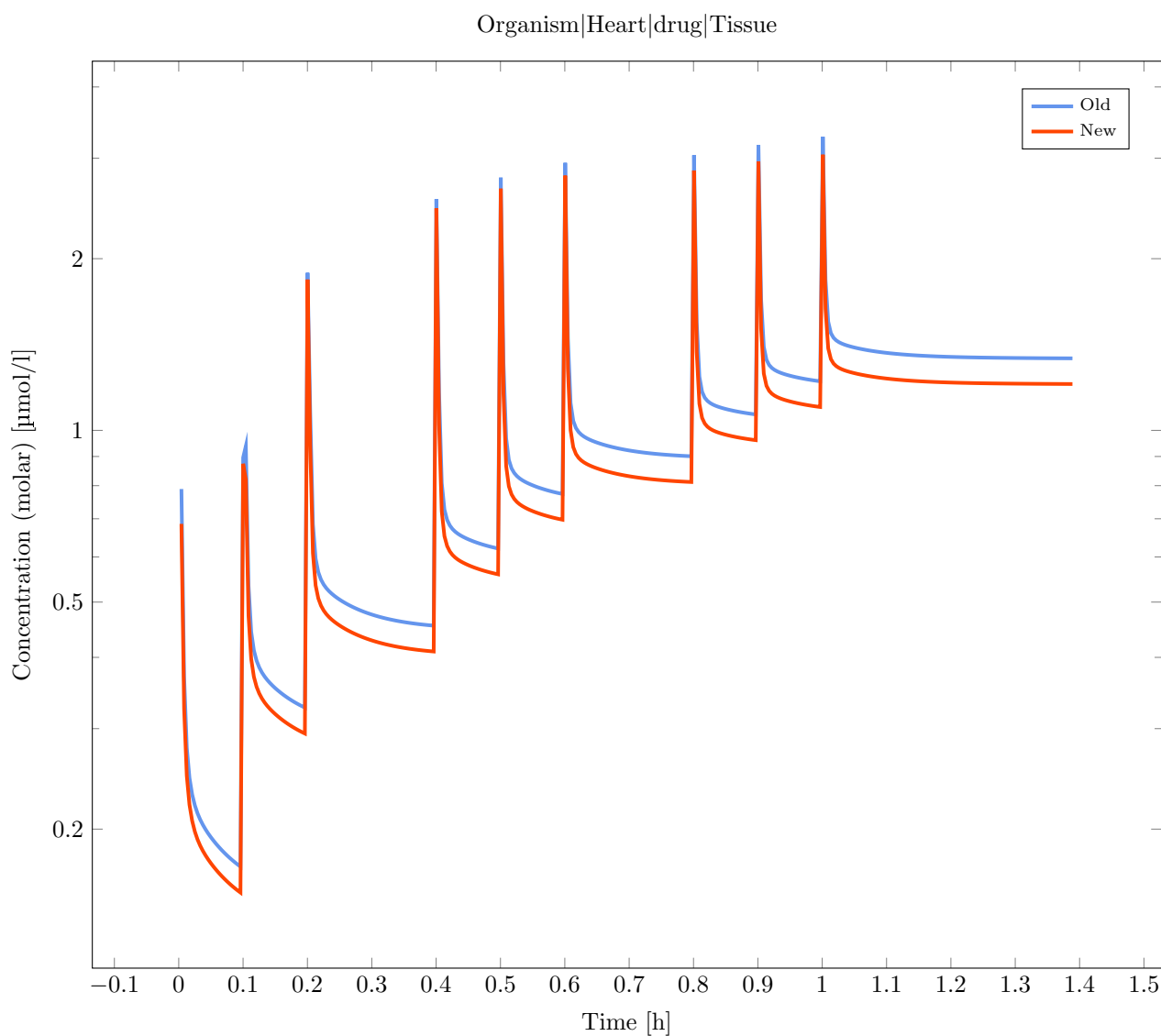
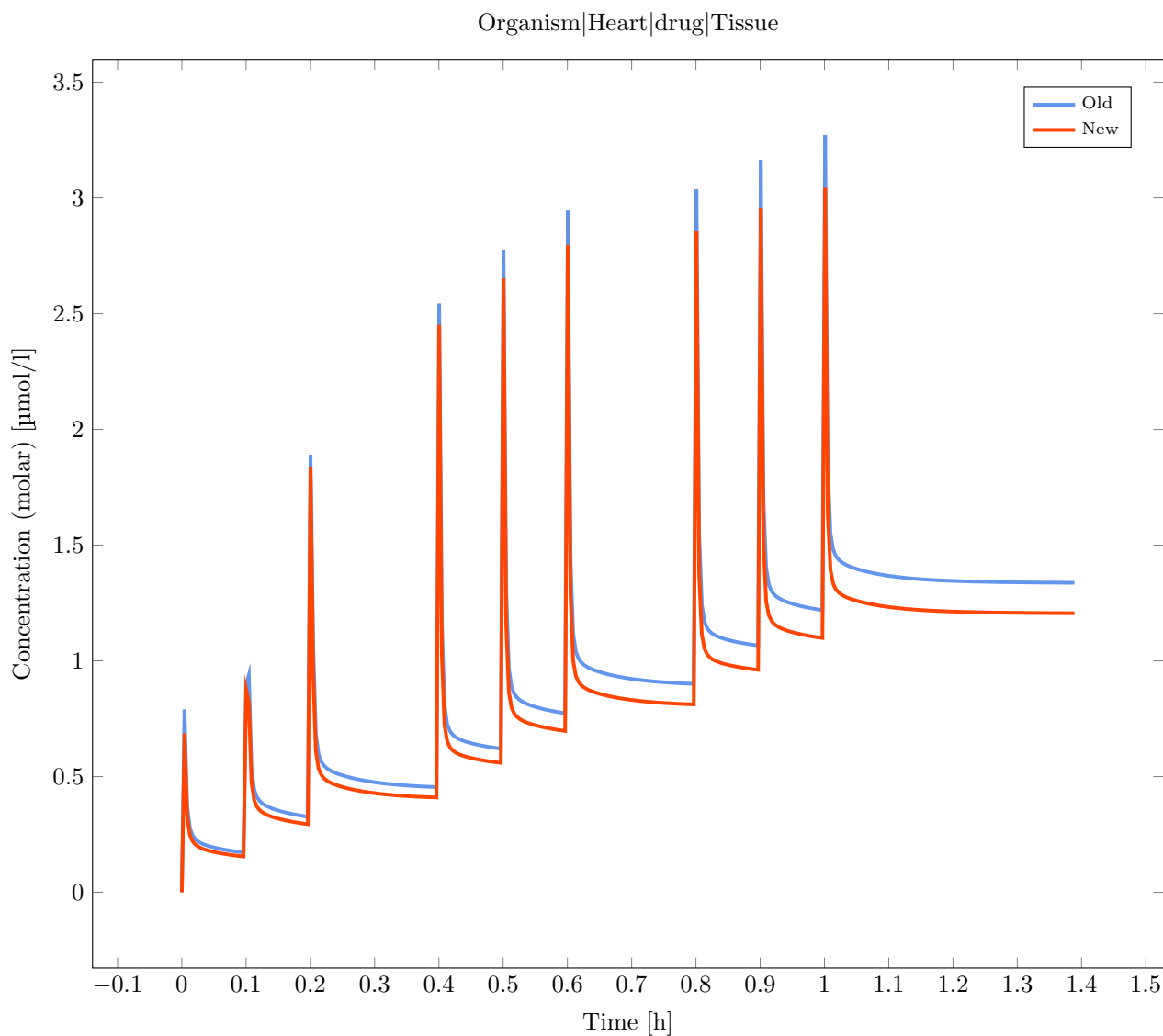


Figure 1.6

Output Path: Organism|Heart|drug|Tissue

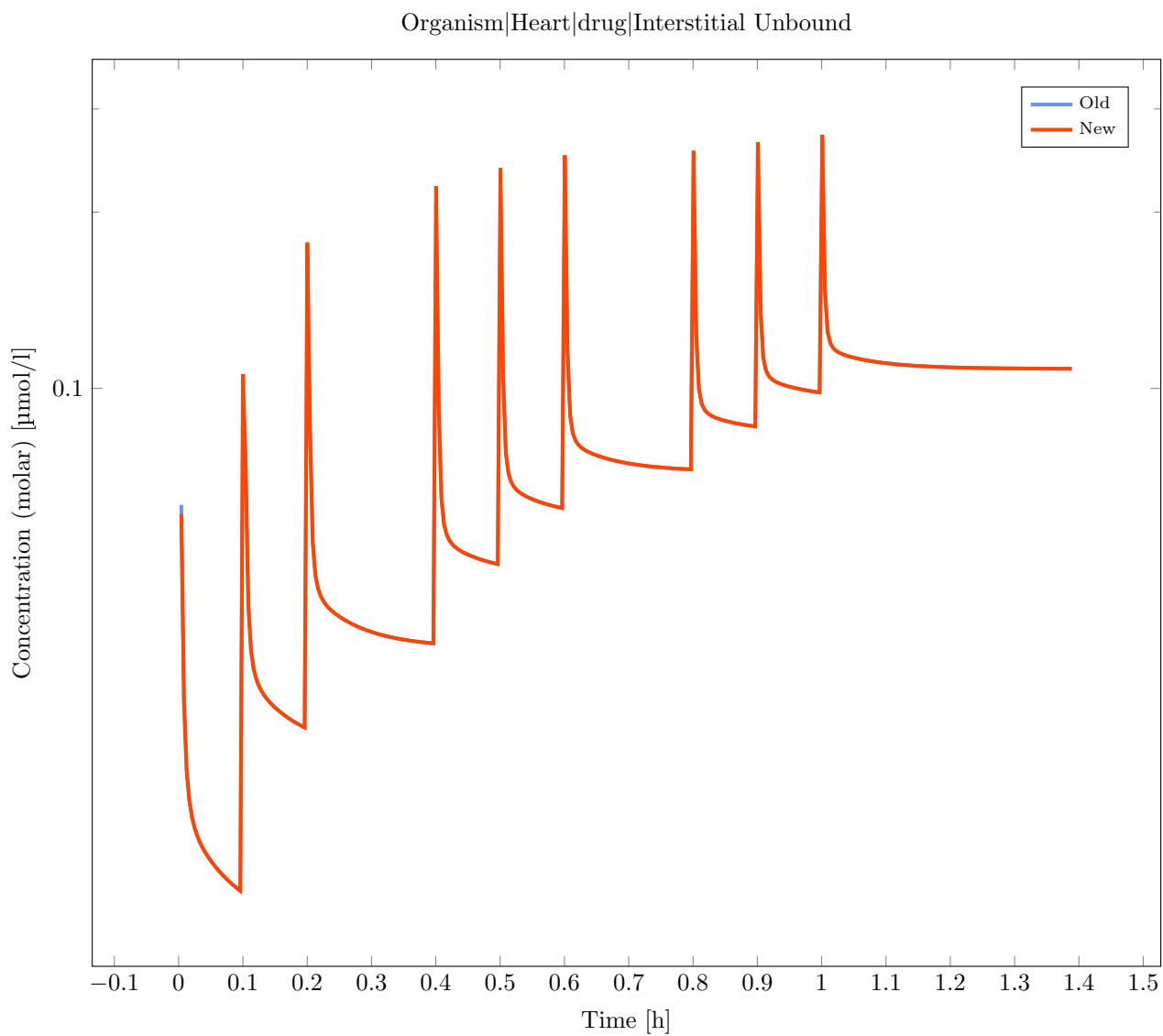
Deviation for 'Organism|Heart|drug|Tissue' is 13.13% and is greater than the allowed max. tolerance of 3.00%
 Deviation: 0.13

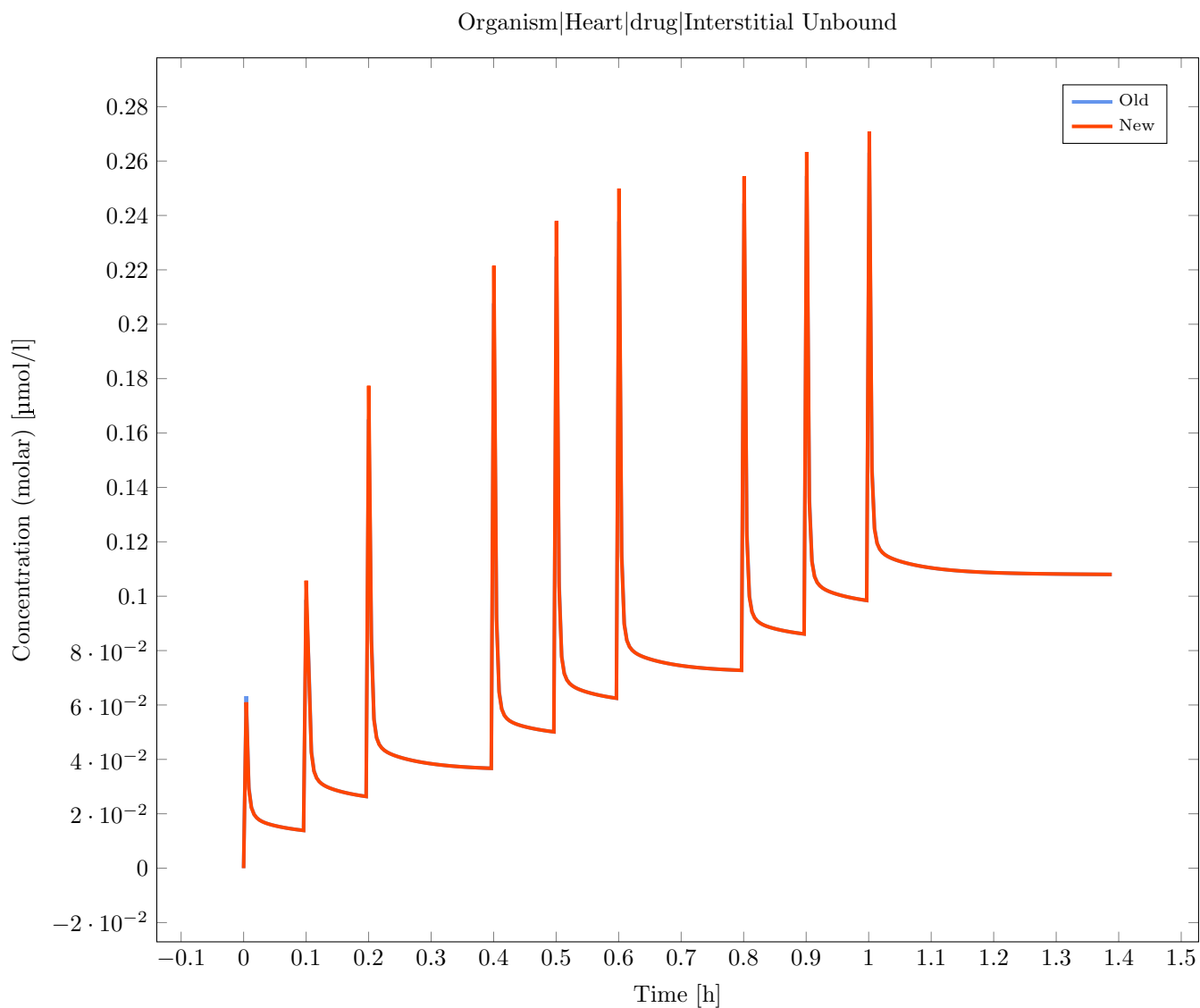
**Figure 1.7**

**Figure 1.8****Output Path: Organism|Heart|drug|Interstitial Unbound**

Deviation for 'Organism|Heart|drug|Interstitial Unbound' is 7.51% and is greater than the allowed max. tolerance of 3.00%

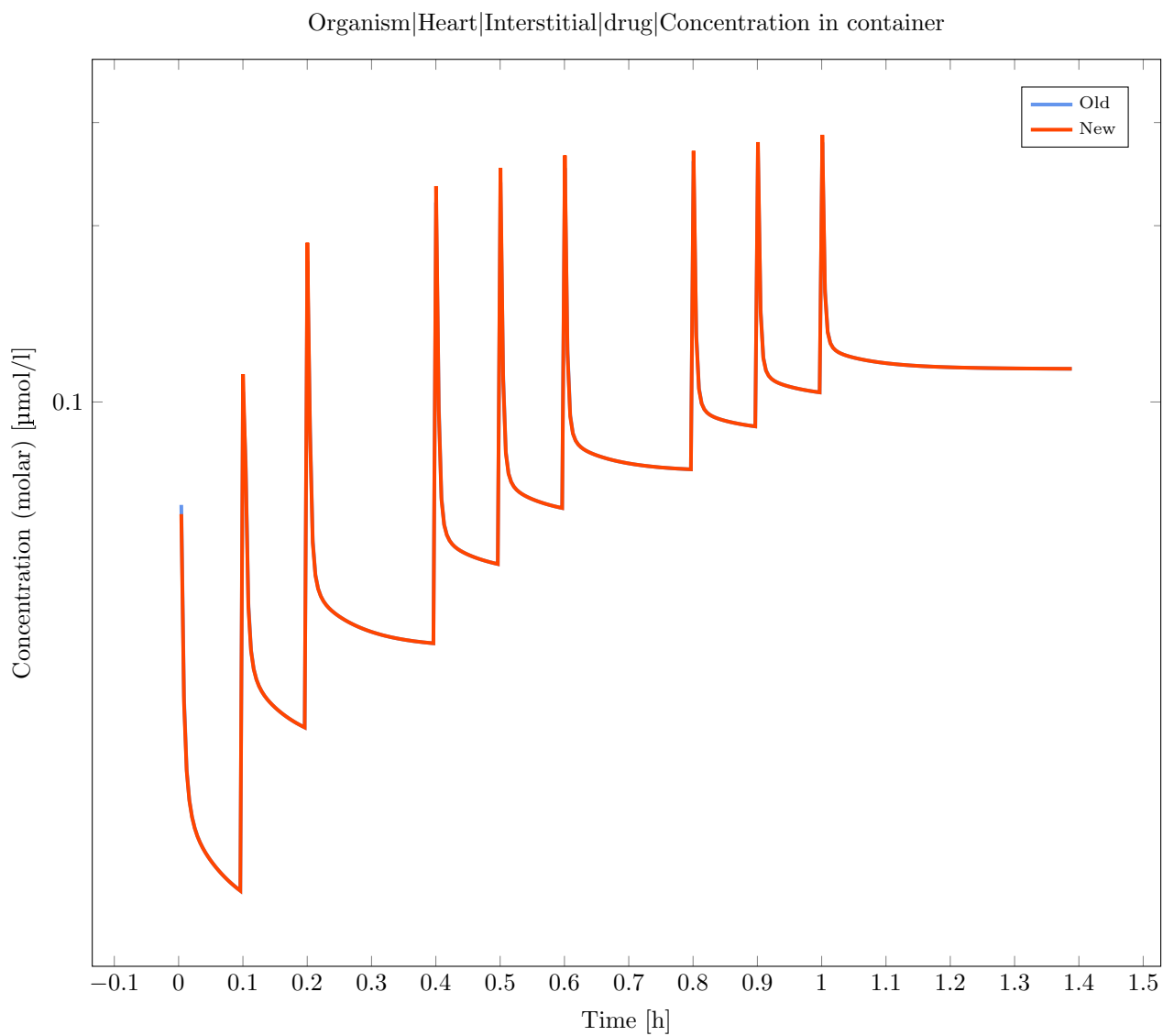
Deviation: 0.08

**Figure 1.9**

**Figure 1.10****Output Path: Organism|Heart|Interstitial|drug|Concentration in container**

Deviation for 'Organism|Heart|Interstitial|drug|Concentration in container' is 7.51% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.08

**Figure 1.11**

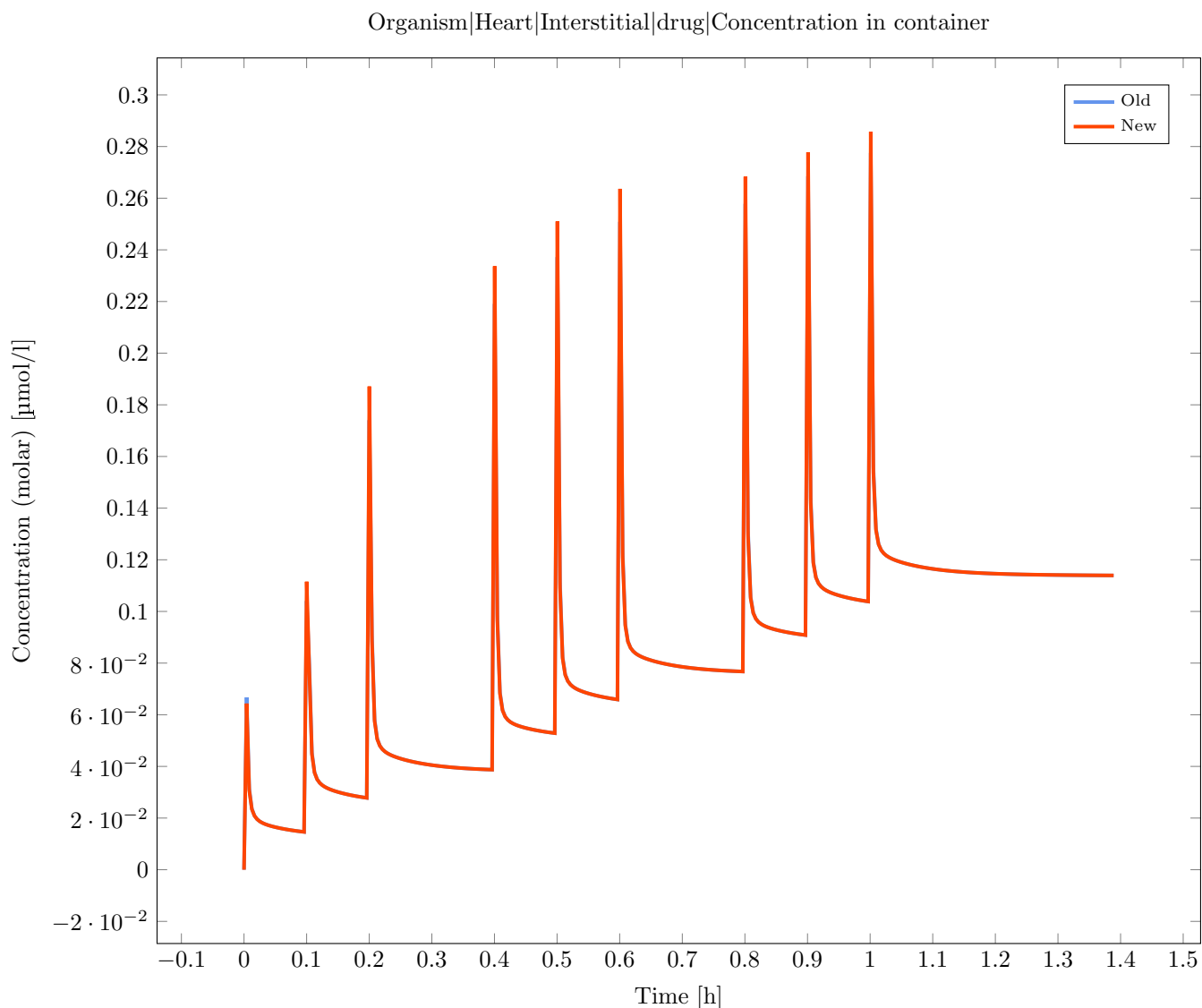


Figure 1.12

Simulation: Human_MultipleIV_PGP-Human_MultipleIV_PGPResult of the validation: **Invalid**

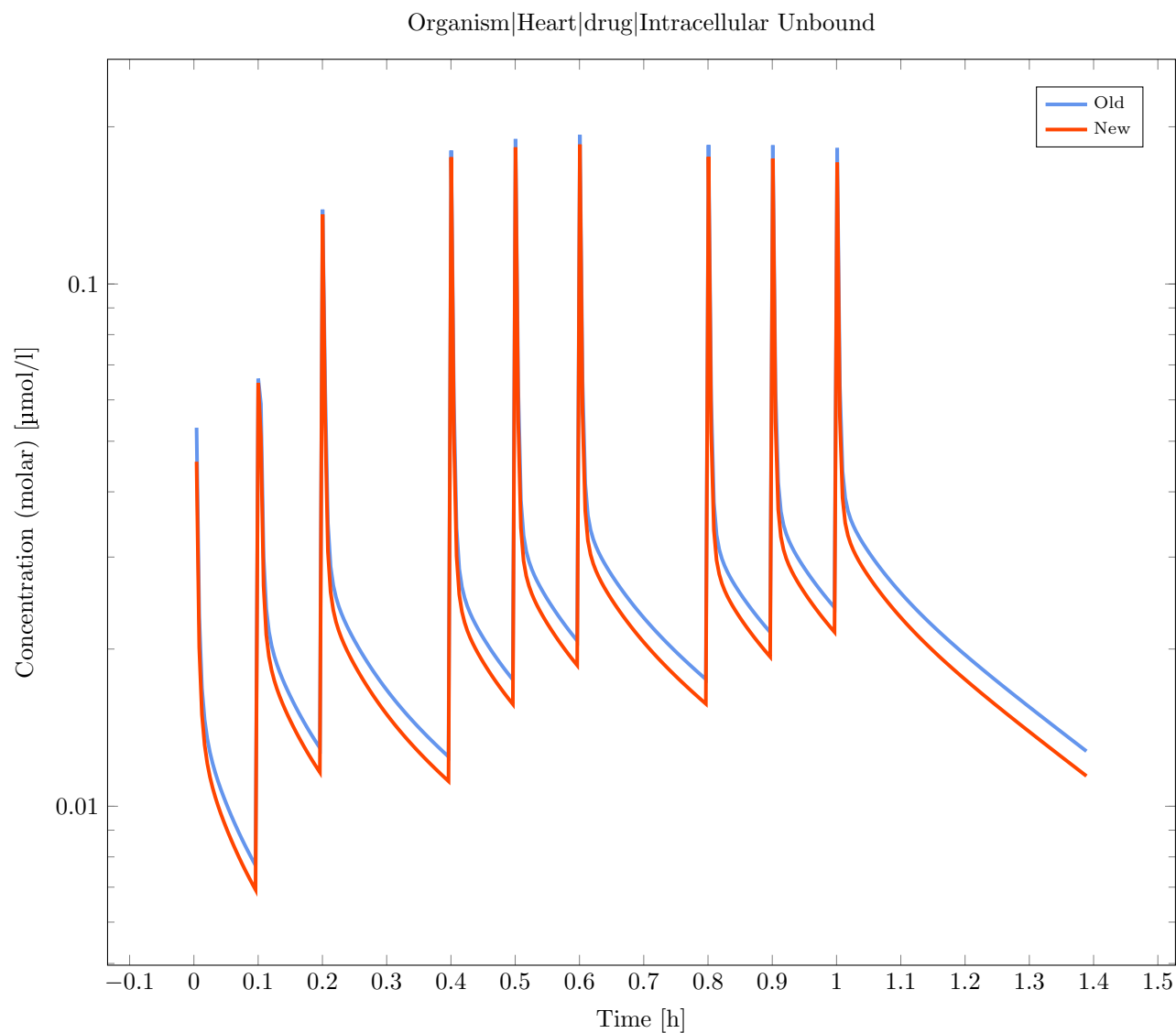
Absolute Tolerance: 1.00E-10

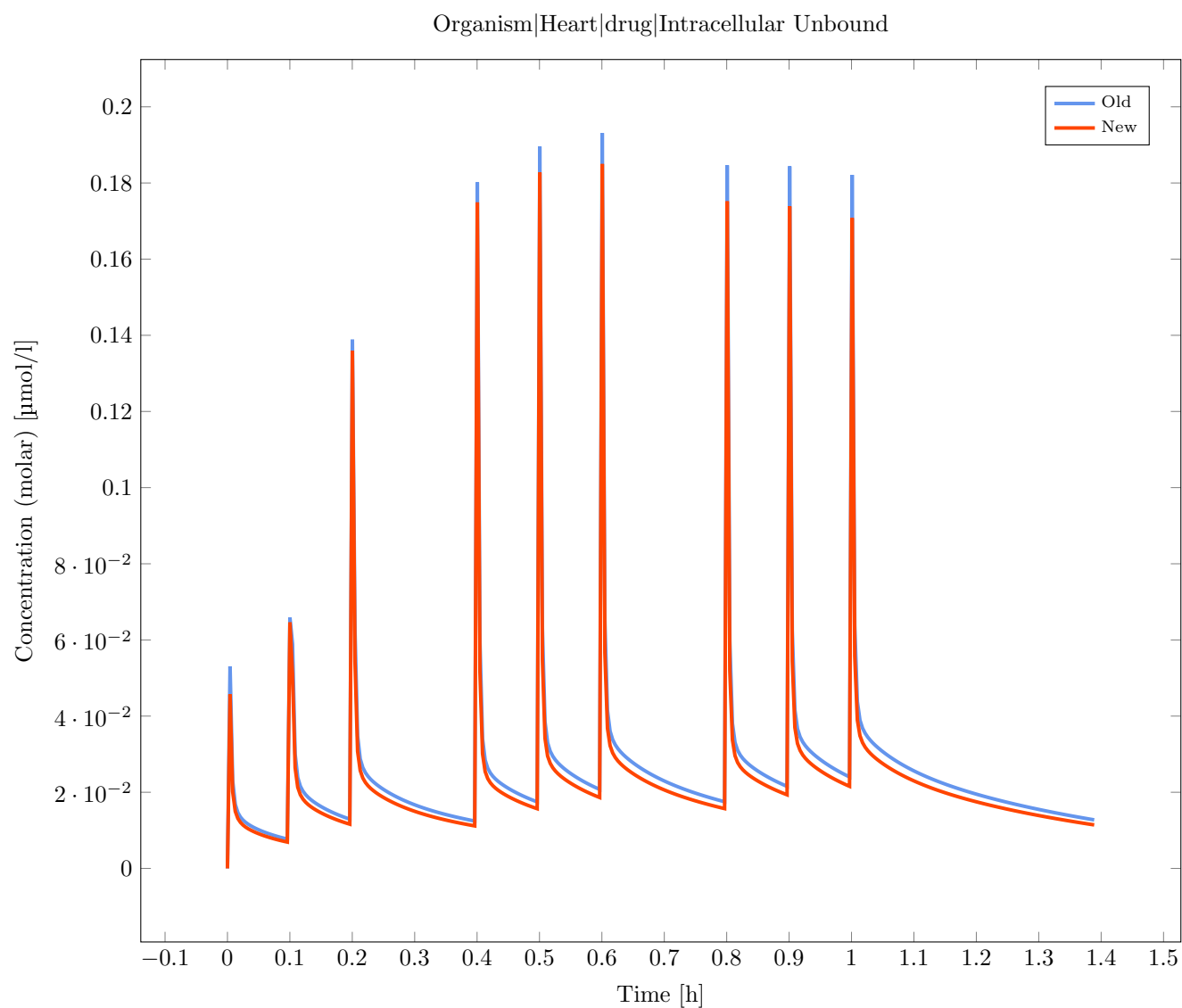
Relative Tolerance: 1.00E-5

Output Path: Organism|Heart|drug|Intracellular Unbound

Deviation for 'Organism|Heart|drug|Intracellular Unbound' is 13.93% and is greater than the allowed max. tolerance of 3.00%

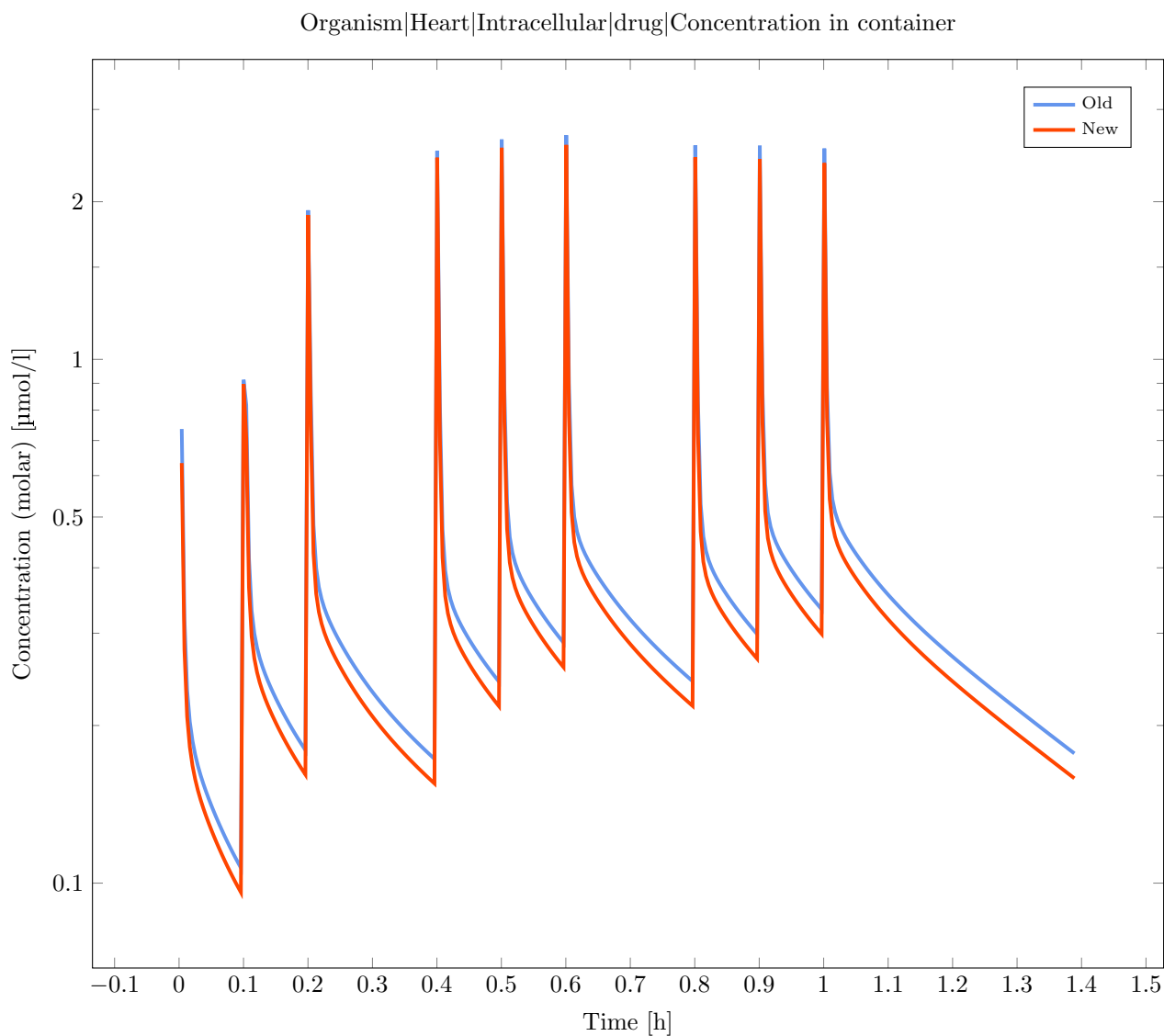
Deviation: 0.14

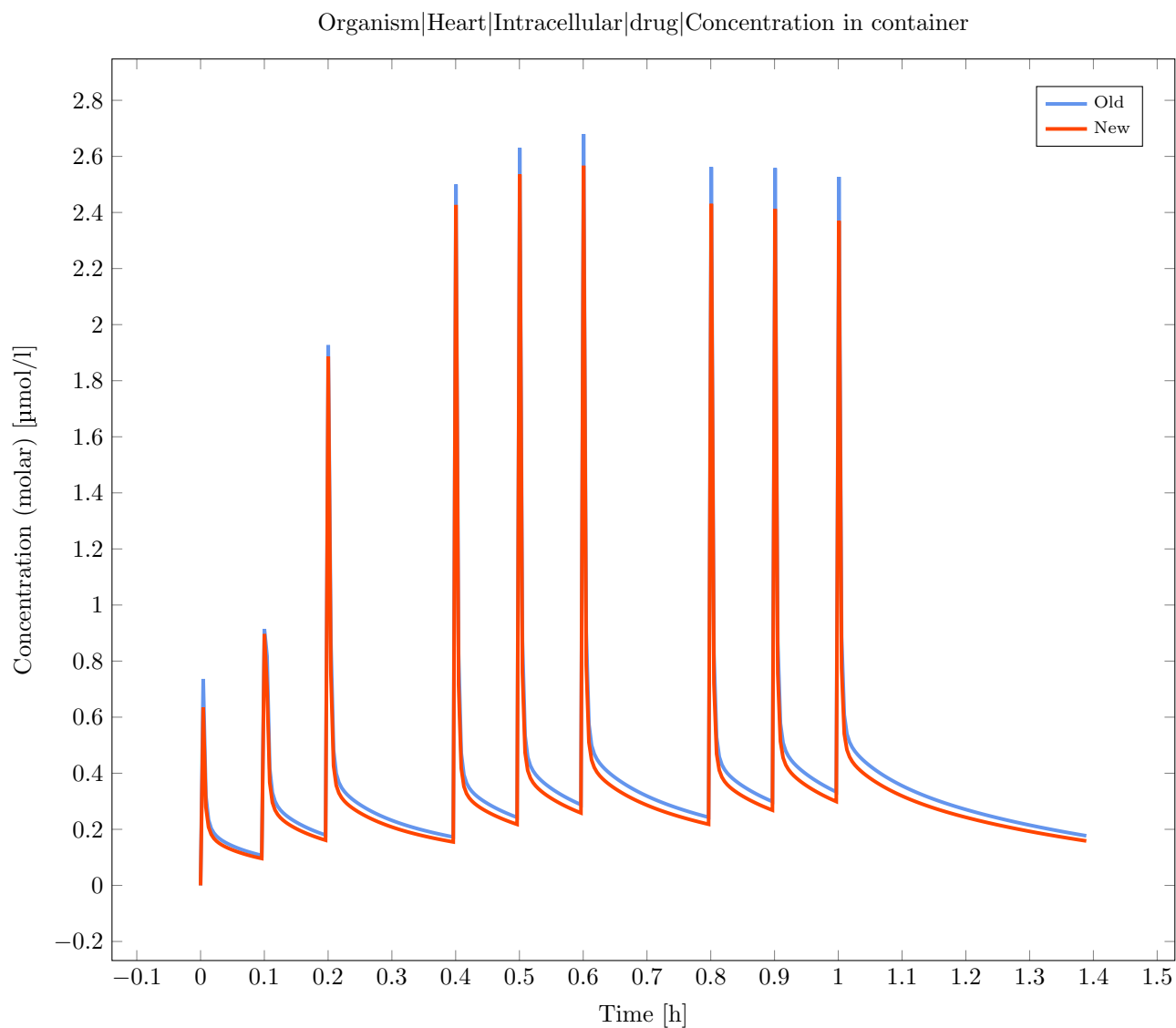
**Figure 1.13**

**Figure 1.14****Output Path: Organism|Heart|Intracellular|drug|Concentration in container**

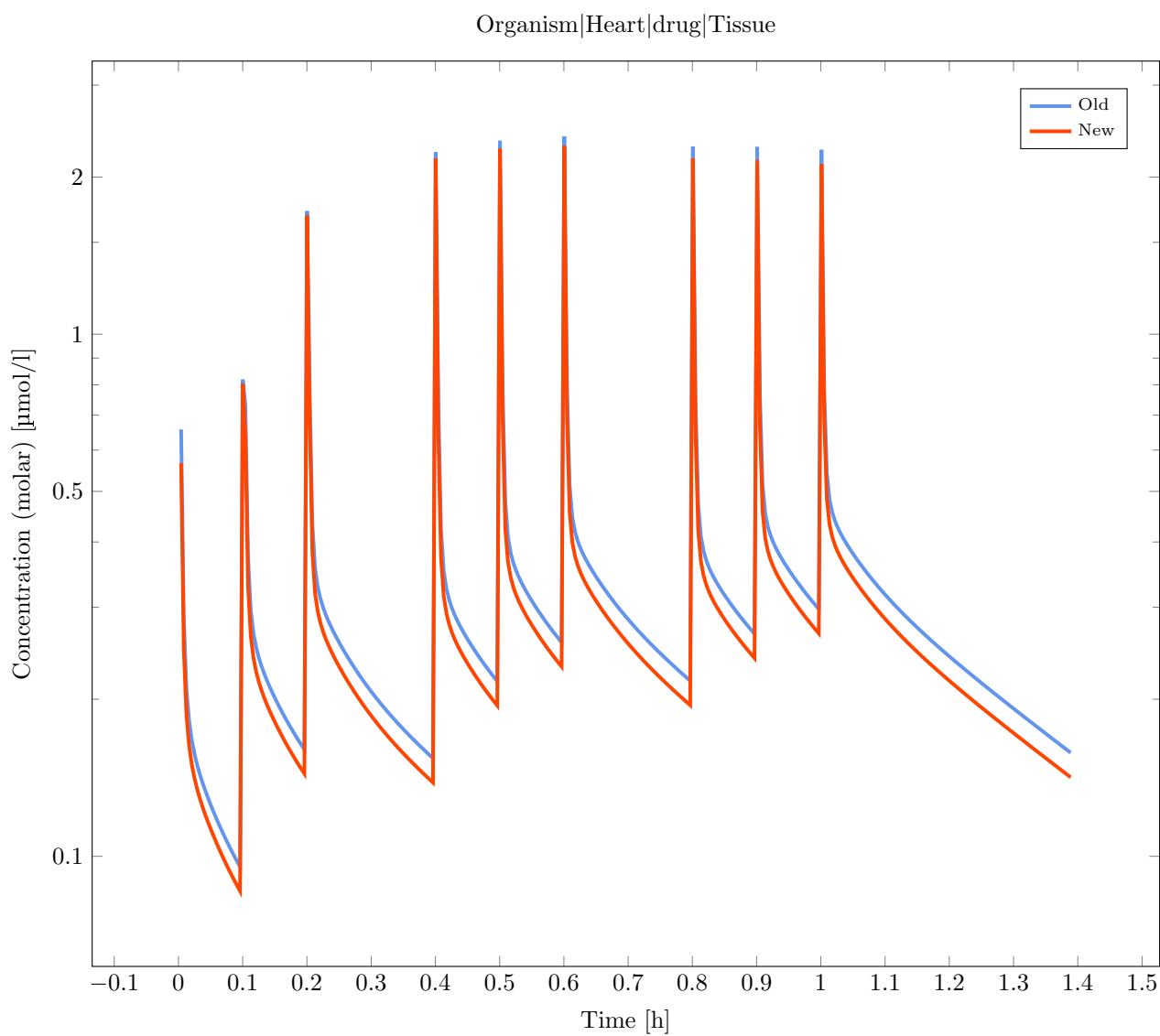
Deviation for 'Organism|Heart|Intracellular|drug|Concentration in container' is 13.93% and is greater than the allowed max. tolerance of 3.00%

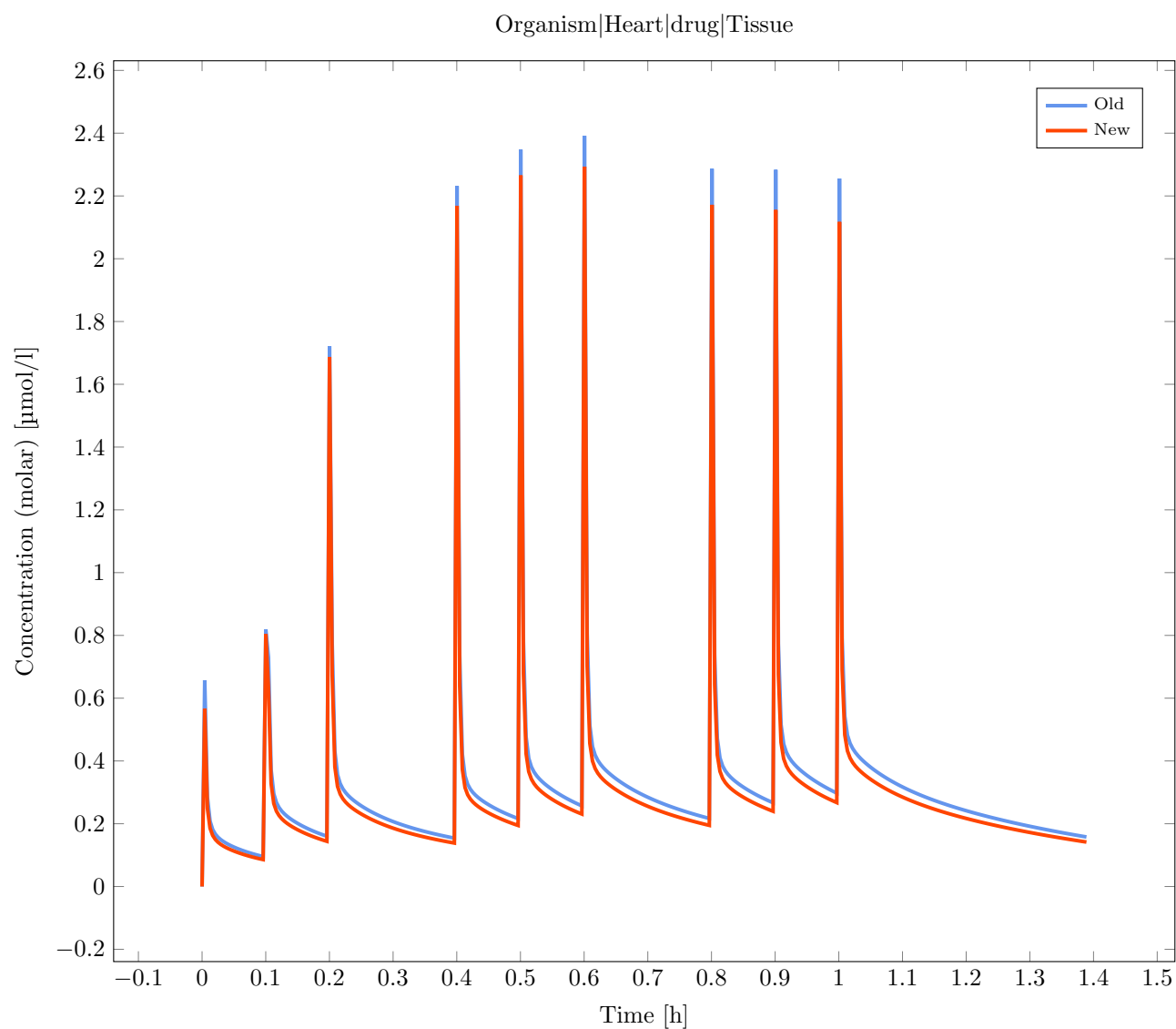
Deviation: 0.14

**Figure 1.15**

**Figure 1.16****Output Path: Organism|Heart|drug|Tissue**

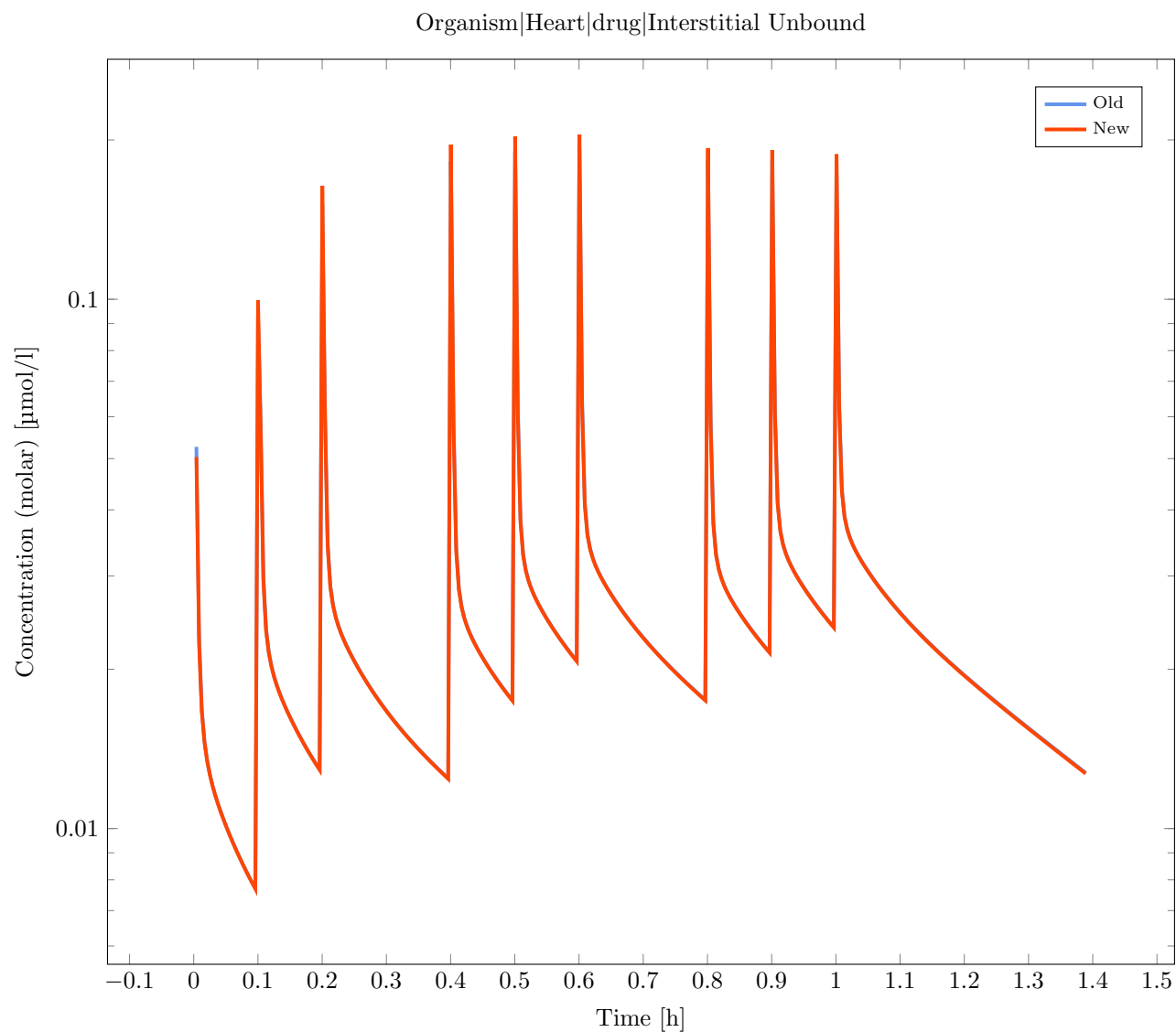
Deviation for 'Organism|Heart|drug|Tissue' is 13.83% and is greater than the allowed max. tolerance of 3.00%
Deviation: 0.14

**Figure 1.17**

**Figure 1.18****Output Path: Organism|Heart|drug|Interstitial Unbound**

Deviation for 'Organism|Heart|drug|Interstitial Unbound' is 8.18% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.08

**Figure 1.19**

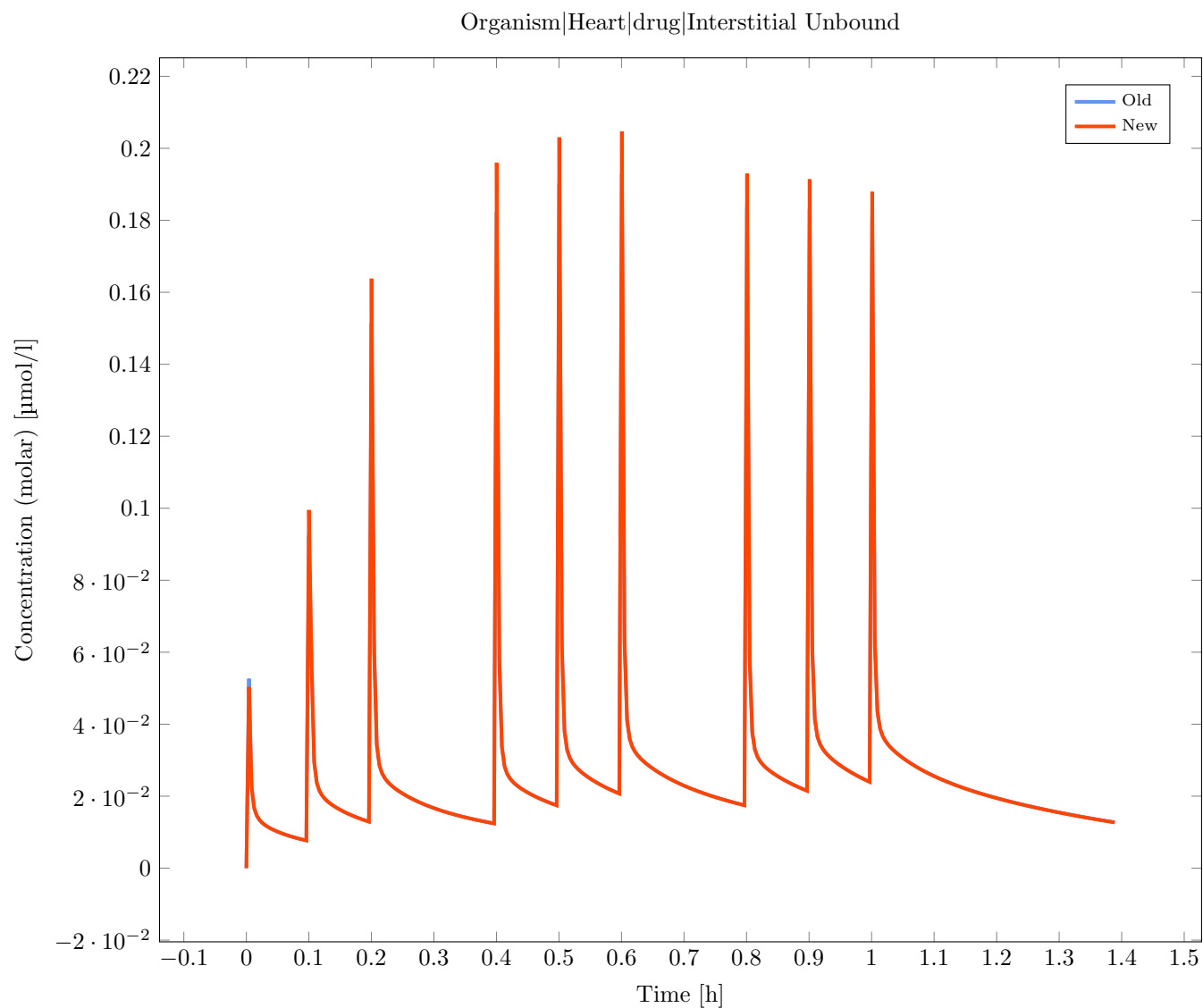
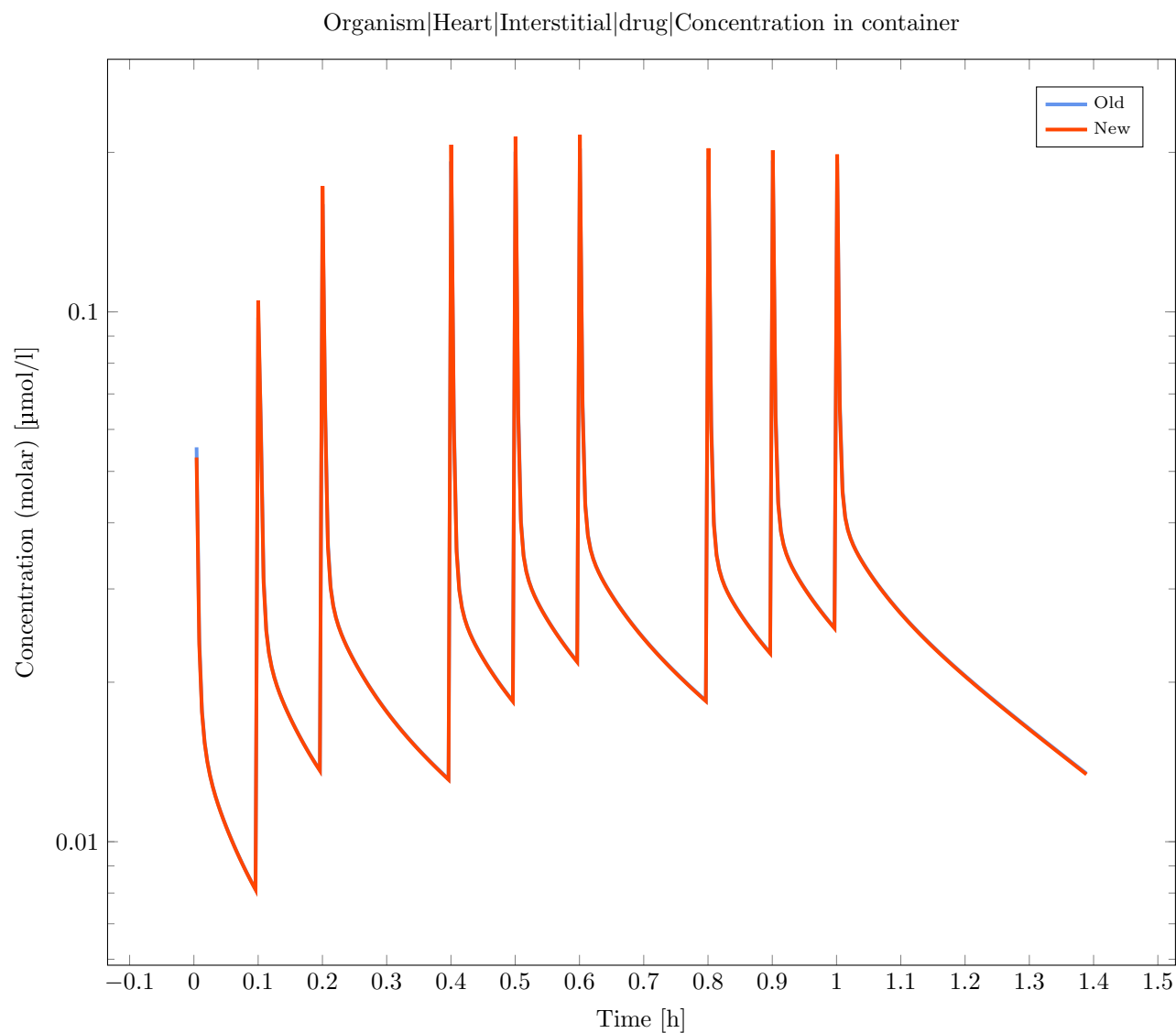


Figure 1.20

Output Path: Organism|Heart|Interstitial|drug|Concentration in container

Deviation for 'Organism|Heart|Interstitial|drug|Concentration in container' is 8.18% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.08

**Figure 1.21**

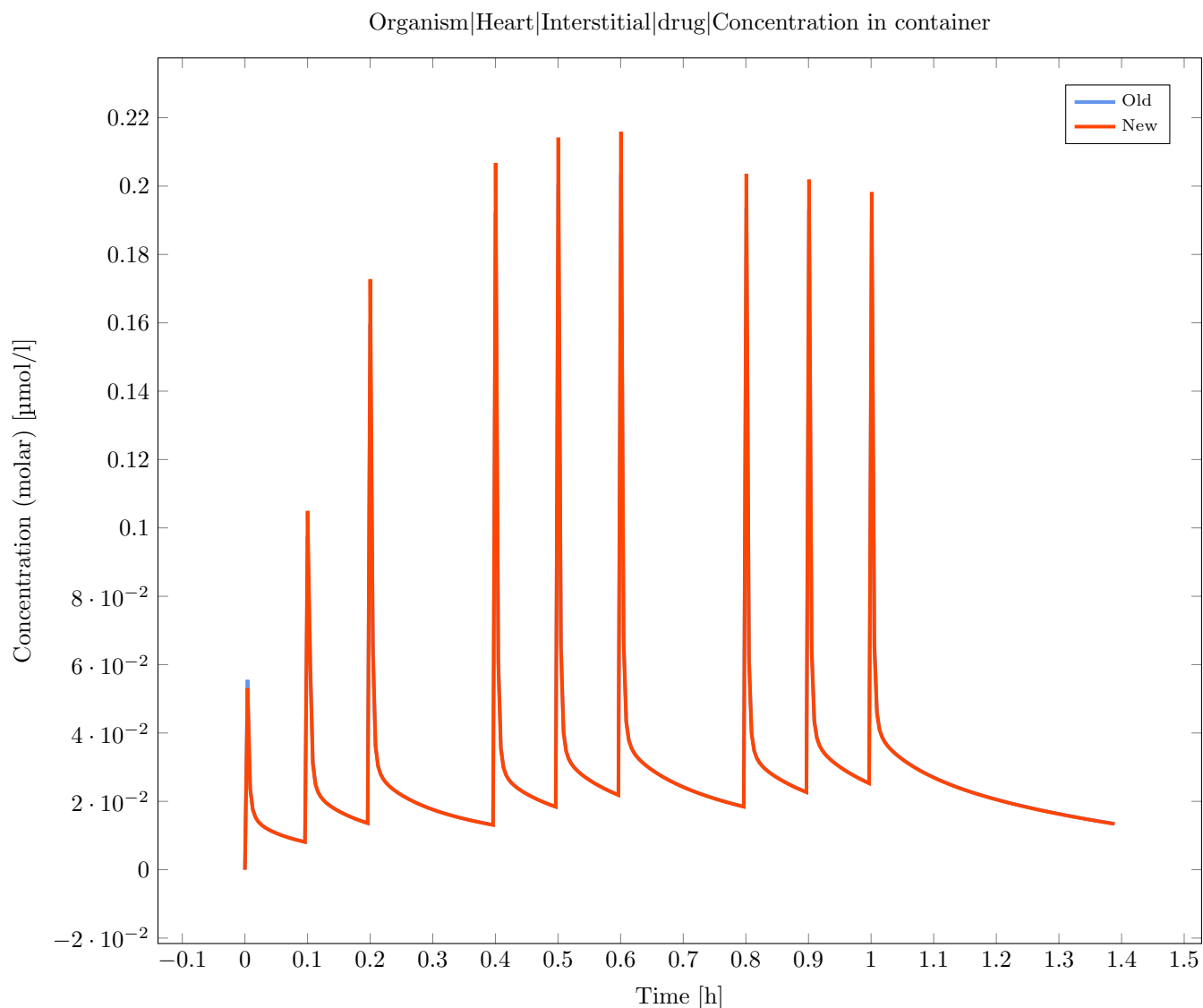


Figure 1.22

Simulation: Human_Oral_BiDaily_TableFormulation-S2_NoSuspensionResult of the validation: **Invalid**

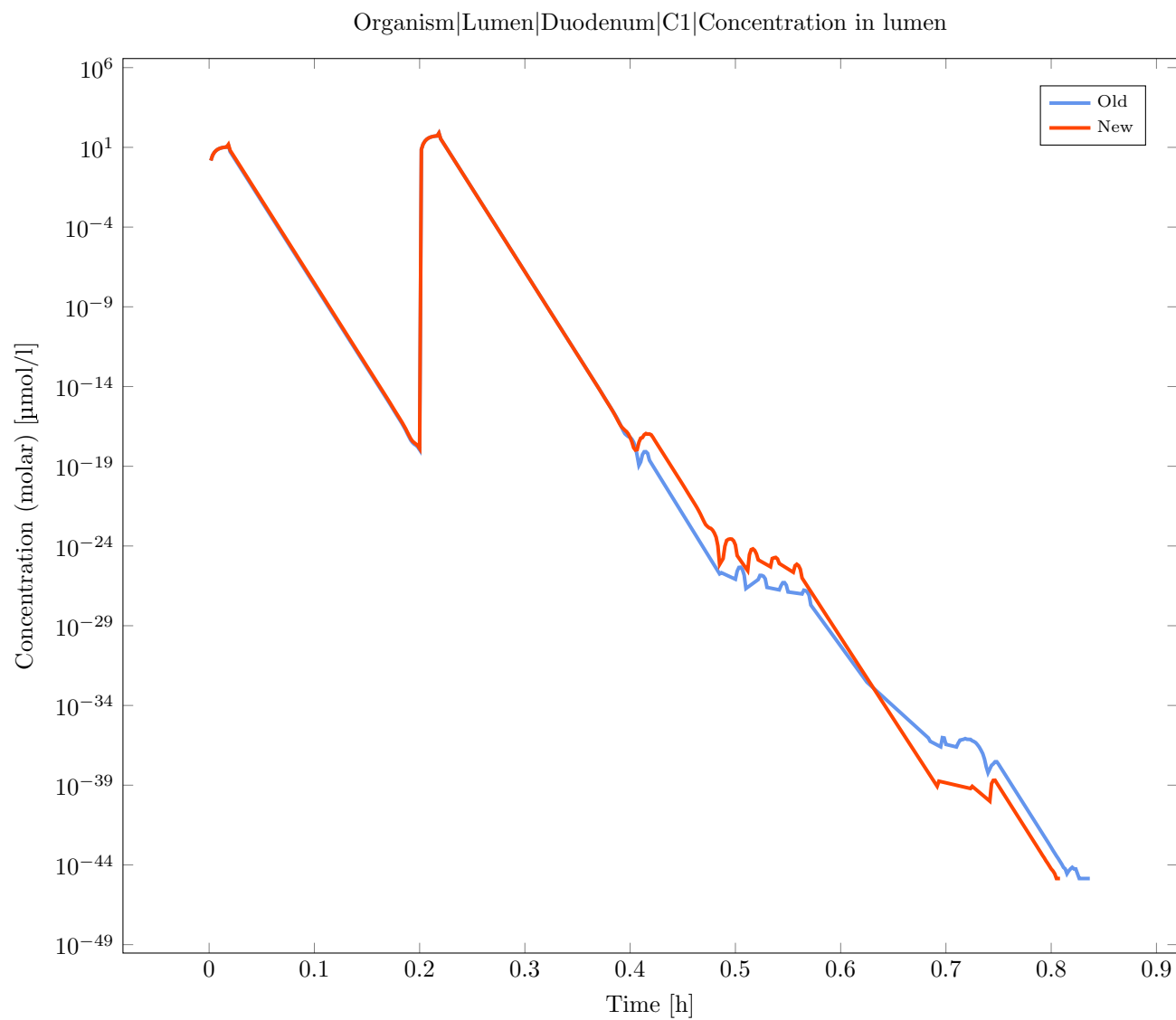
Absolute Tolerance: 1.00E-10

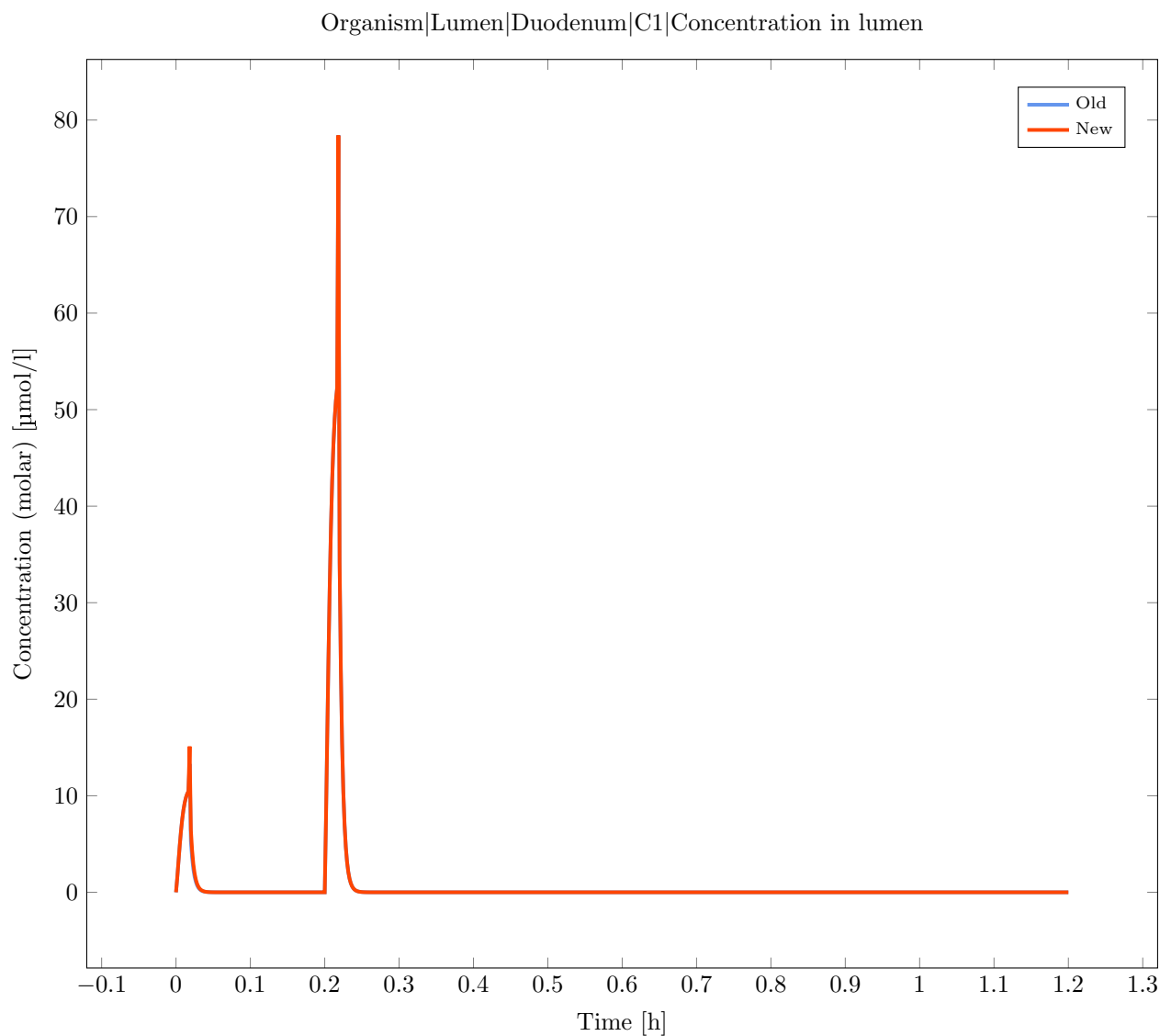
Relative Tolerance: 1.00E-5

Output Path: Organism|Lumen|Duodenum|C1|Concentration in lumen

Deviation for 'Organism|Lumen|Duodenum|C1|Concentration in lumen' is 22.20% and is greater than the allowed max. tolerance of 3.00%

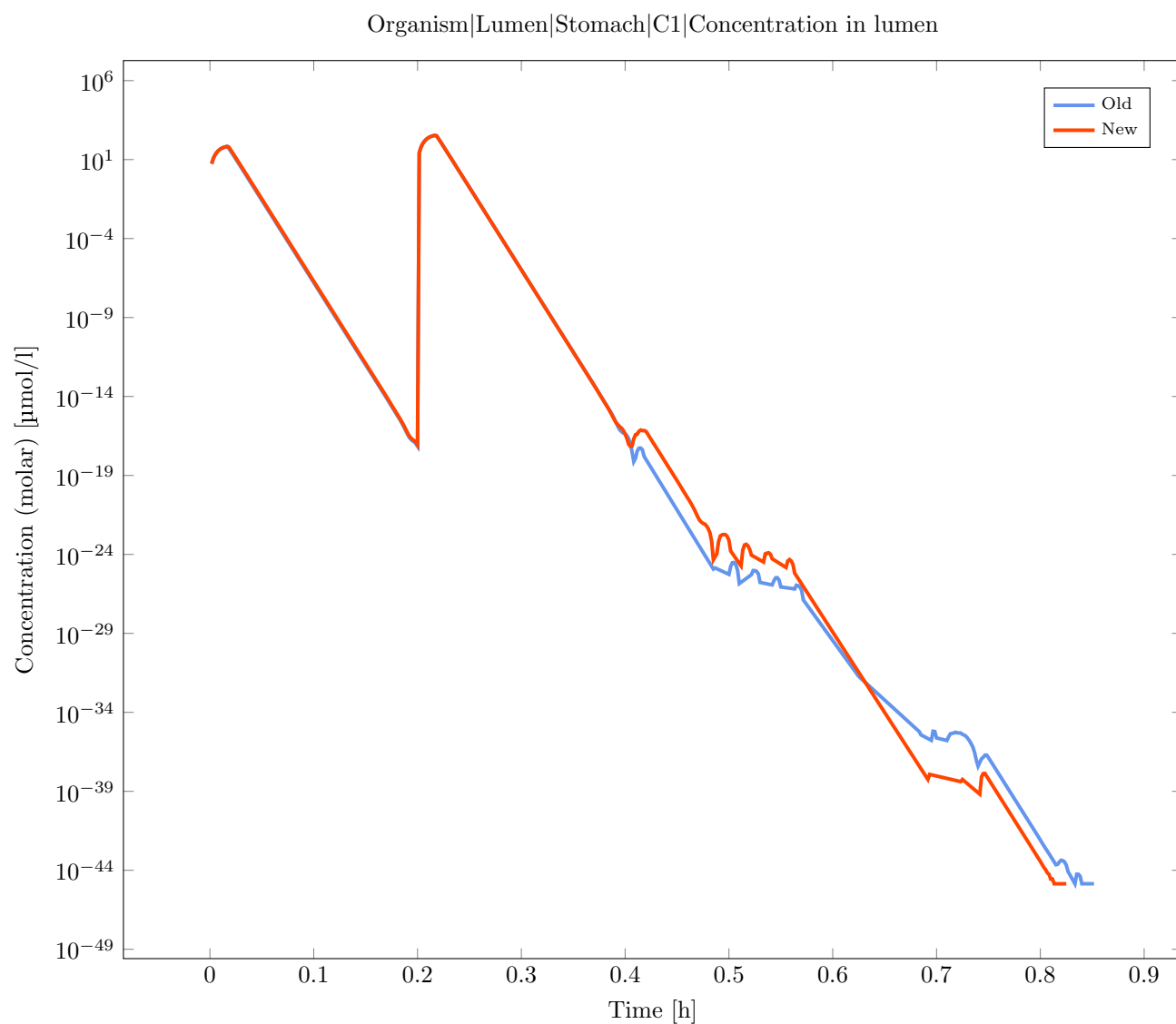
Deviation: 0.22

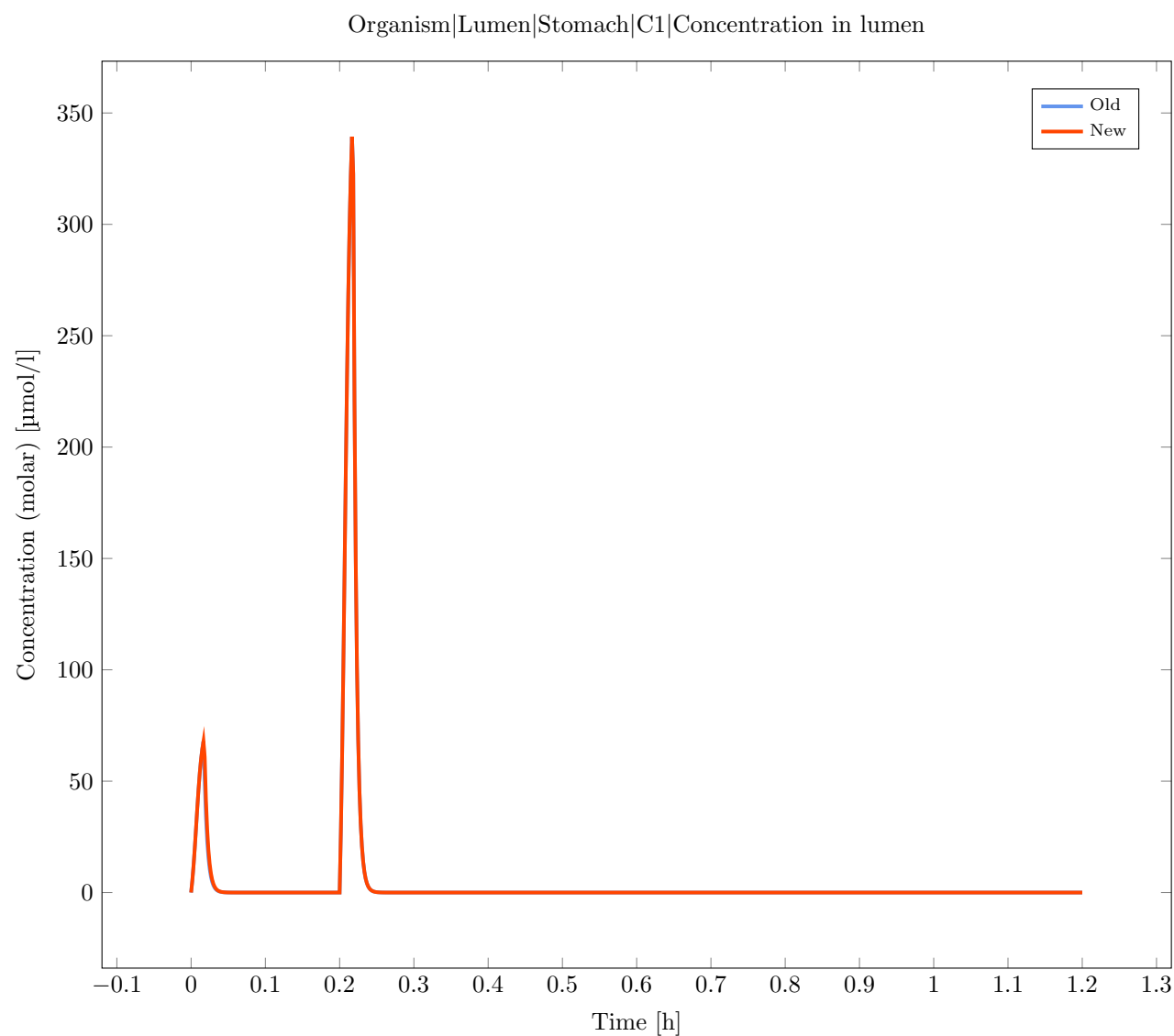
**Figure 1.23**

**Figure 1.24****Output Path: Organism|Lumen|Stomach|C1|Concentration in lumen**

Deviation for 'Organism|Lumen|Stomach|C1|Concentration in lumen' is 22.20% and is greater than the allowed max. tolerance of 3.00%

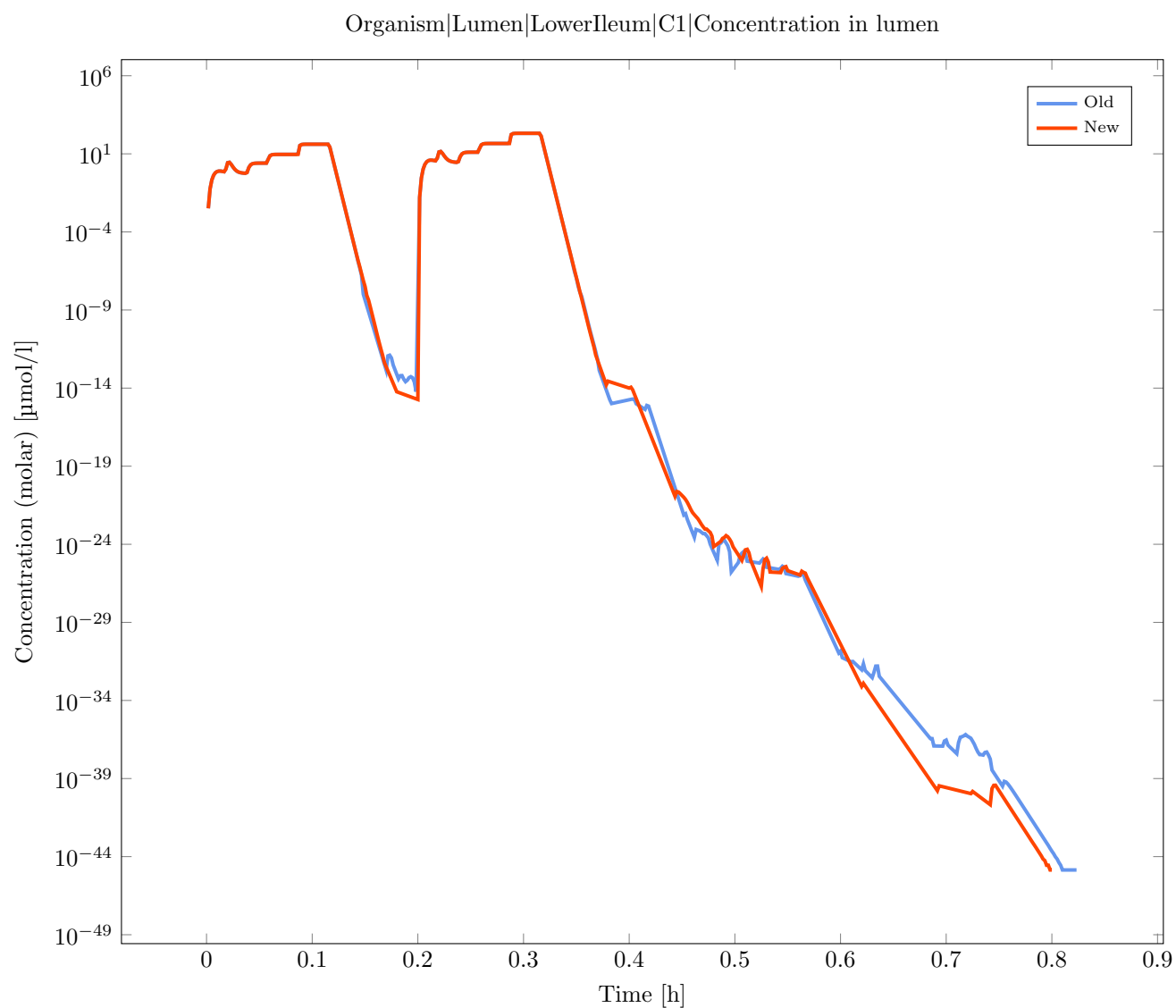
Deviation: 0.22

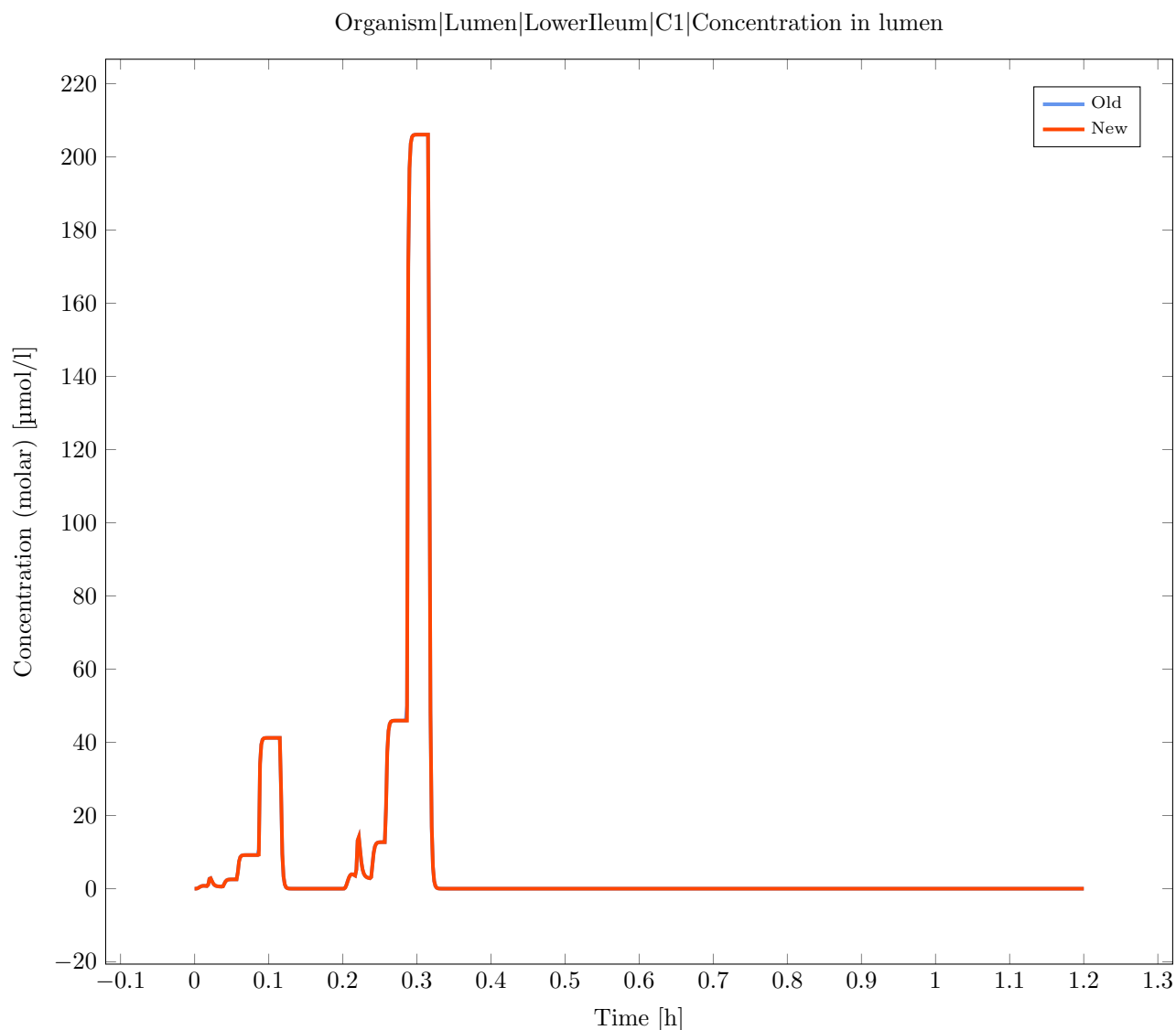
**Figure 1.25**

**Figure 1.26****Output Path: Organism|Lumen|LowerIleum|C1|Concentration in lumen**

Deviation for 'Organism|Lumen|LowerIleum|C1|Concentration in lumen' is 13.15% and is greater than the allowed max. tolerance of 3.00%

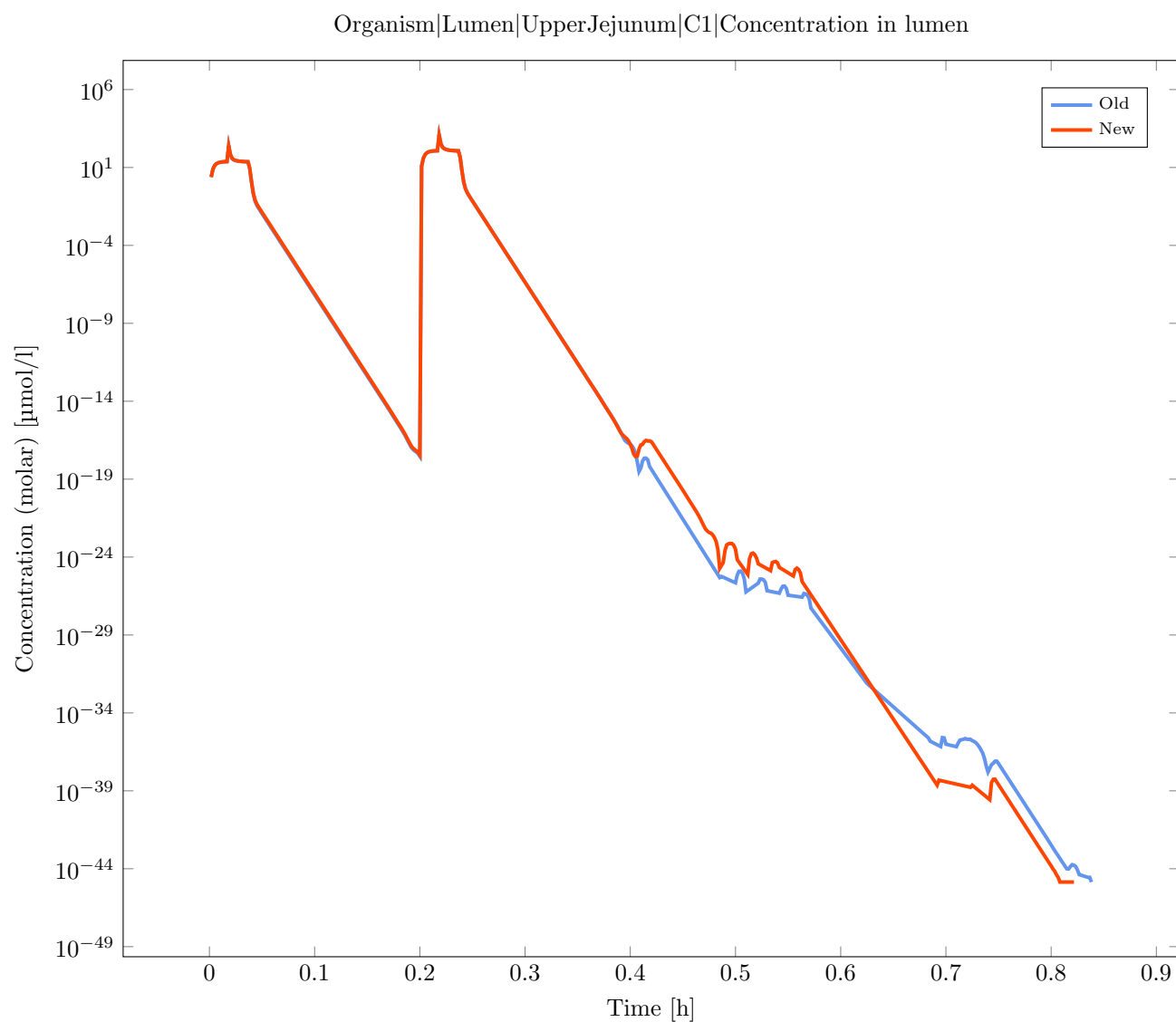
Deviation: 0.13

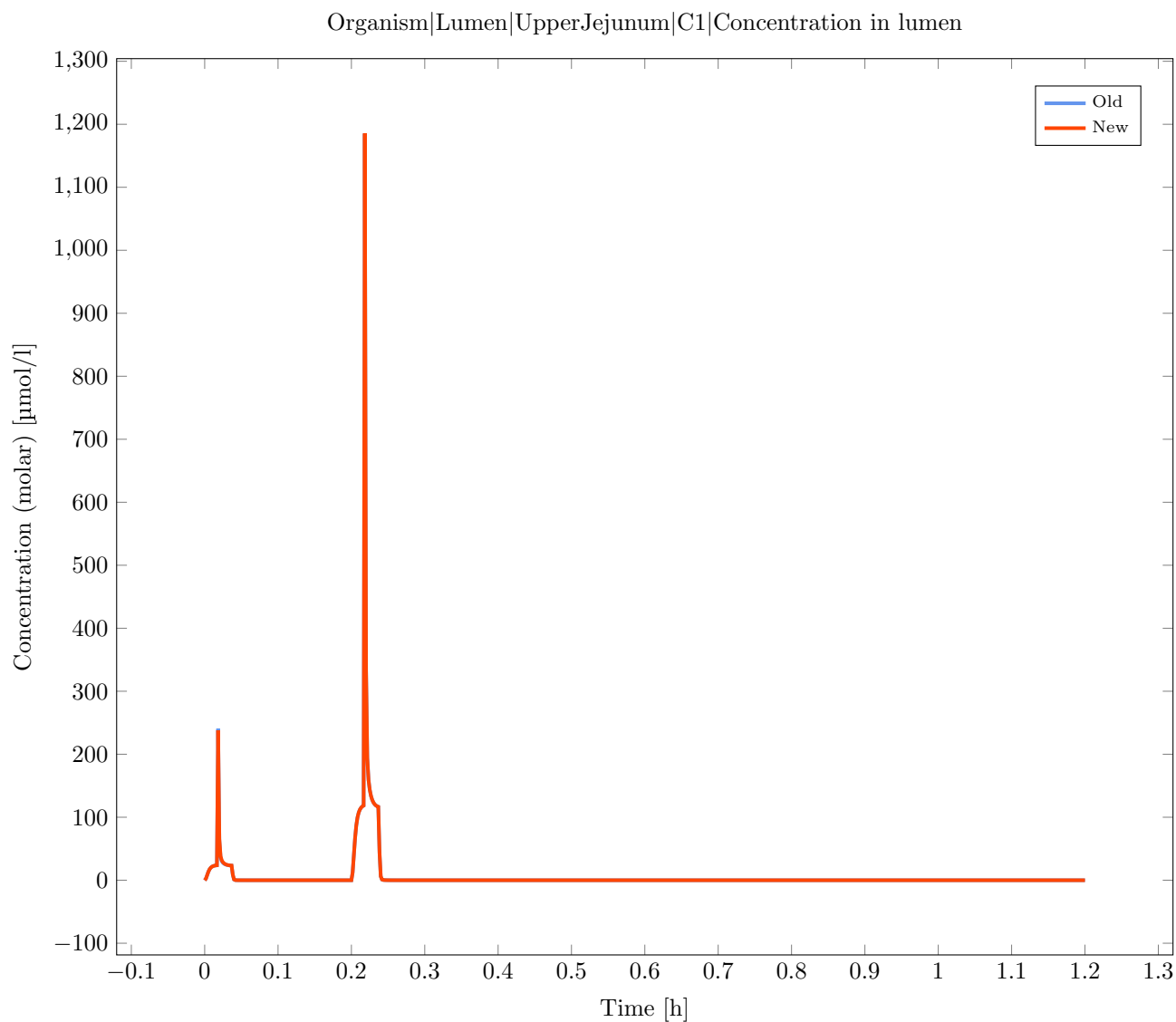
**Figure 1.27**

**Figure 1.28****Output Path: Organism|Lumen|UpperJejunum|C1|Concentration in lumen**

Deviation for 'Organism|Lumen|UpperJejunum|C1|Concentration in lumen' is 7.78% and is greater than the allowed max. tolerance of 3.00%

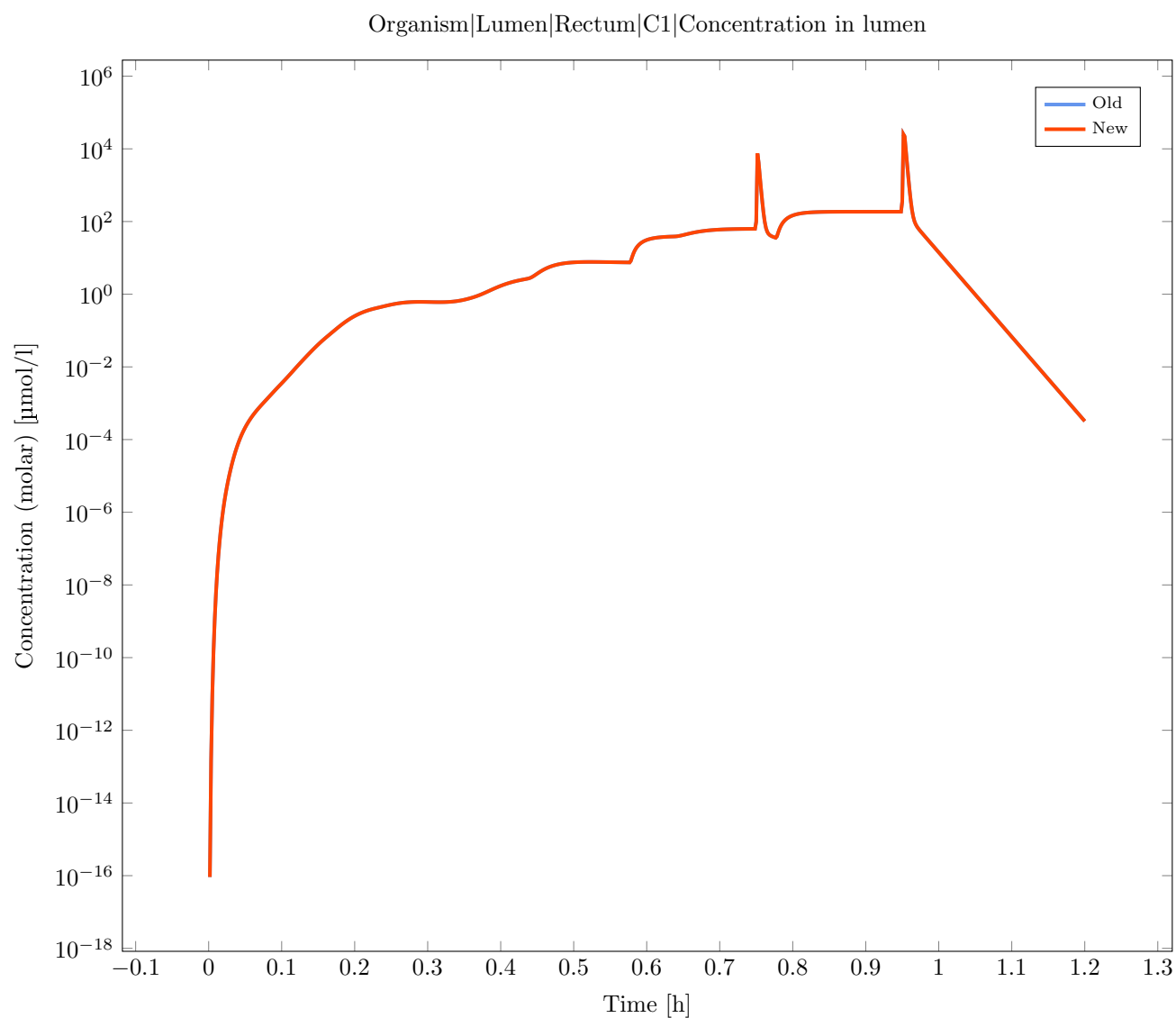
Deviation: 0.08

**Figure 1.29**

**Figure 1.30****Output Path: Organism|Lumen|Rectum|C1|Concentration in lumen**

Deviation for 'Organism|Lumen|Rectum|C1|Concentration in lumen' is 6.77% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.07

**Figure 1.31**

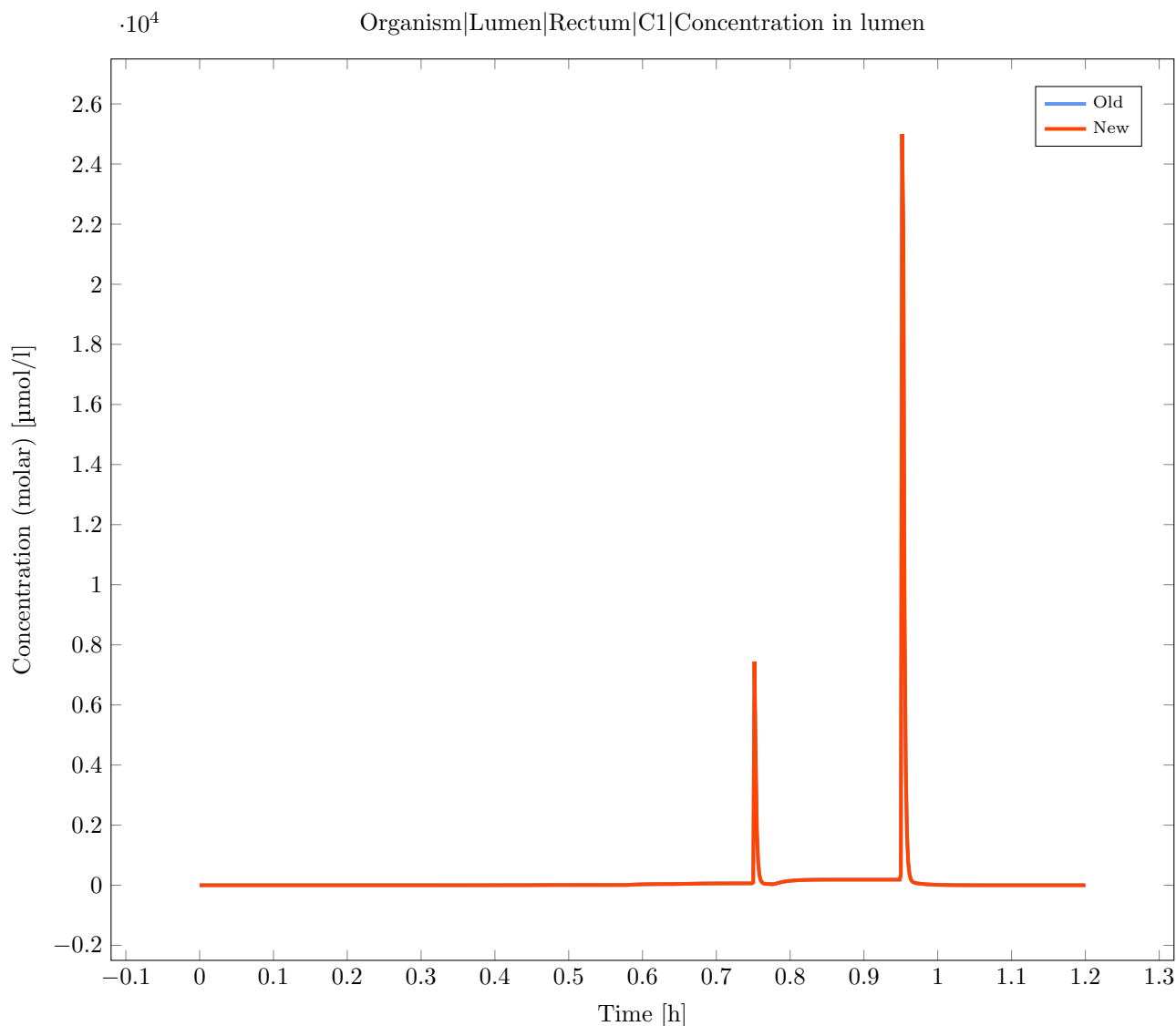


Figure 1.32

Simulation: Human_SingleORAL_MonoParticles_AsSuspention-Human_SingleORAL_MonoParticles_-AsSuspention

Result of the validation: **Invalid**

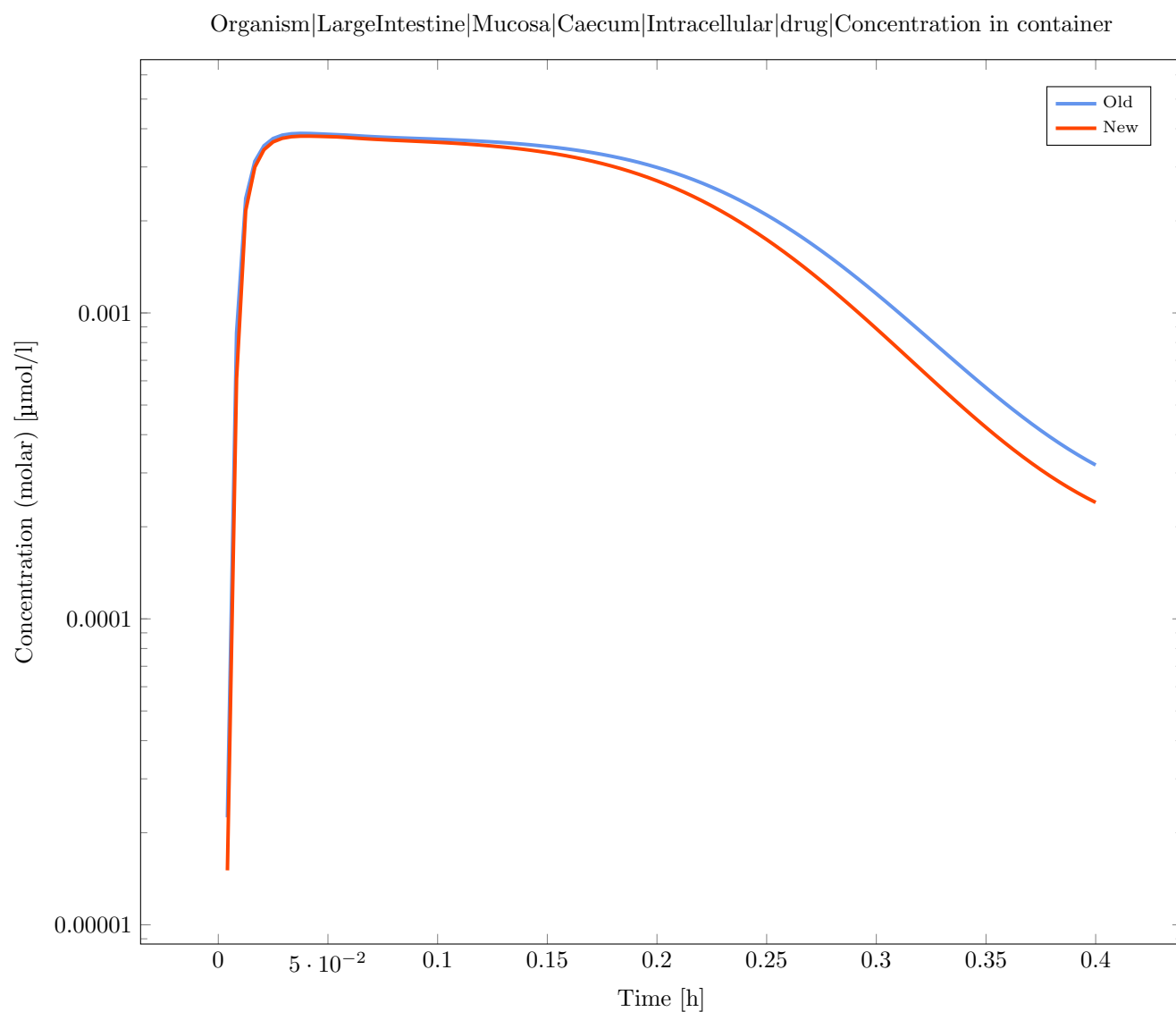
Absolute Tolerance: 1.00E-10

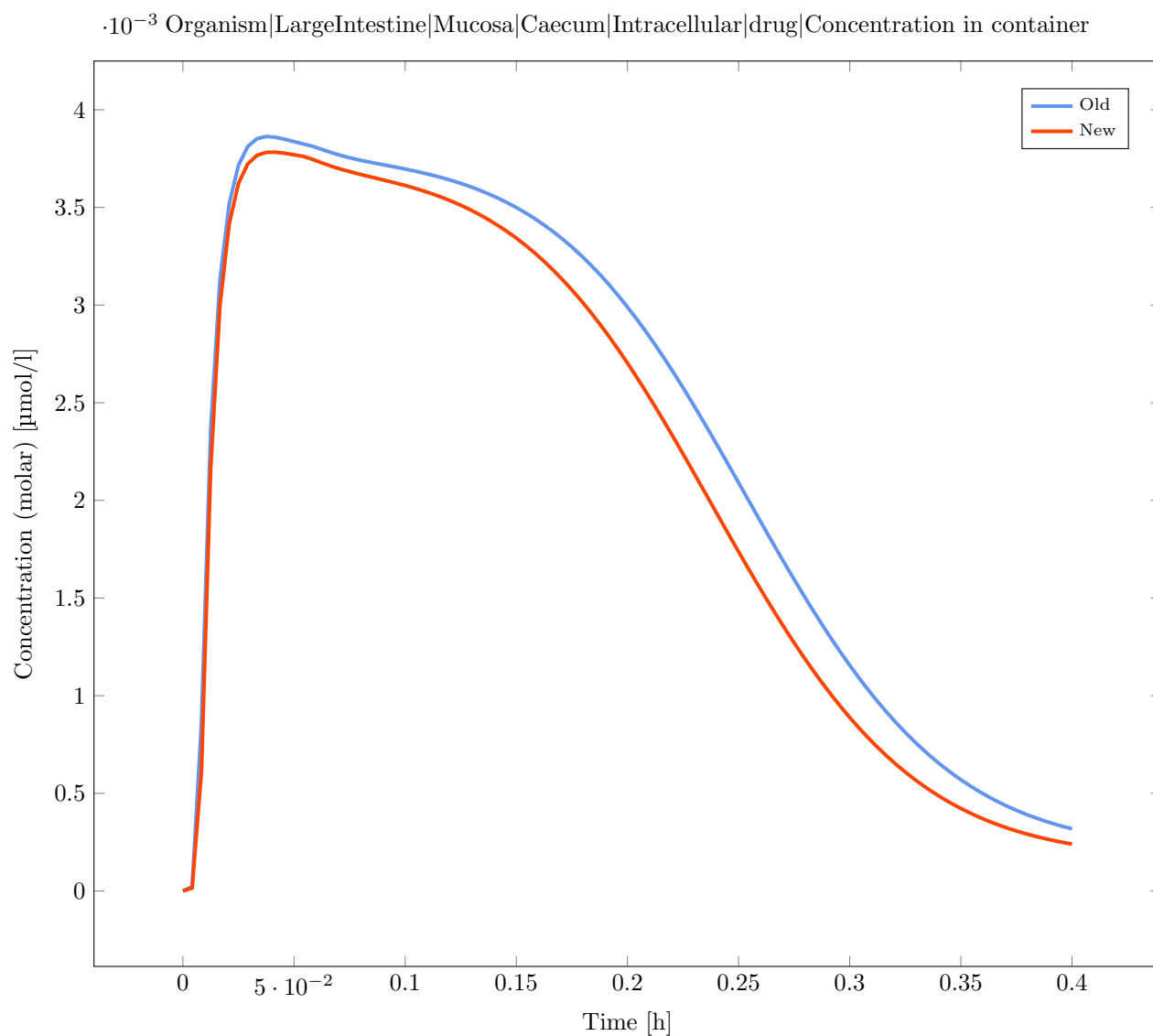
Relative Tolerance: 1.00E-5

Output Path: Organism|LargeIntestine|Mucosa|Caecum|Intracellular|drug|Concentration in container

Deviation for 'Organism|LargeIntestine|Mucosa|Caecum|Intracellular|drug|Concentration in container' is 32.90% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

**Figure 1.33**

**Figure 1.34**

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container' is 32.82% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

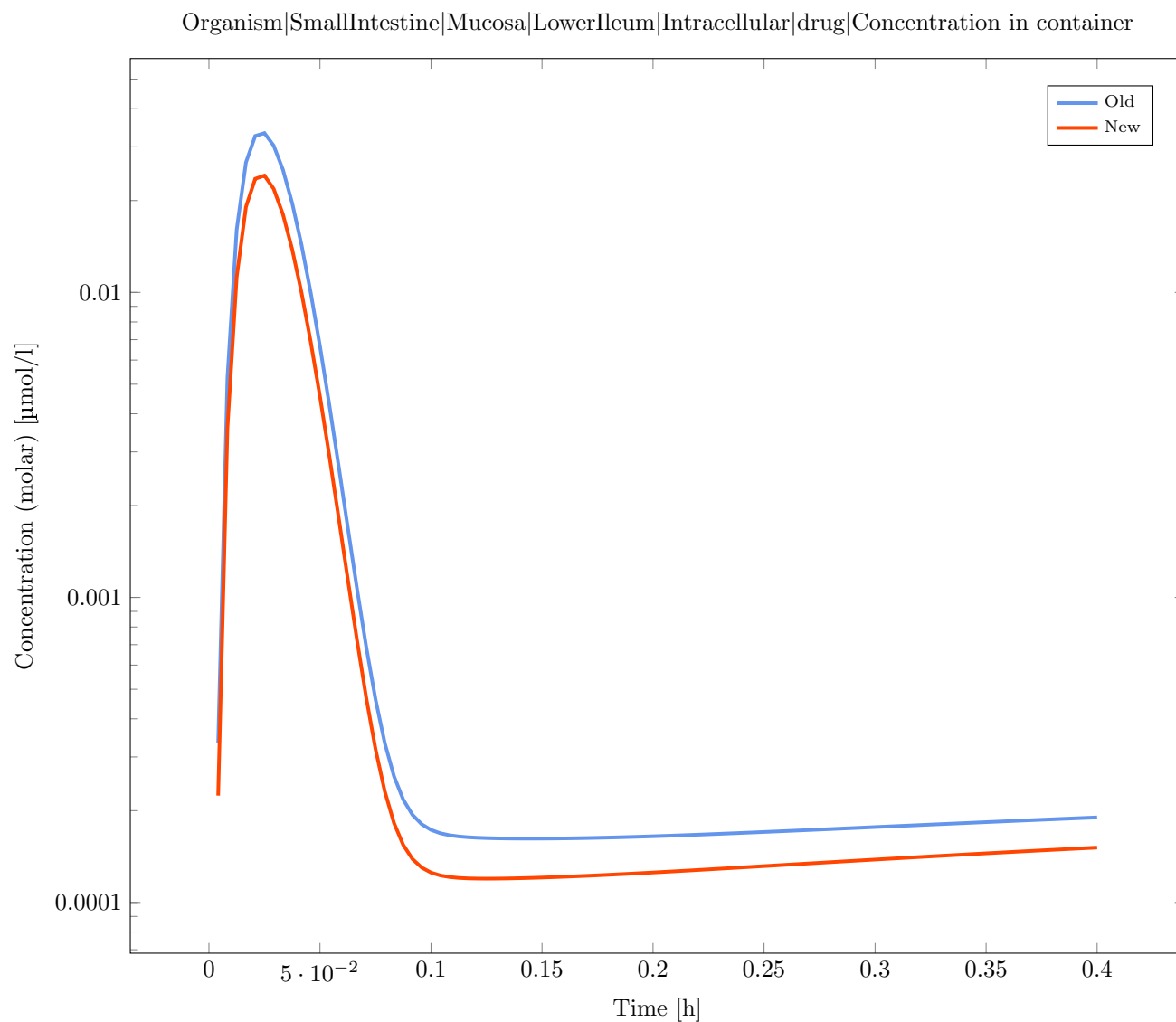


Figure 1.35

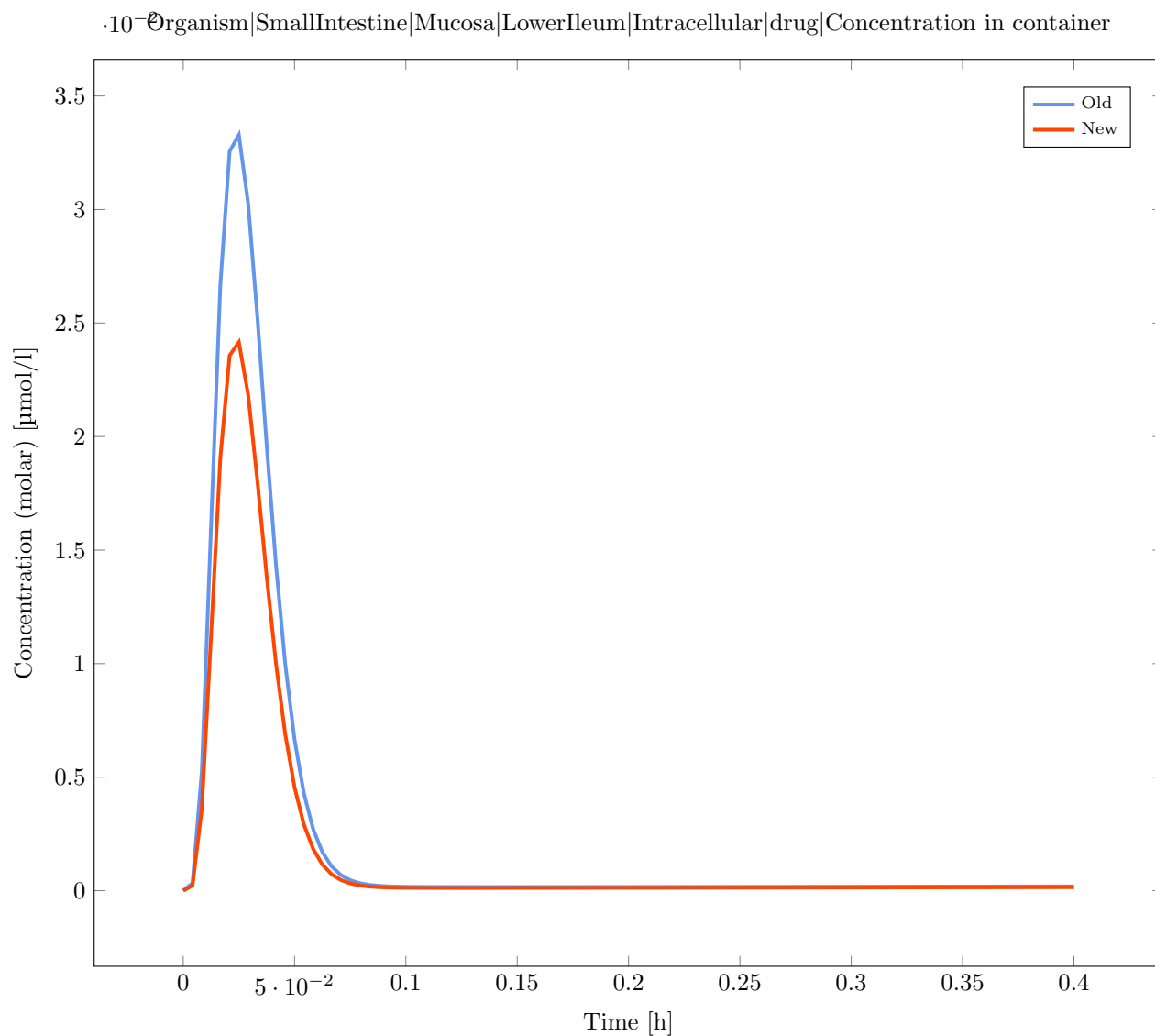


Figure 1.36

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Interstitial|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Interstitial|drug|Concentration in container' is 32.71% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

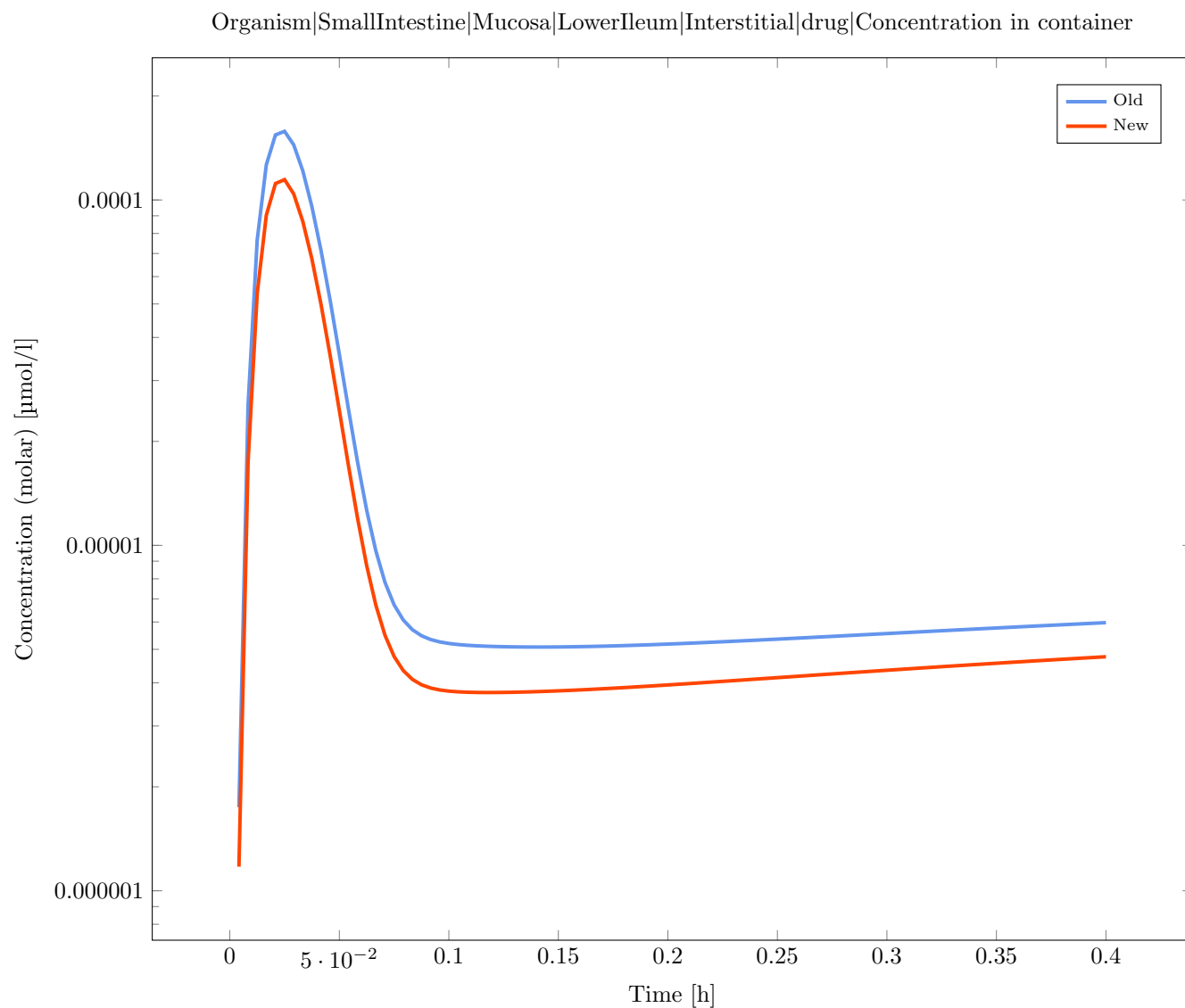


Figure 1.37

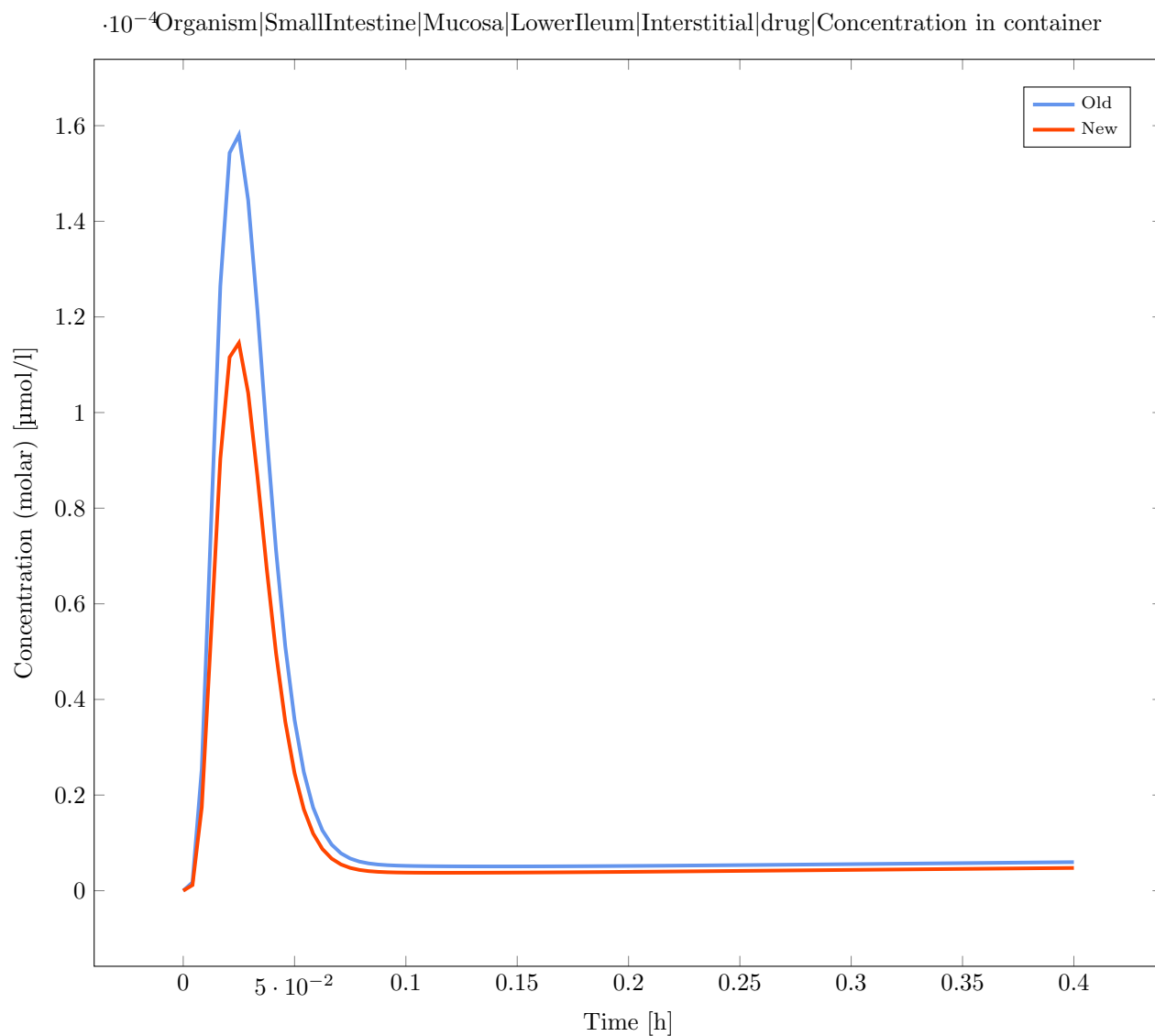


Figure 1.38

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Plasma|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Plasma|drug|Concentration in container' is 32.71% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

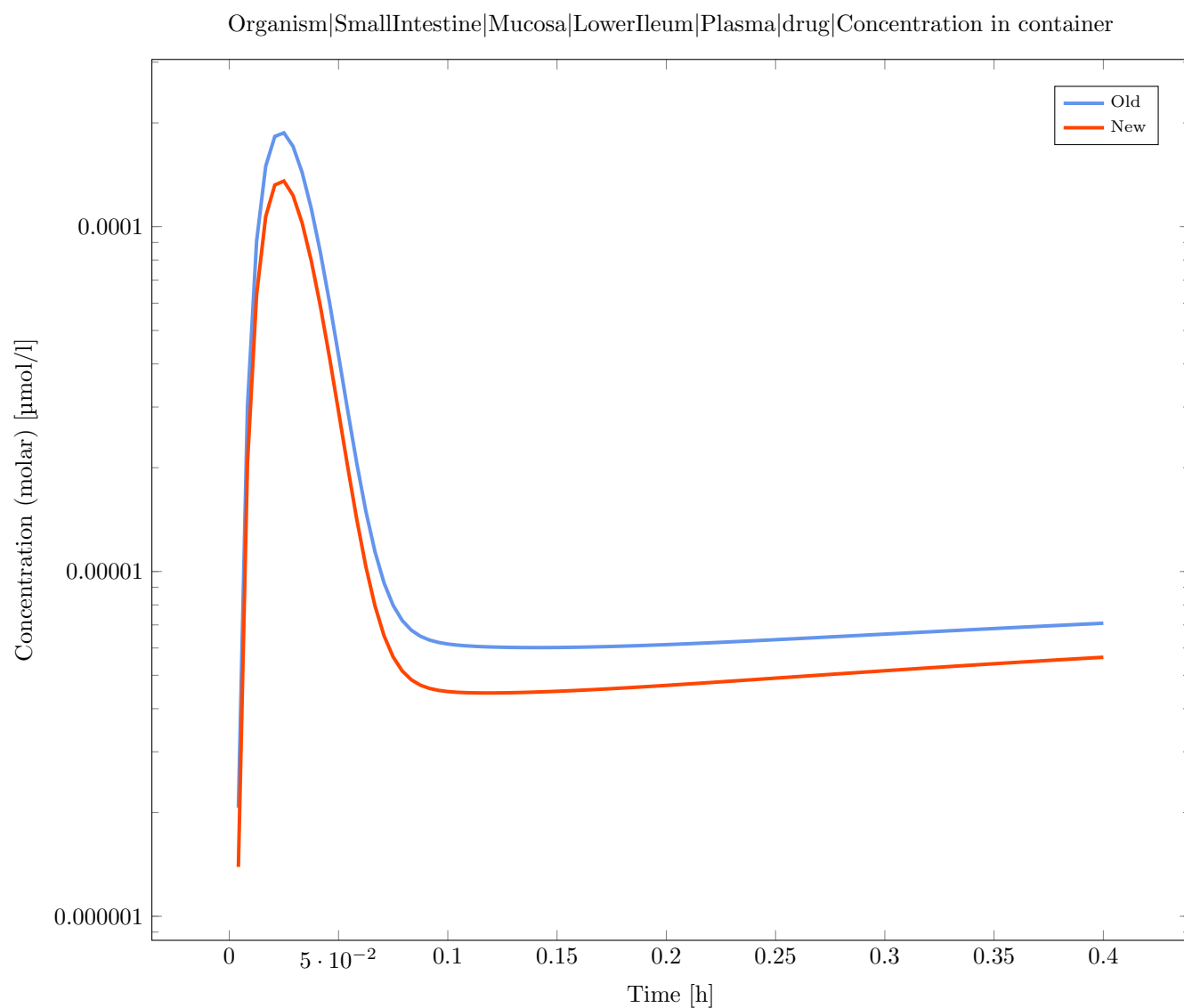


Figure 1.39

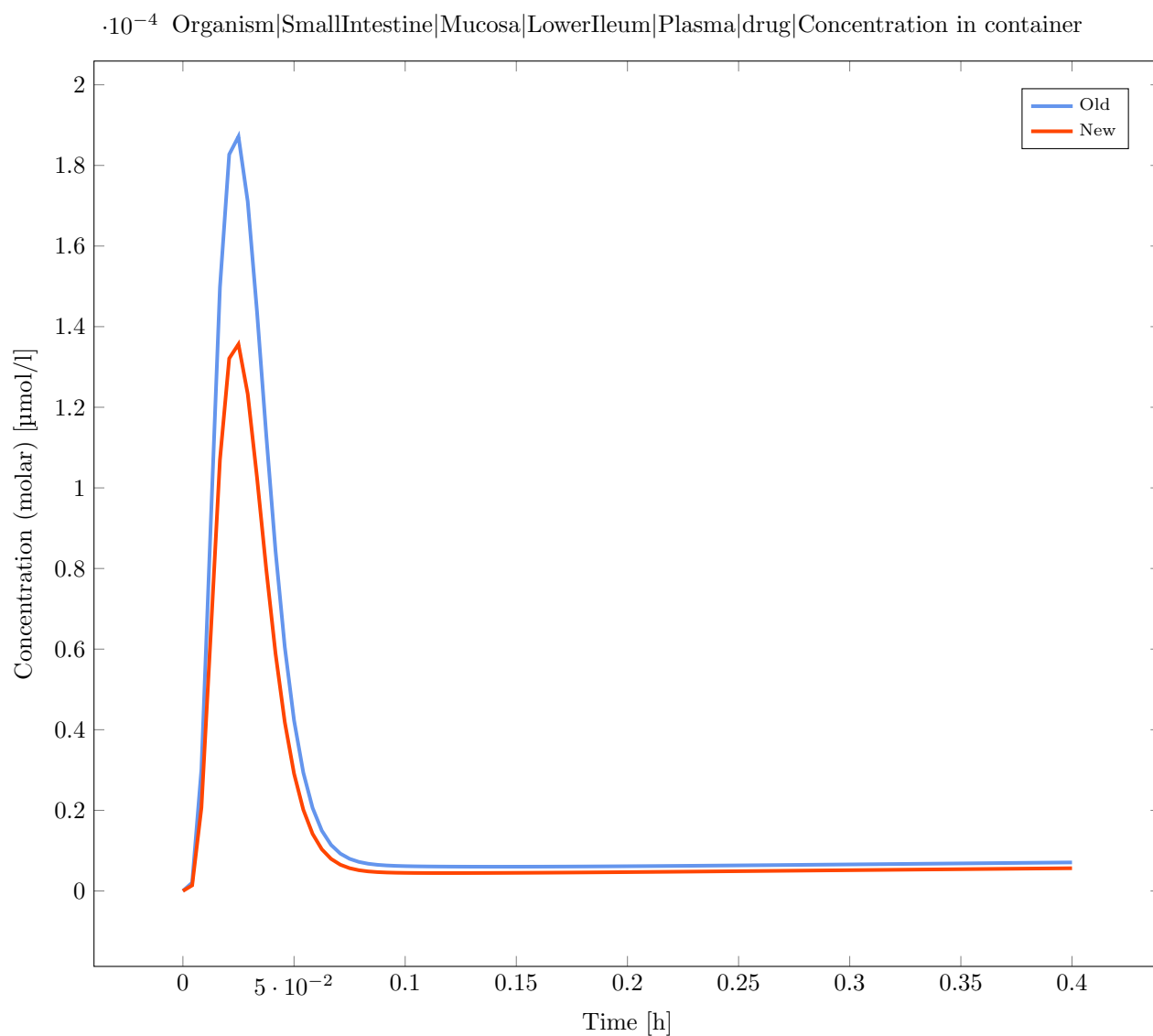
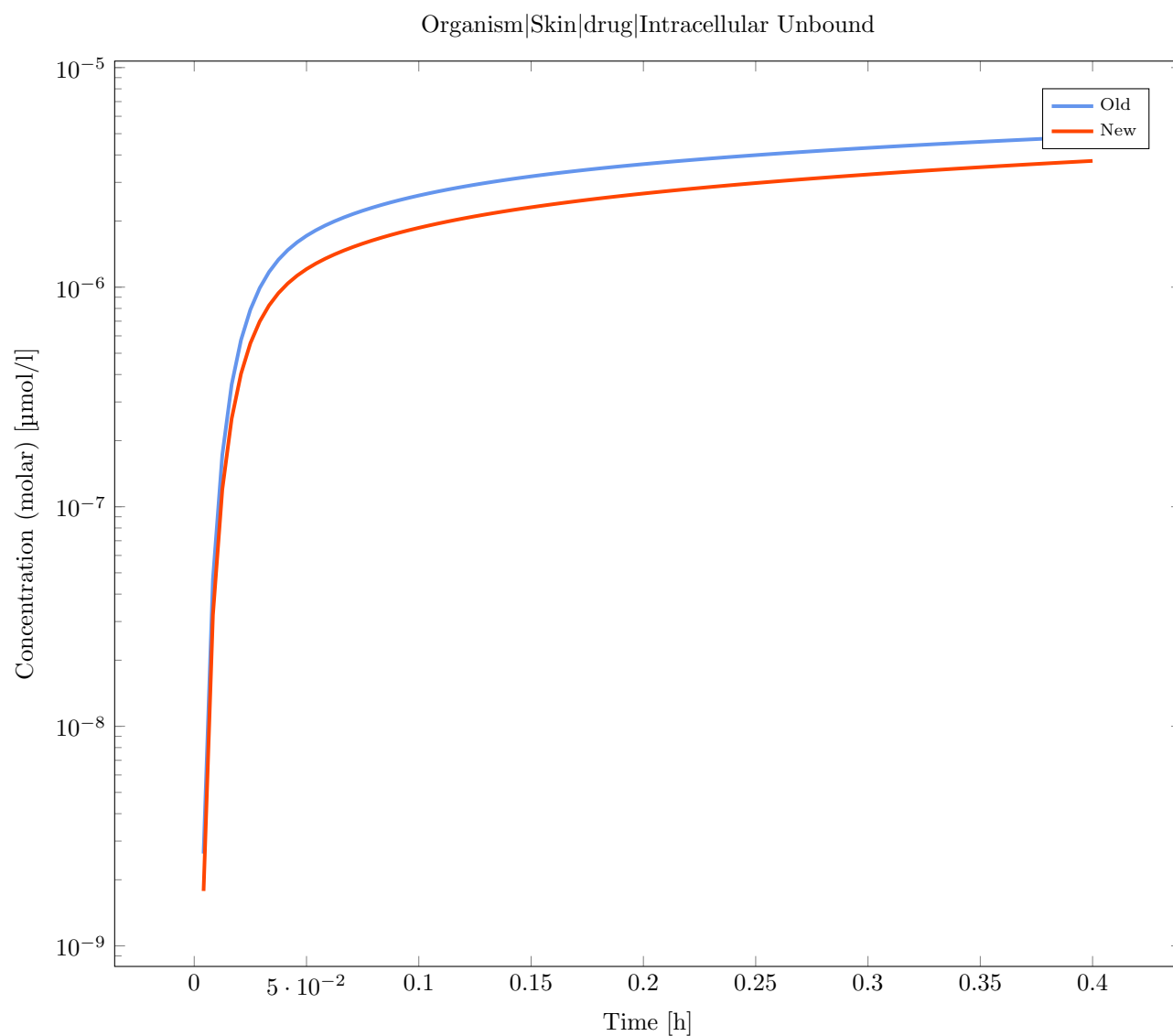


Figure 1.40

Output Path: Organism|Skin|drug|Intracellular Unbound

Deviation for 'Organism|Skin|drug|Intracellular Unbound' is 32.45% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.32

**Figure 1.41**

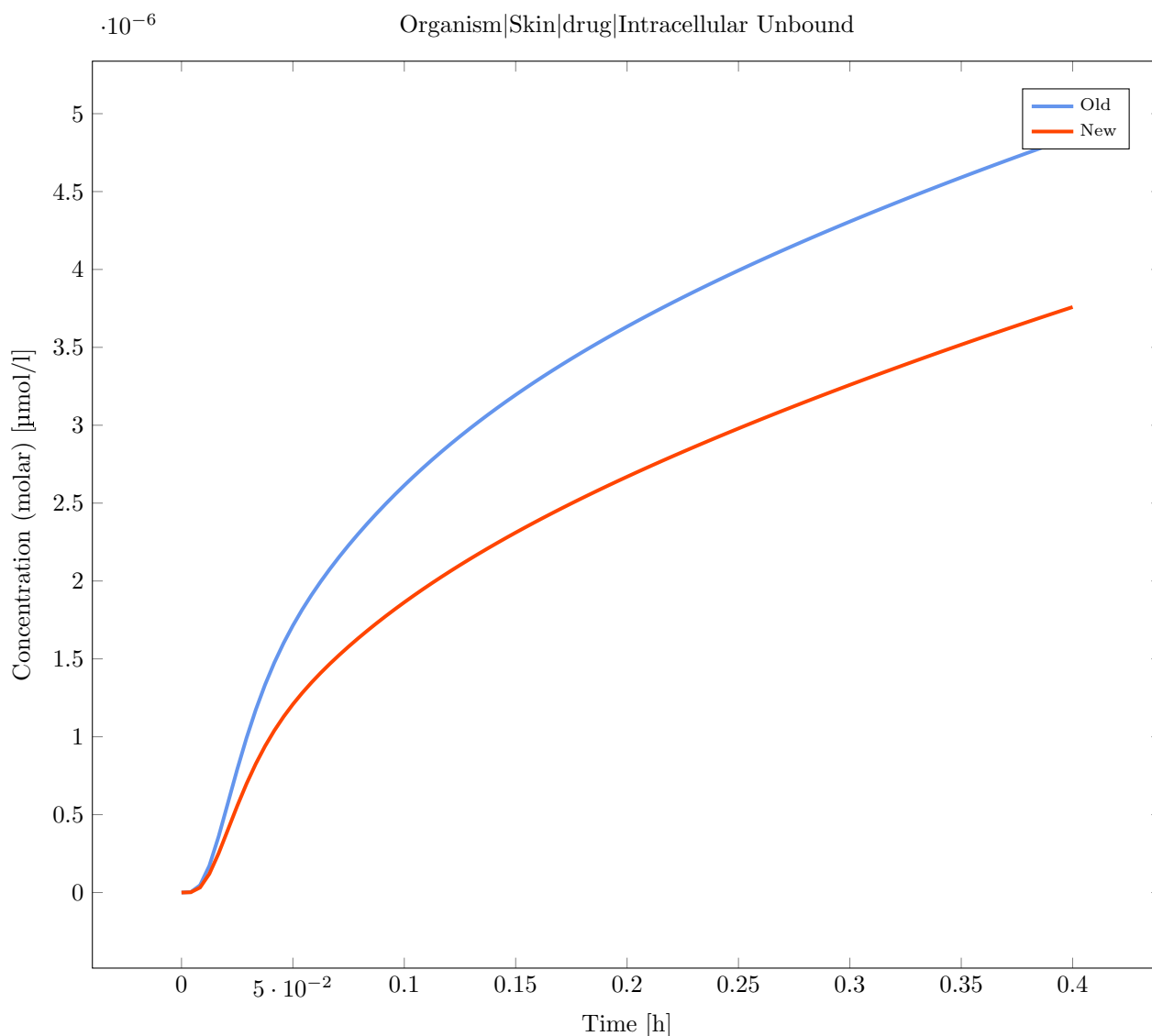


Figure 1.42

Simulation: Human_SingleORAL_PolyParticlesLogNormal_AsSuspention-Human_SingleORAL_PolyParticlesLogNormal_AsSuspention

Result of the validation: **Invalid**

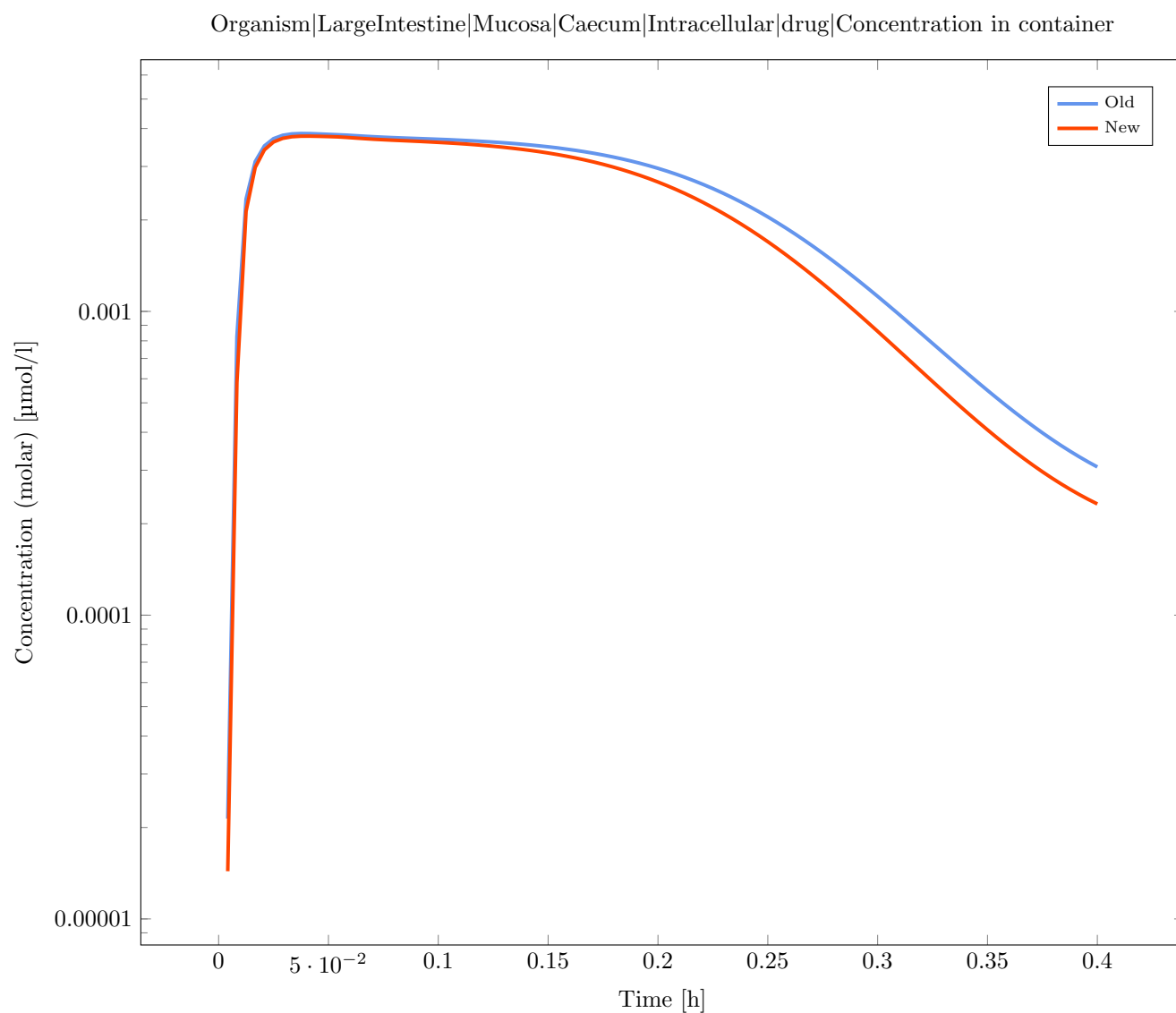
Absolute Tolerance: 1.00E-10

Relative Tolerance: 1.00E-5

Output Path: Organism|LargeIntestine|Mucosa|Caecum|Intracellular|drug|Concentration in container

Deviation for 'Organism|LargeIntestine|Mucosa|Caecum|Intracellular|drug|Concentration in container' is 32.92% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

**Figure 1.43**

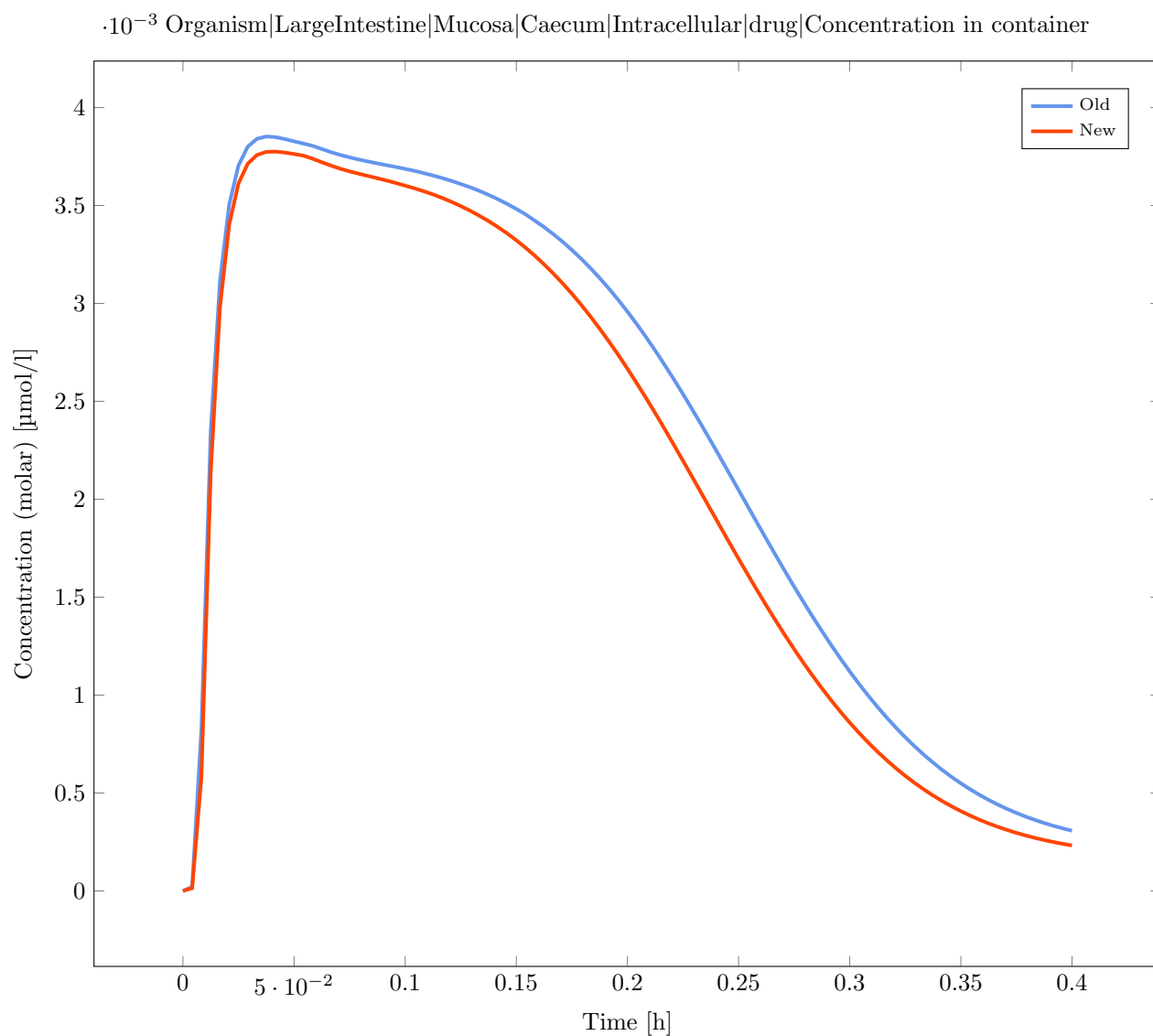


Figure 1.44

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container' is 32.84% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

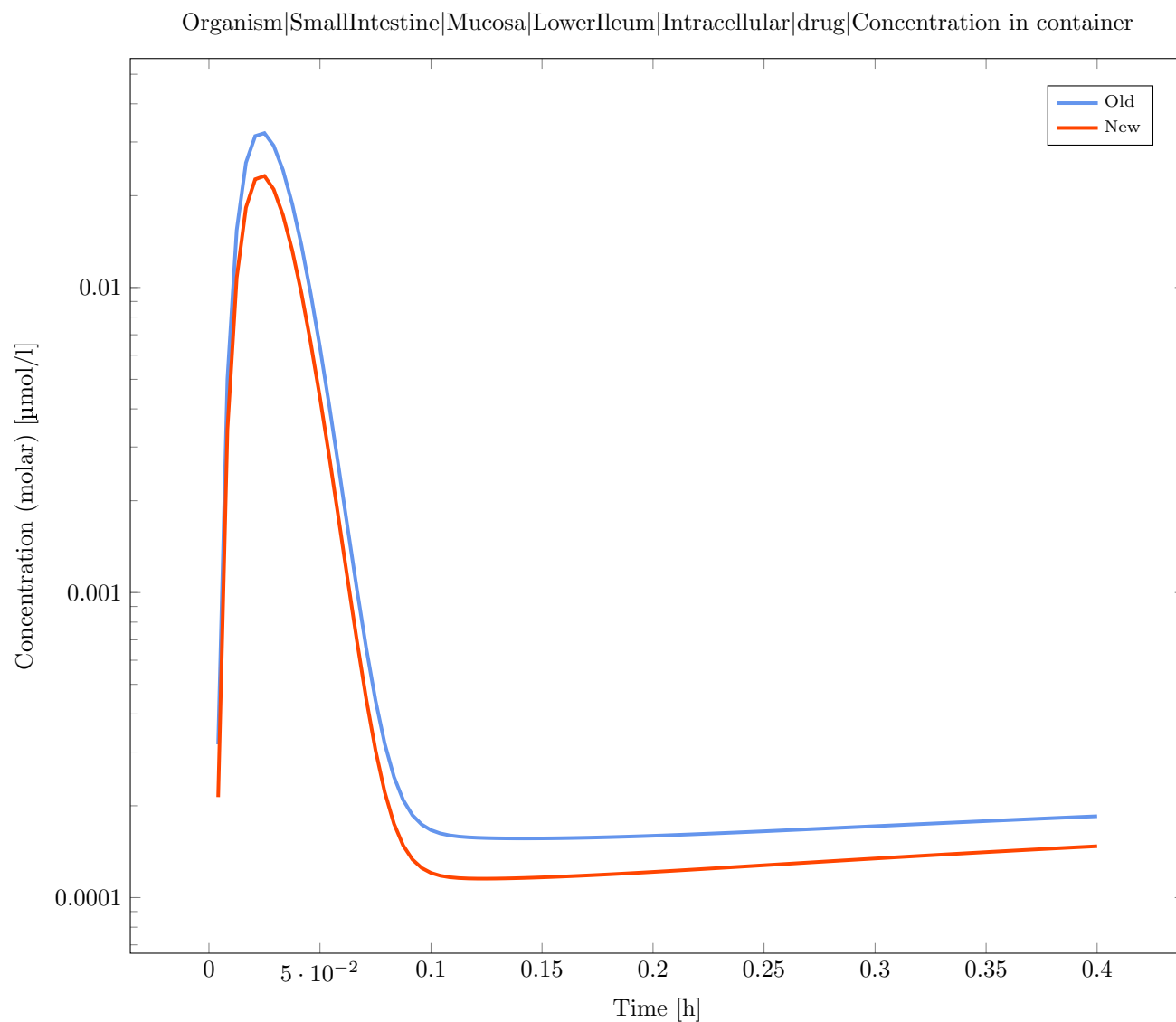


Figure 1.45

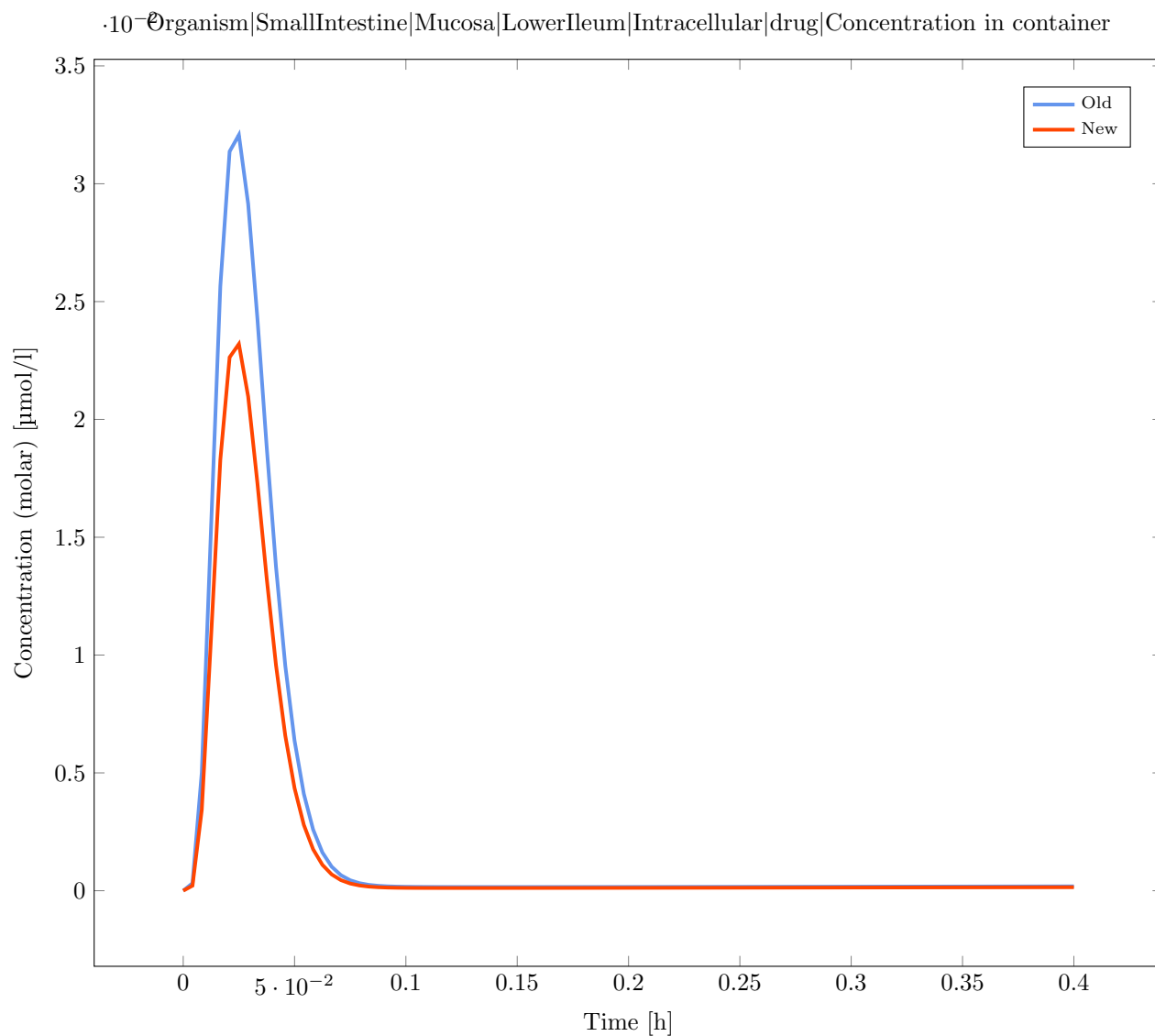


Figure 1.46

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Interstitial|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Interstitial|drug|Concentration in container' is 32.74% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

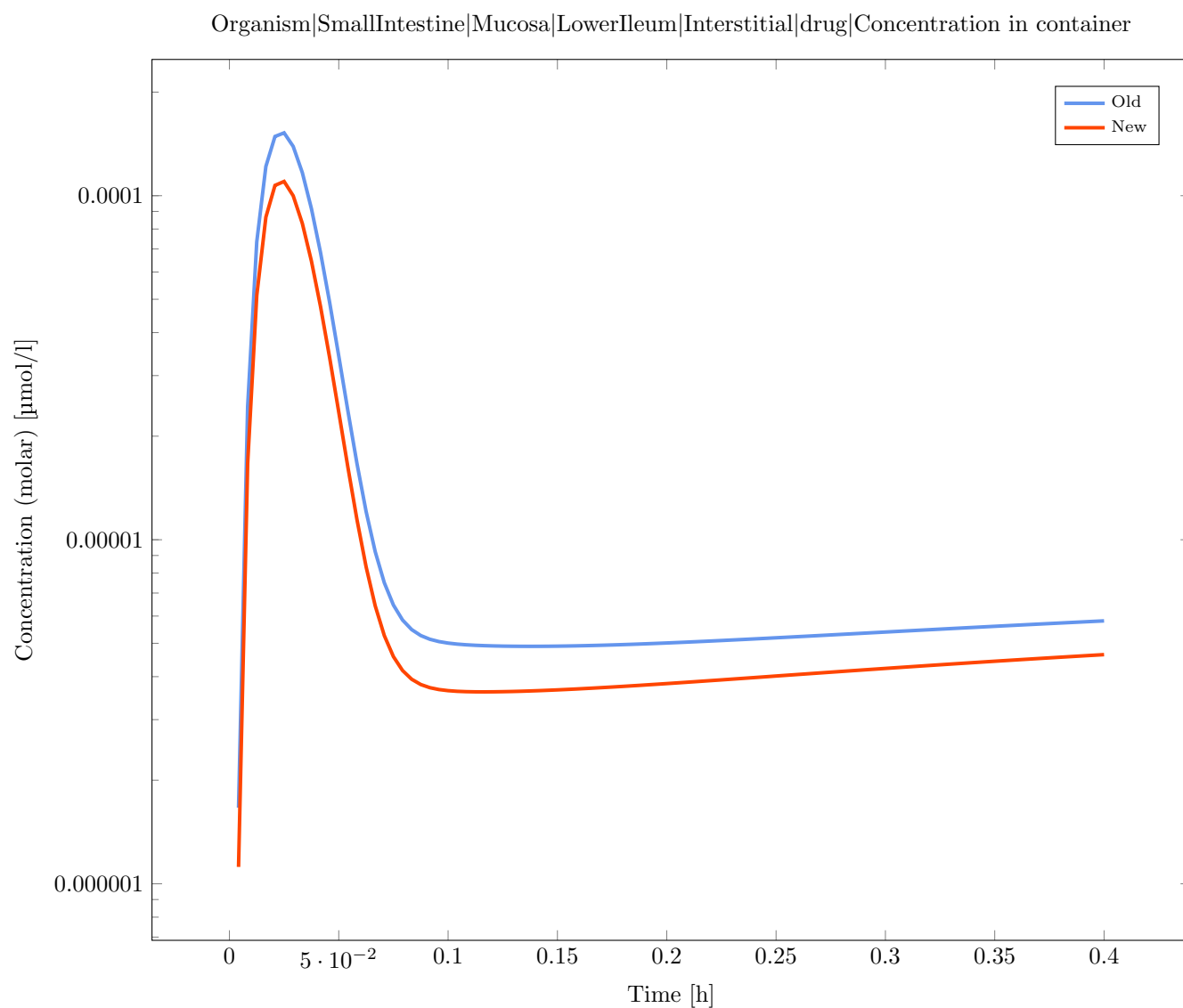


Figure 1.47

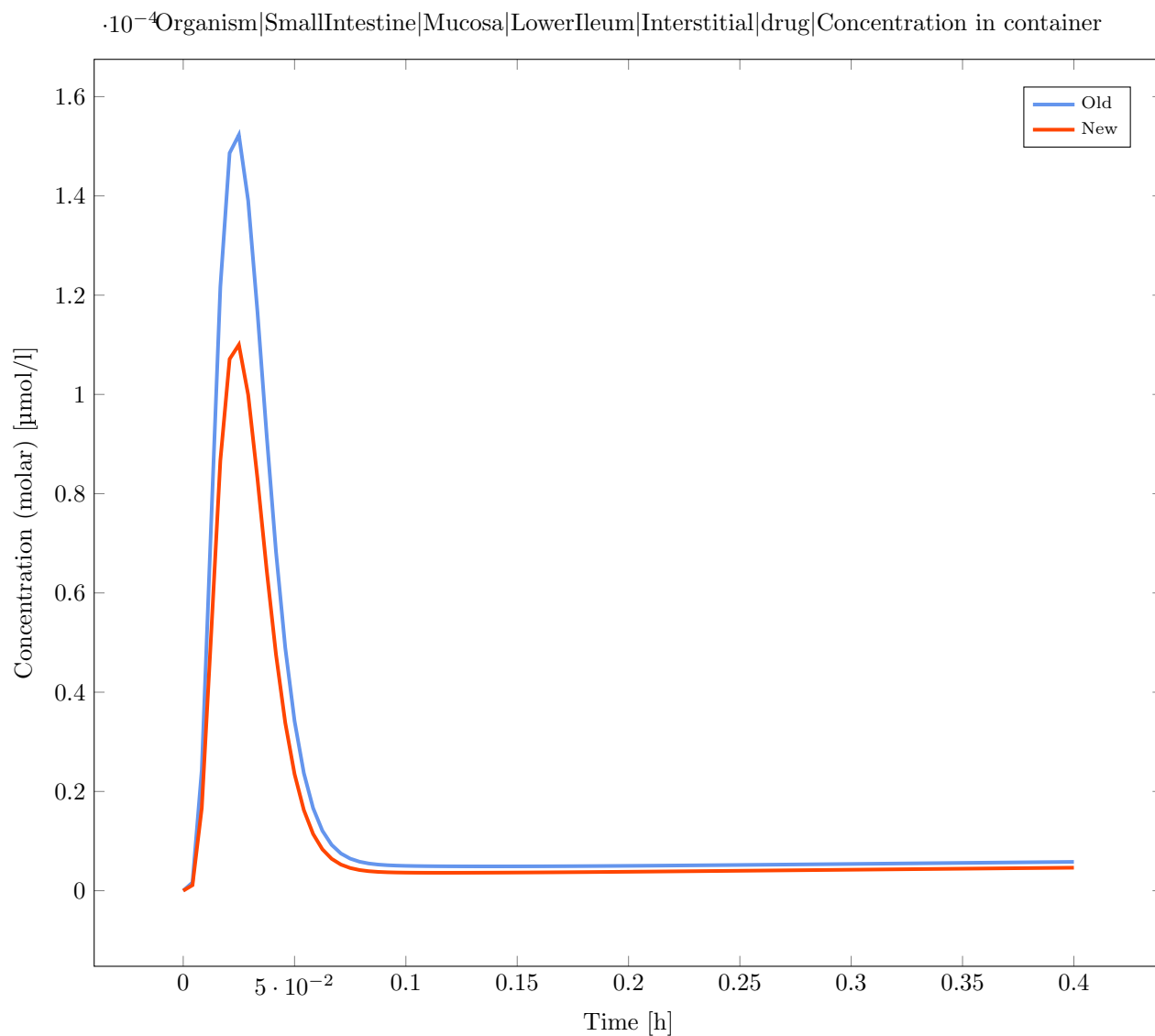
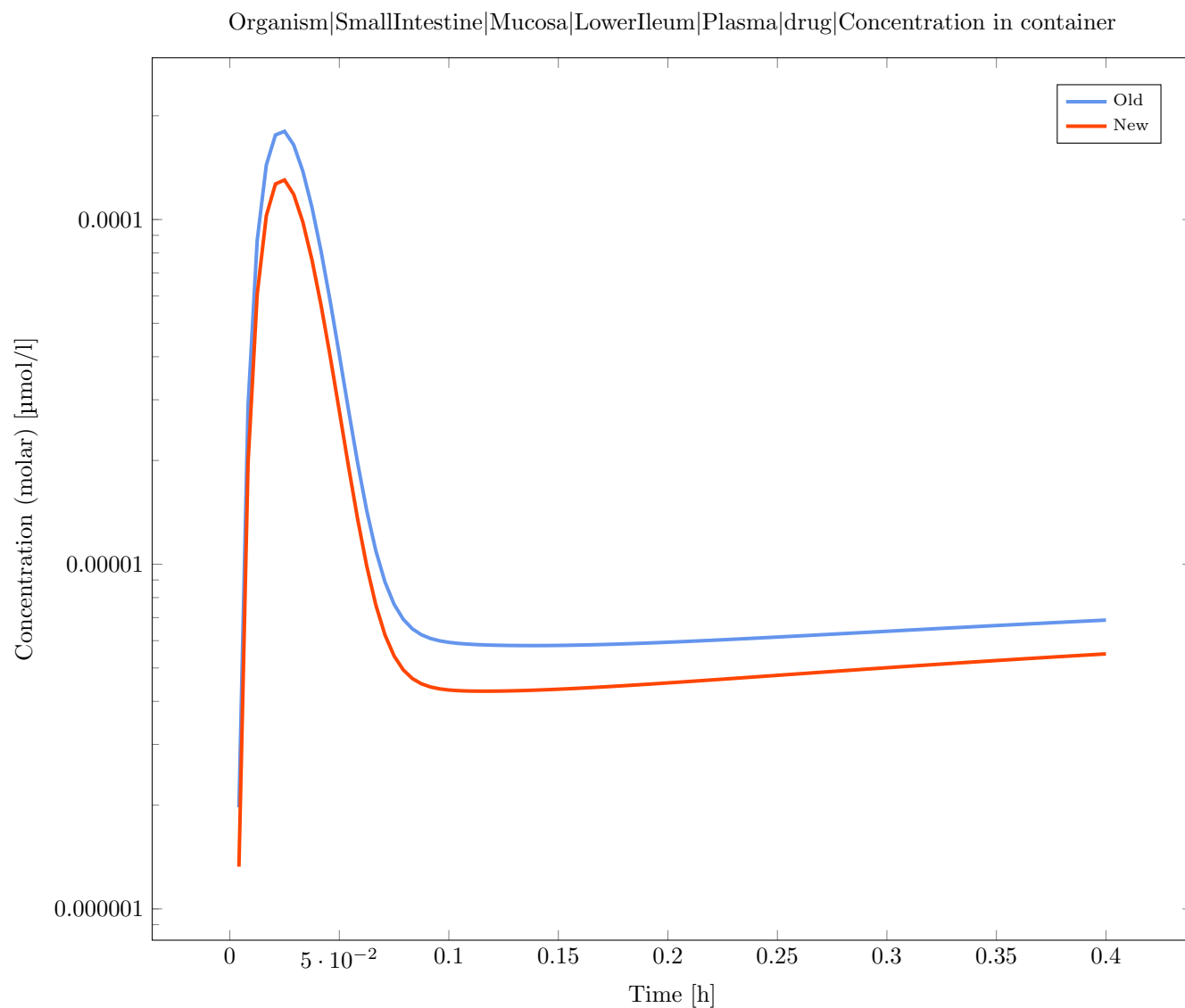


Figure 1.48

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Plasma|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Plasma|drug|Concentration in container' is 32.74% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

**Figure 1.49**

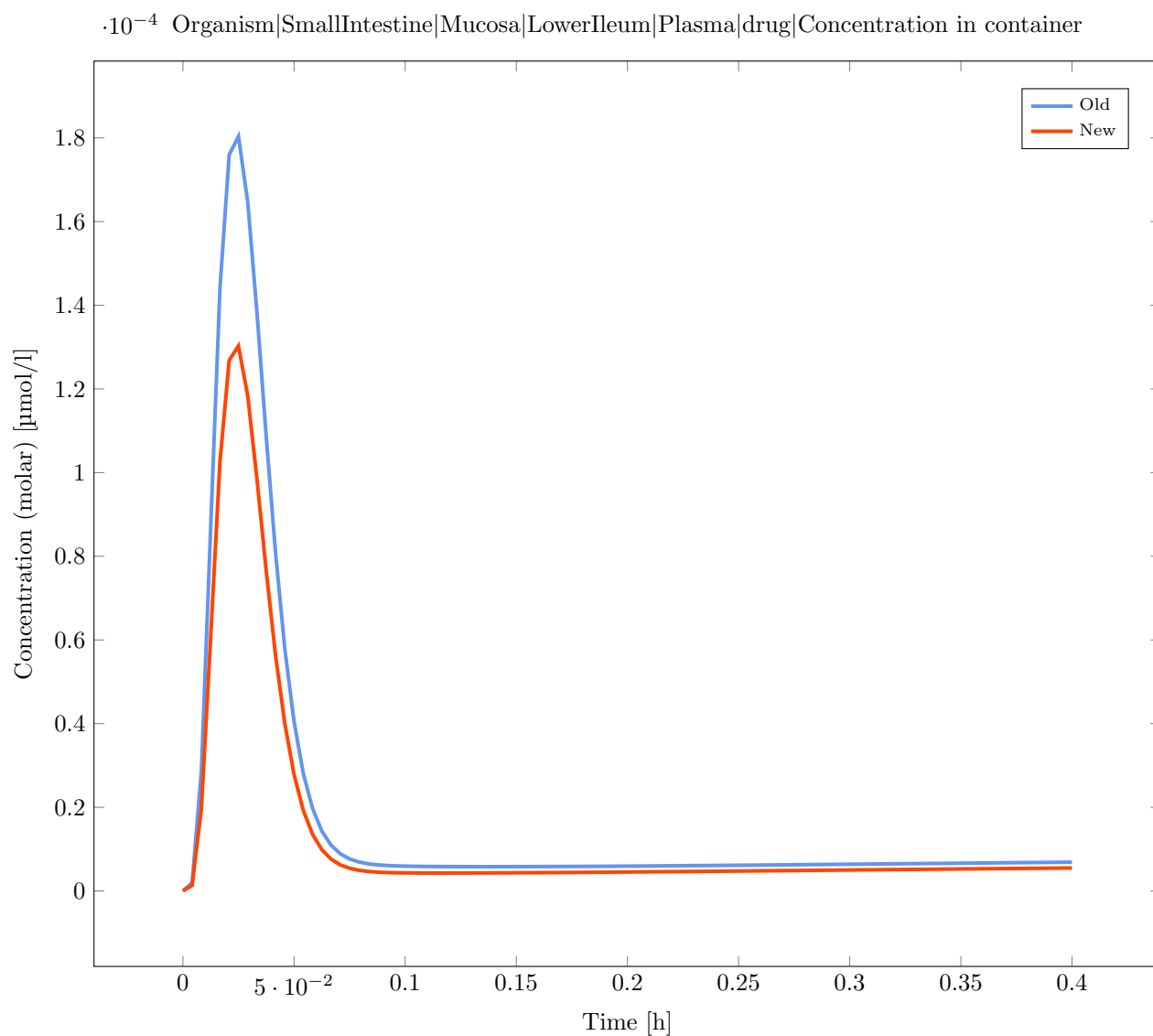
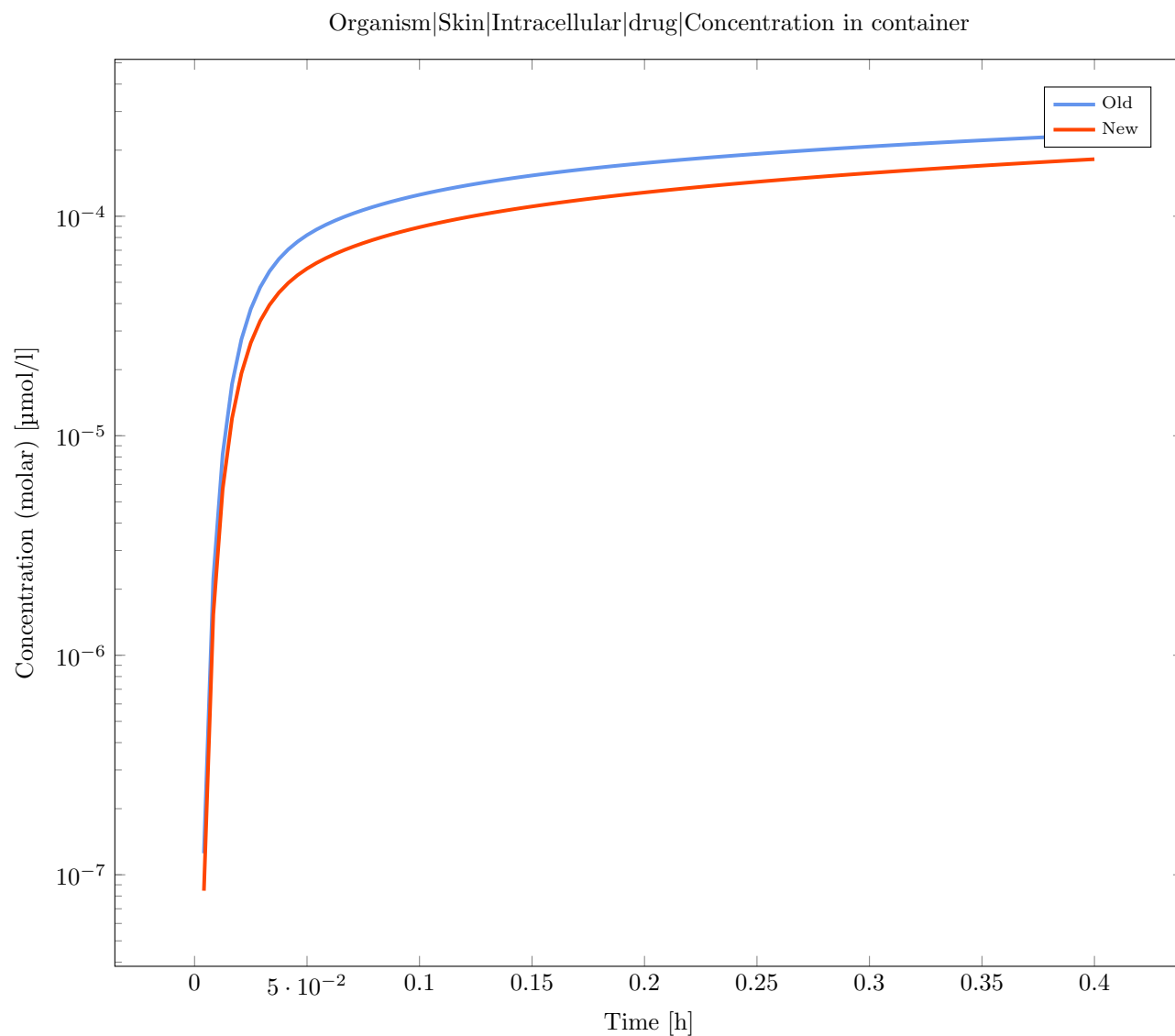


Figure 1.50

Output Path: Organism|Skin|Intracellular|drug|Concentration in container

Deviation for 'Organism|Skin|Intracellular|drug|Concentration in container' is 32.49% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.32

**Figure 1.51**

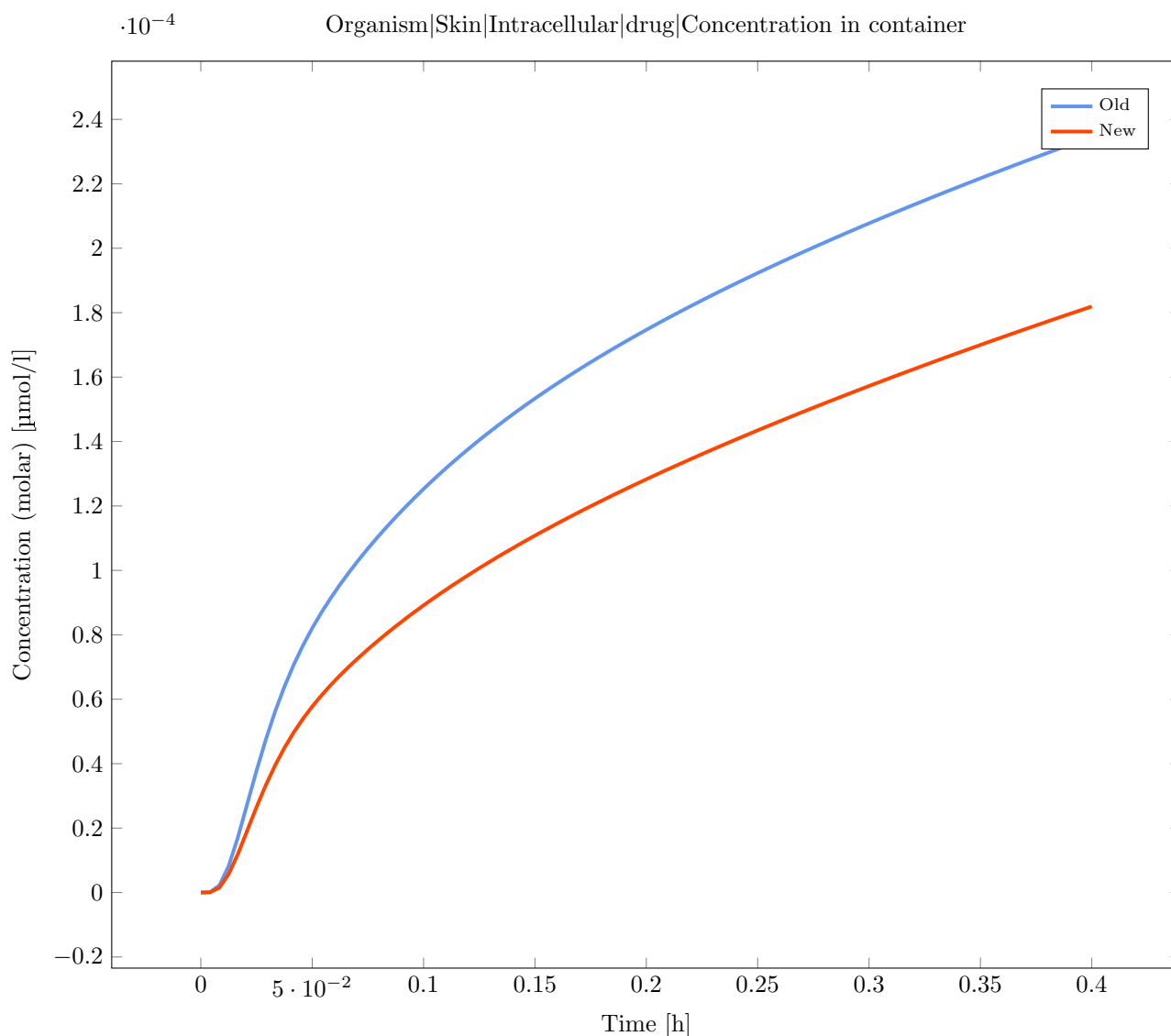


Figure 1.52

Simulation: Human_SingleORAL_PolyParticlesNormal_AsSuspention-Human_SingleORAL_PolyParticlesNormal_AsSuspention

Result of the validation: **Invalid**

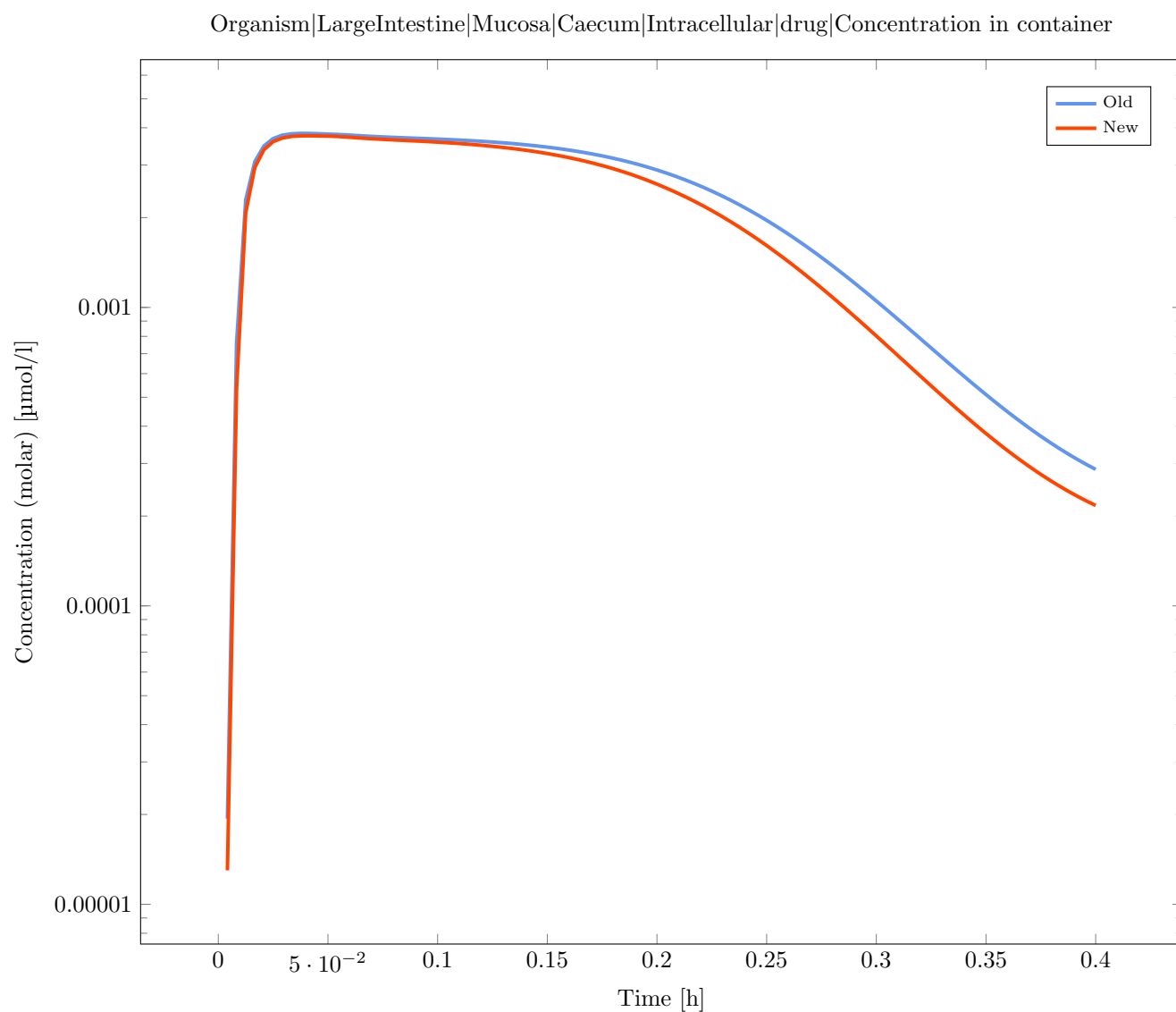
Absolute Tolerance: 1.00E-10

Relative Tolerance: 1.00E-5

Output Path: Organism|LargeIntestine|Mucosa|Caecum|Intracellular|drug|Concentration in container

Deviation for 'Organism|LargeIntestine|Mucosa|Caecum|Intracellular|drug|Concentration in container' is 32.96% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

**Figure 1.53**

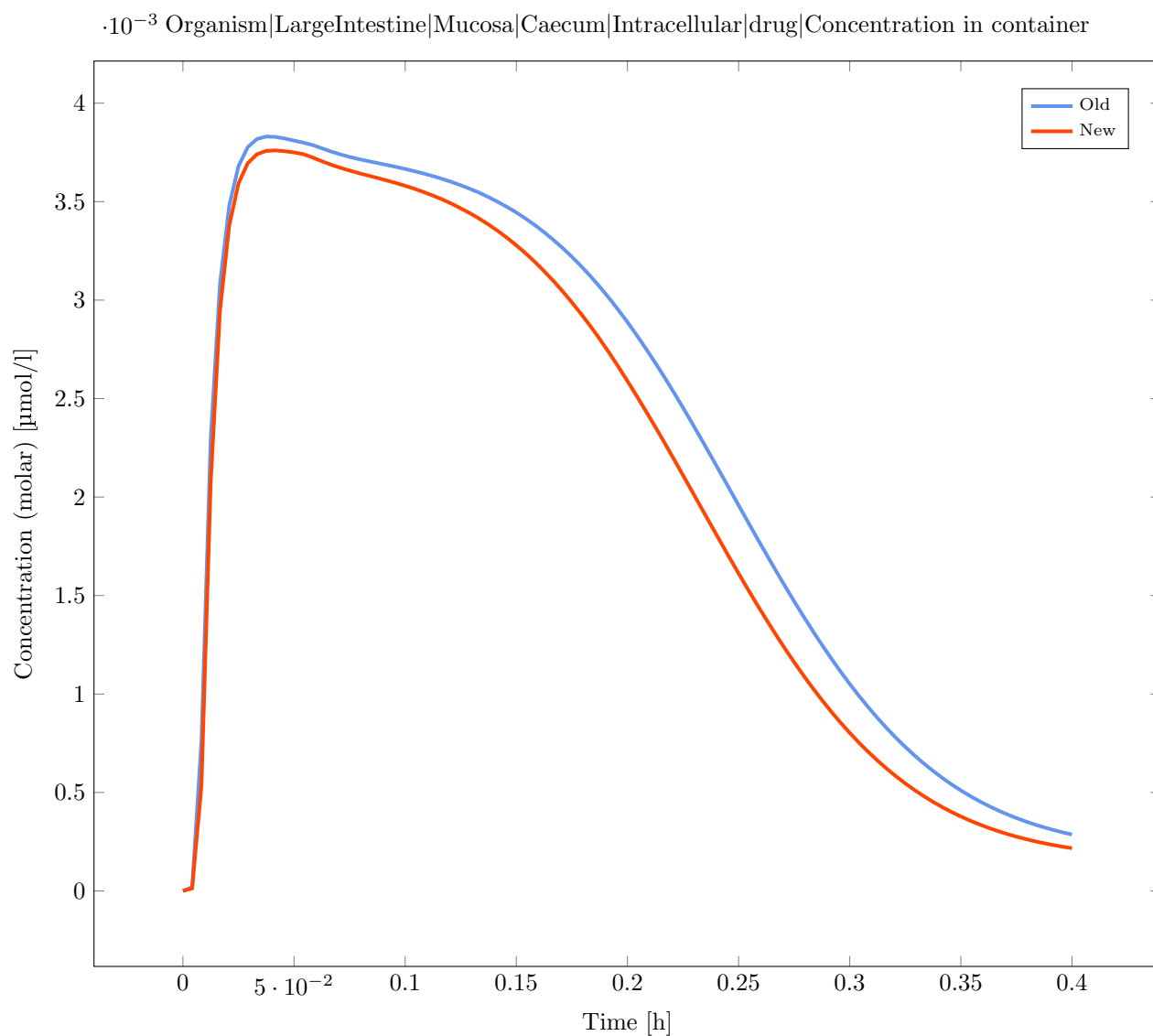


Figure 1.54

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container' is 32.88% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

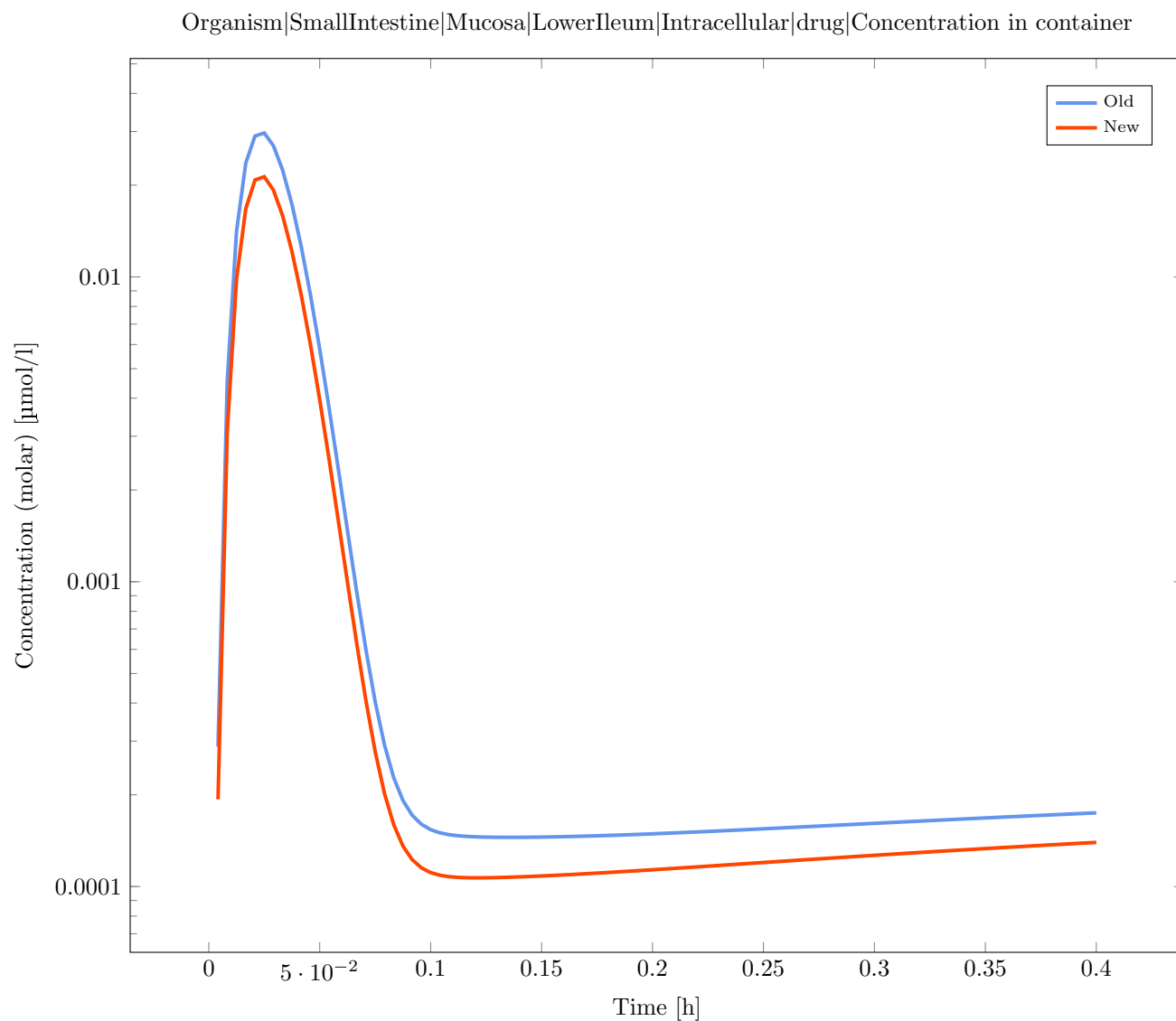


Figure 1.55

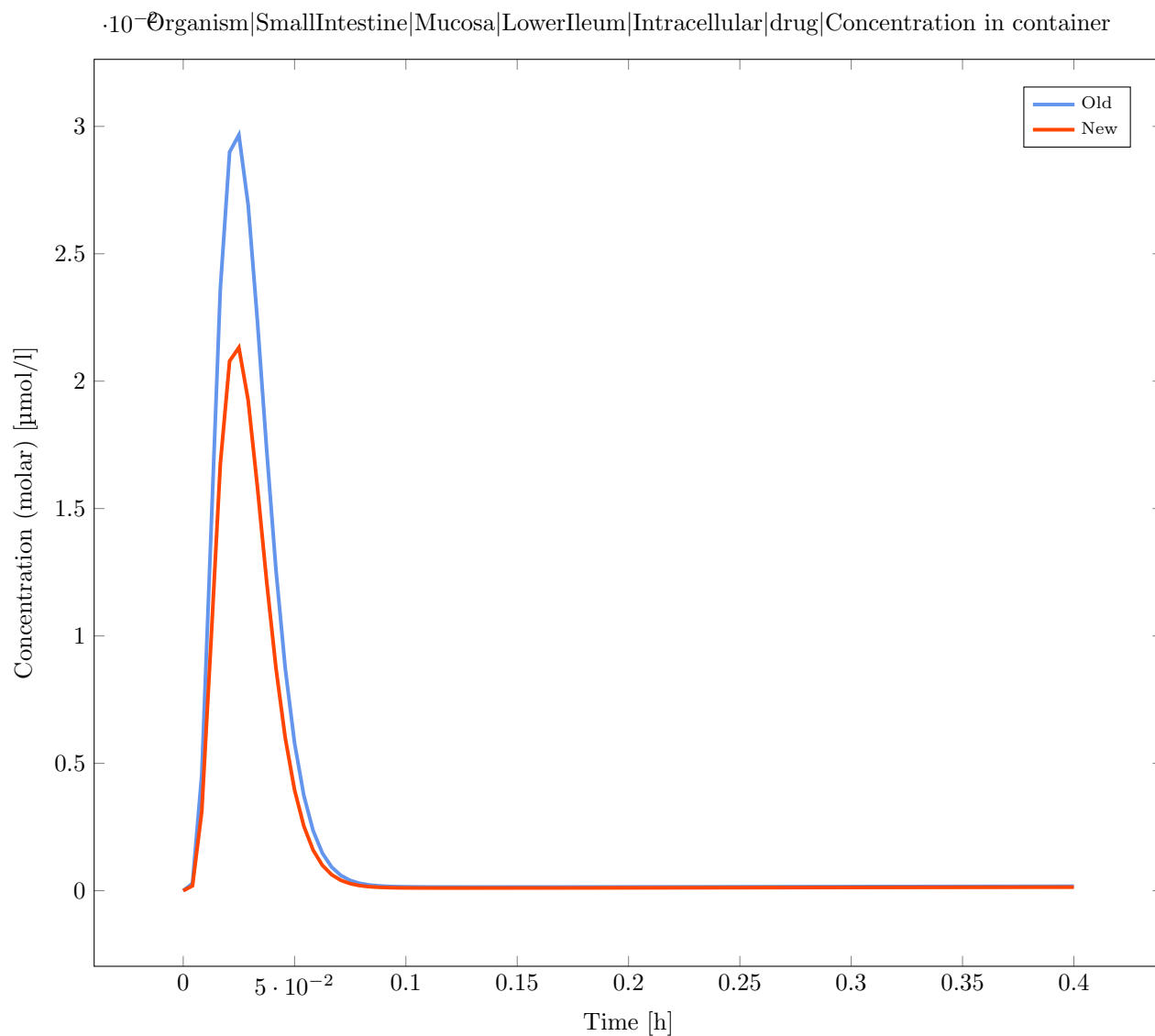


Figure 1.56

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Interstitial|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Interstitial|drug|Concentration in container' is 32.80% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

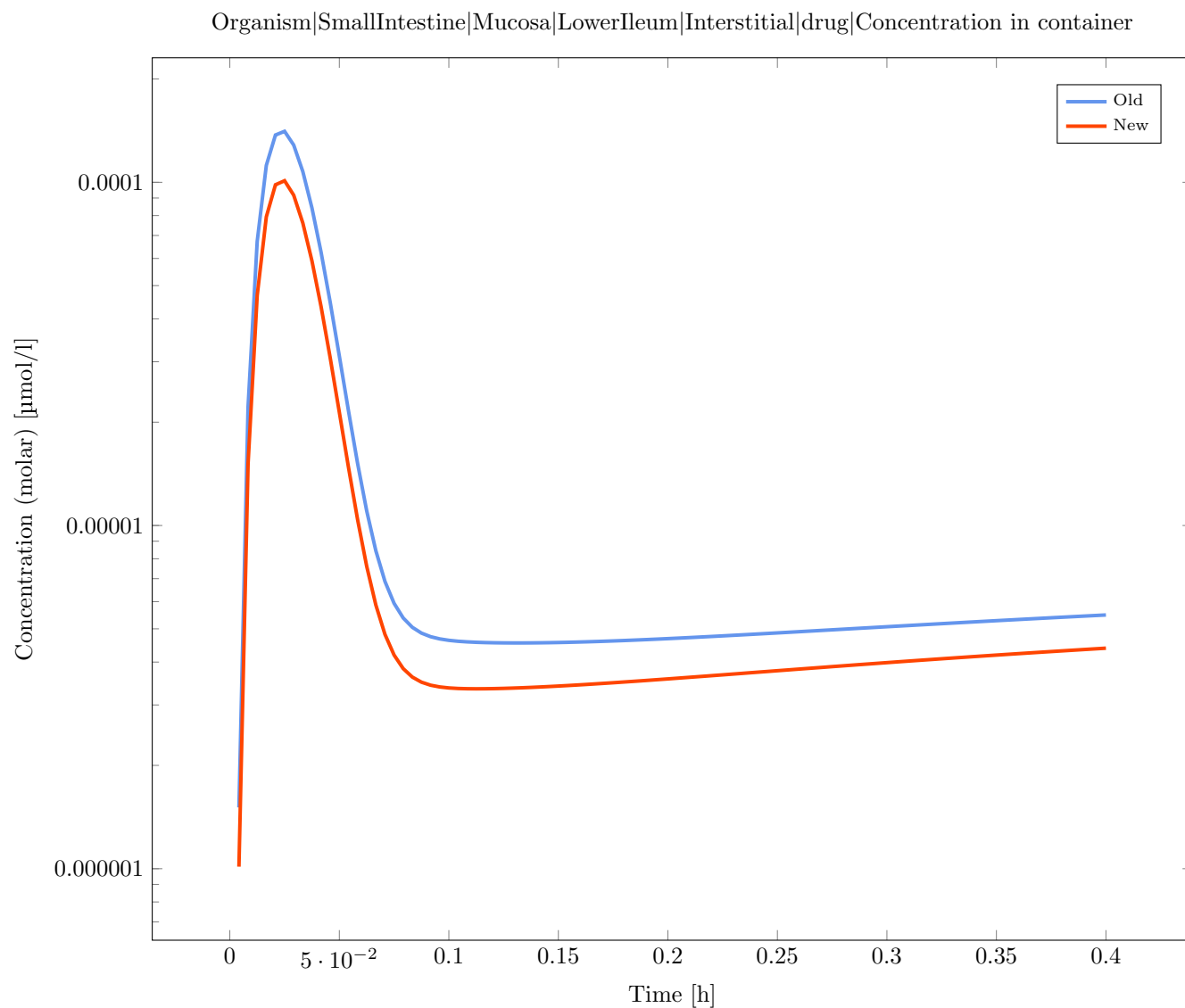


Figure 1.57

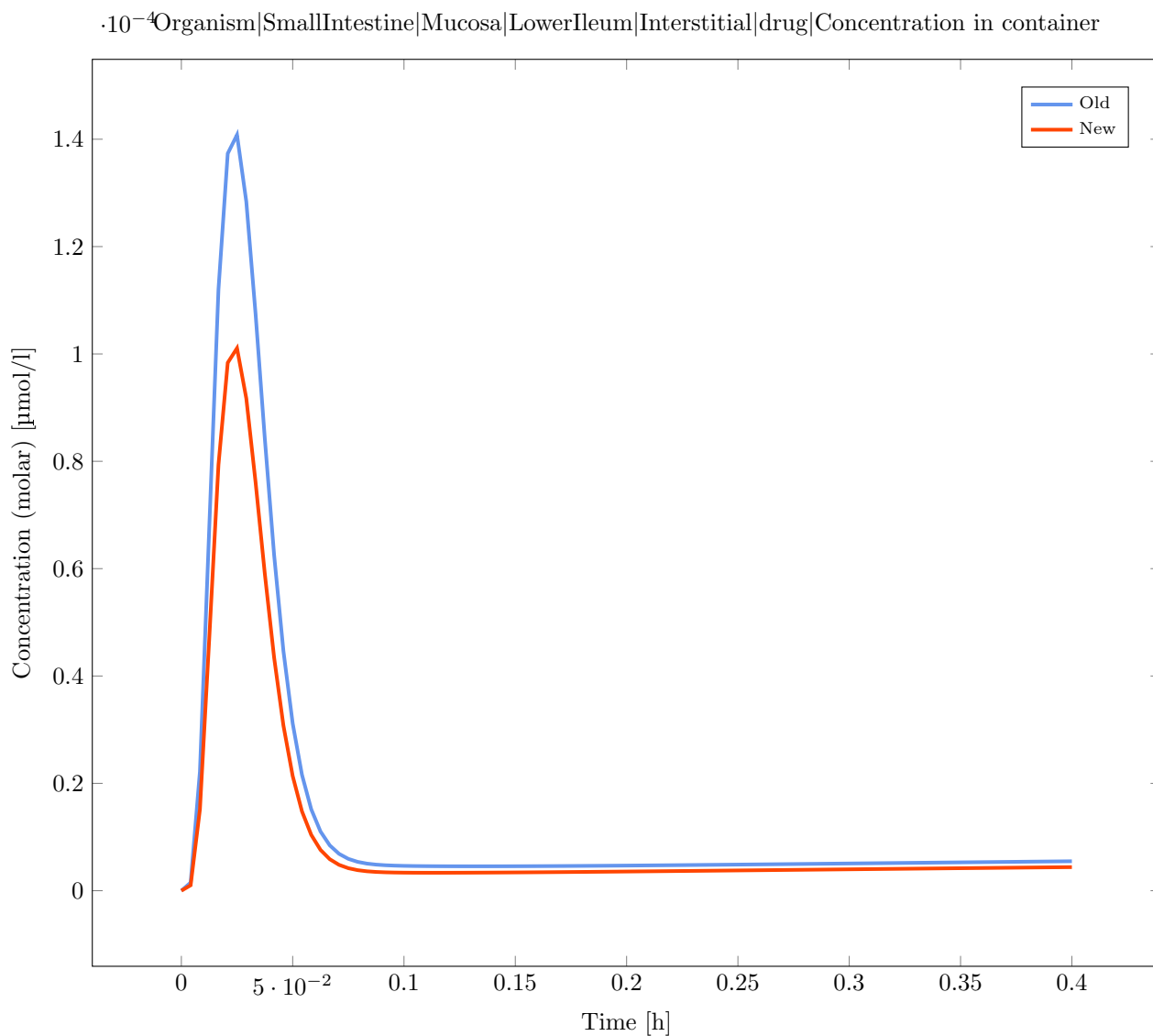
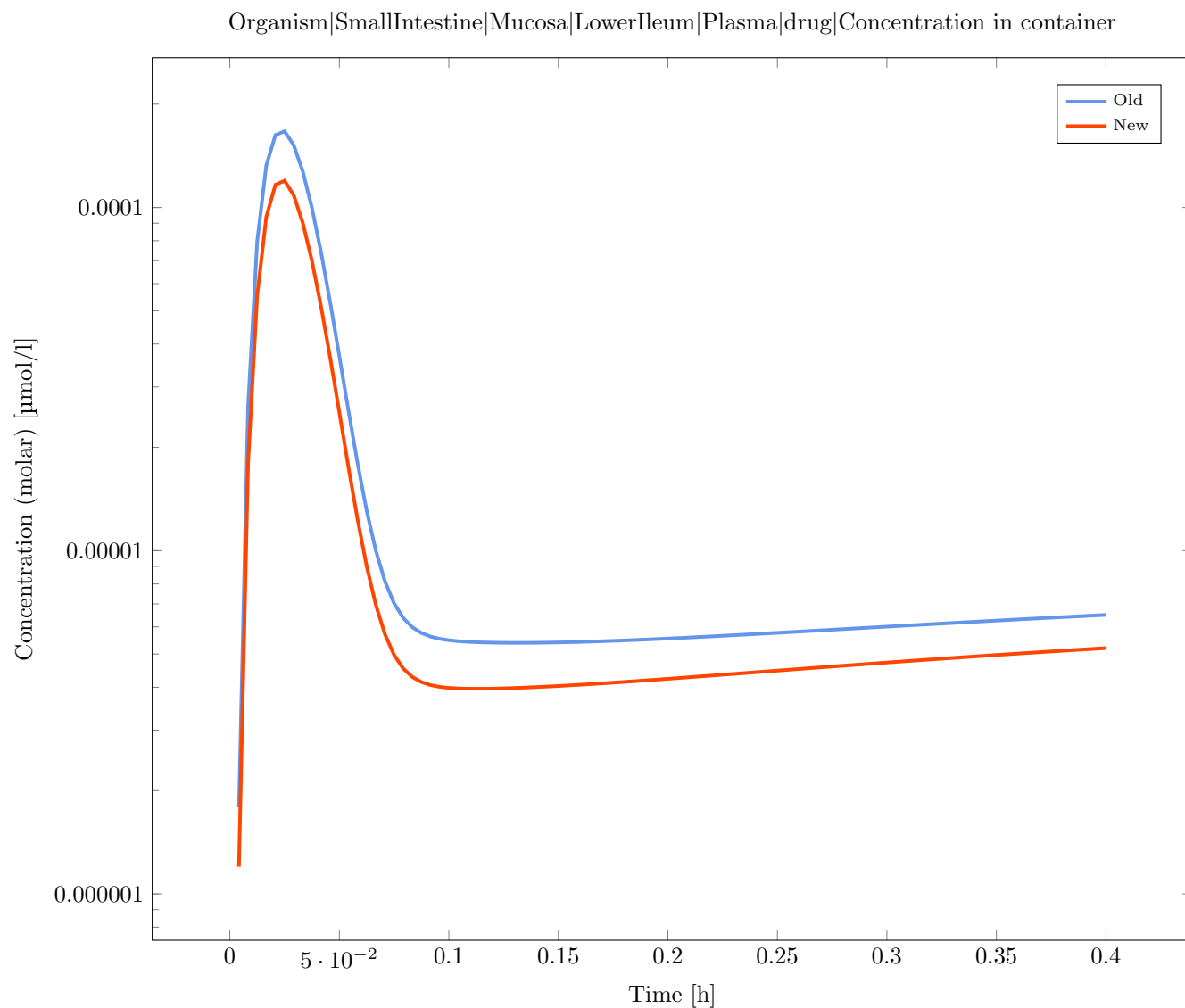


Figure 1.58

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Plasma|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Plasma|drug|Concentration in container' is 32.80% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

**Figure 1.59**

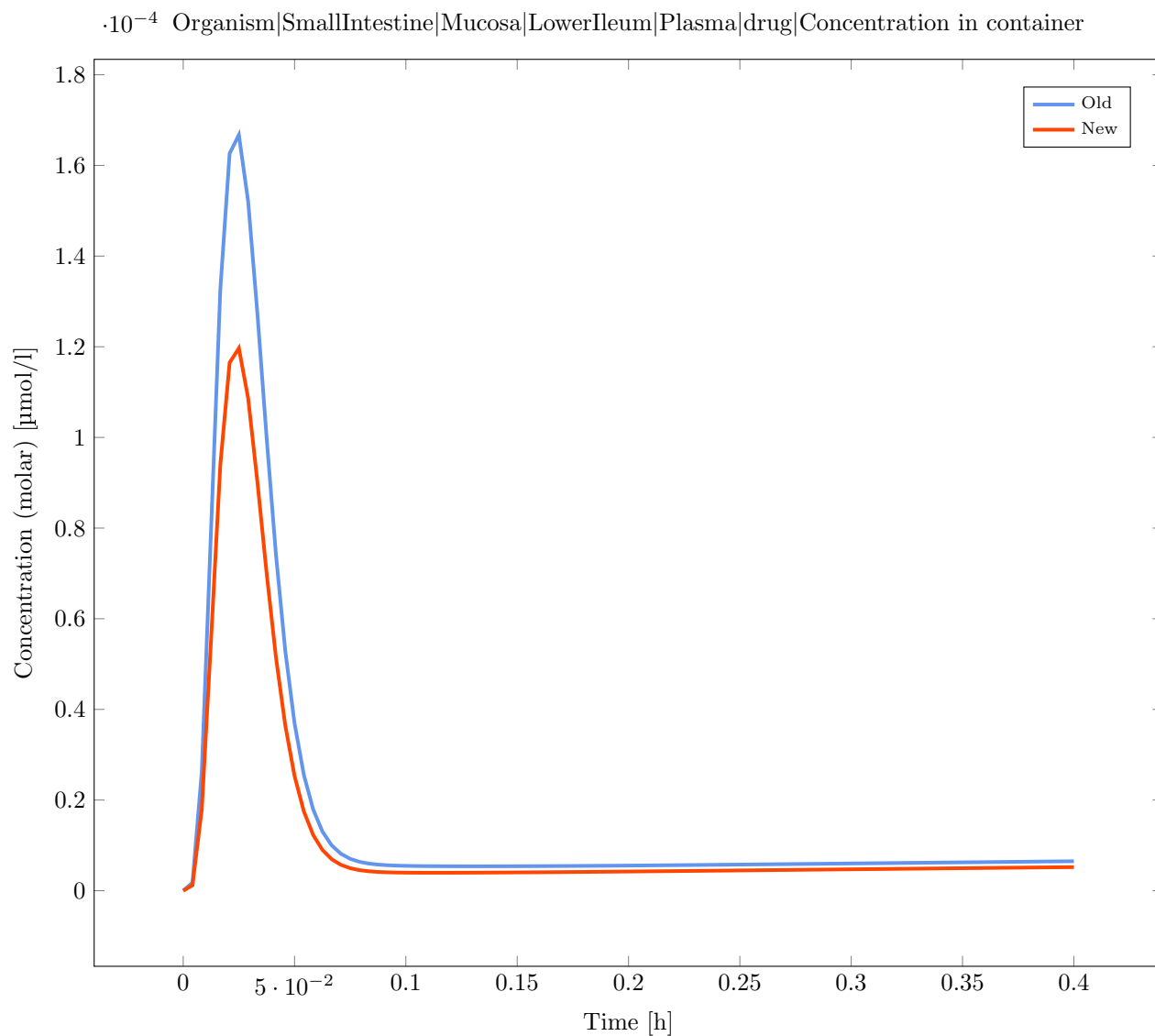
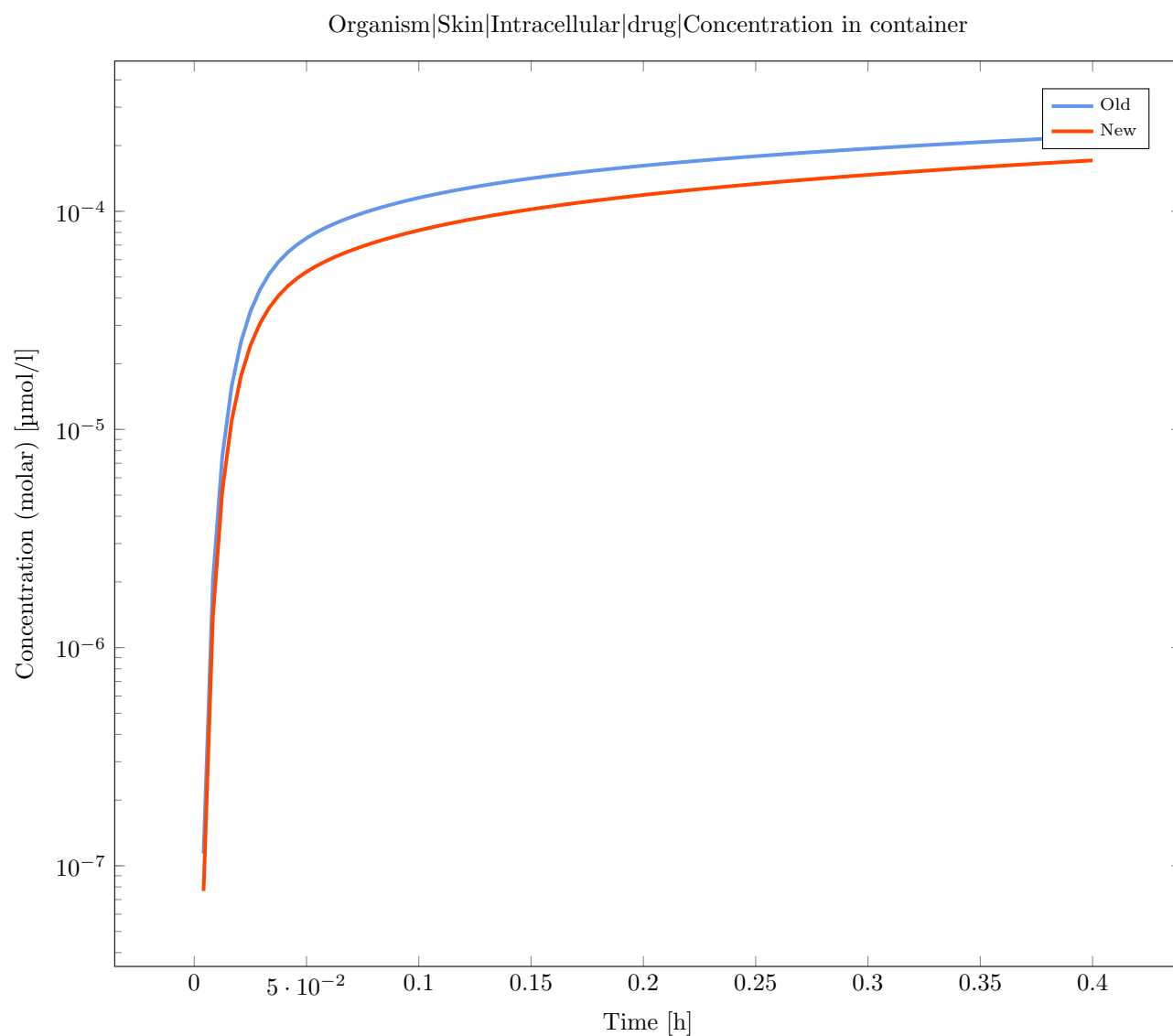


Figure 1.60

Output Path: Organism|Skin|Intracellular|drug|Concentration in container

Deviation for 'Organism|Skin|Intracellular|drug|Concentration in container' is 32.57% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

**Figure 1.61**

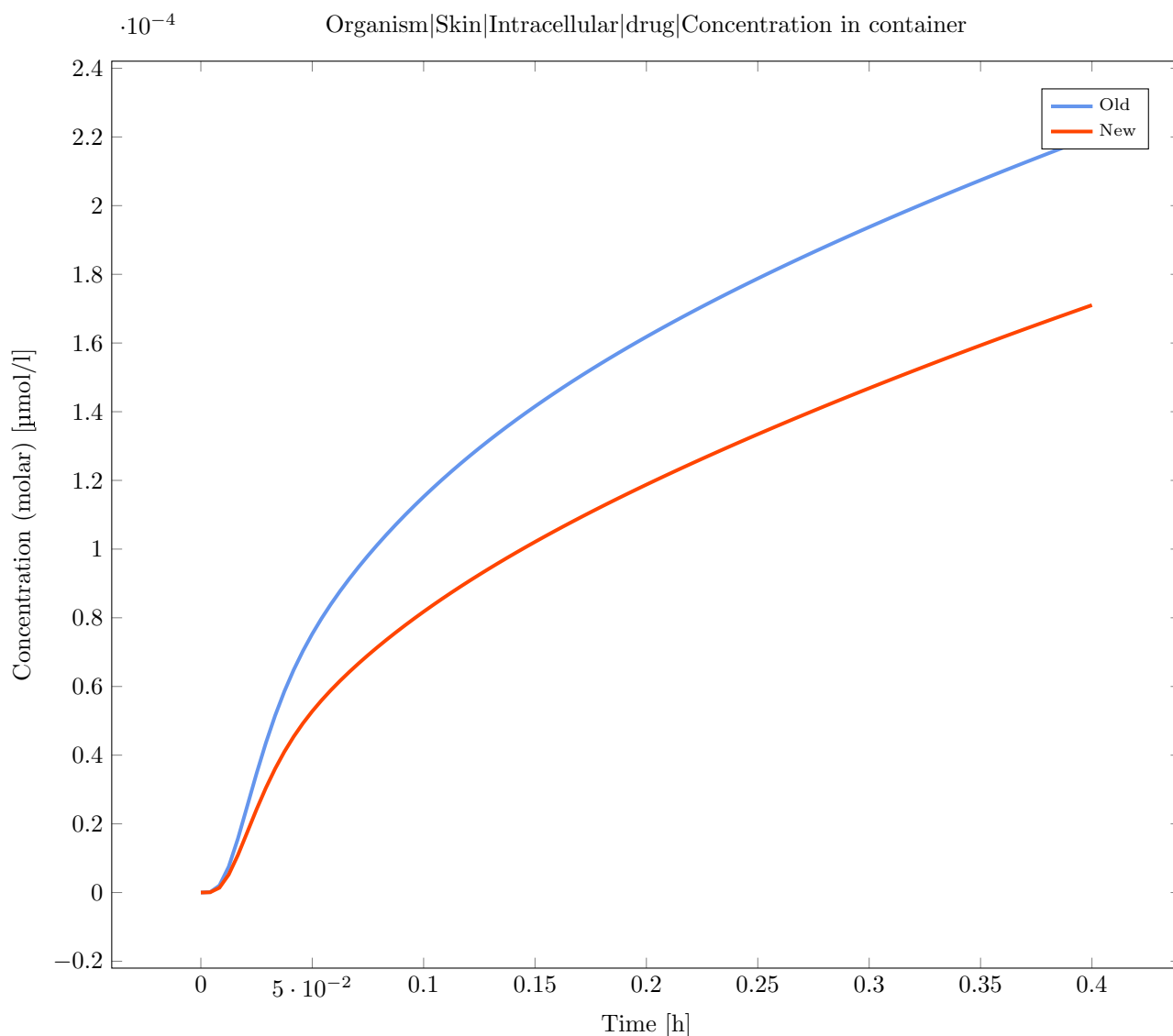


Figure 1.62

Simulation: Human_SingleORAL_PolyParticlesNormal_AsSuspention-Human_SingleORAL_PolyParticlesNormal_AsSuspention_dissolved_radius

Result of the validation: **Invalid**

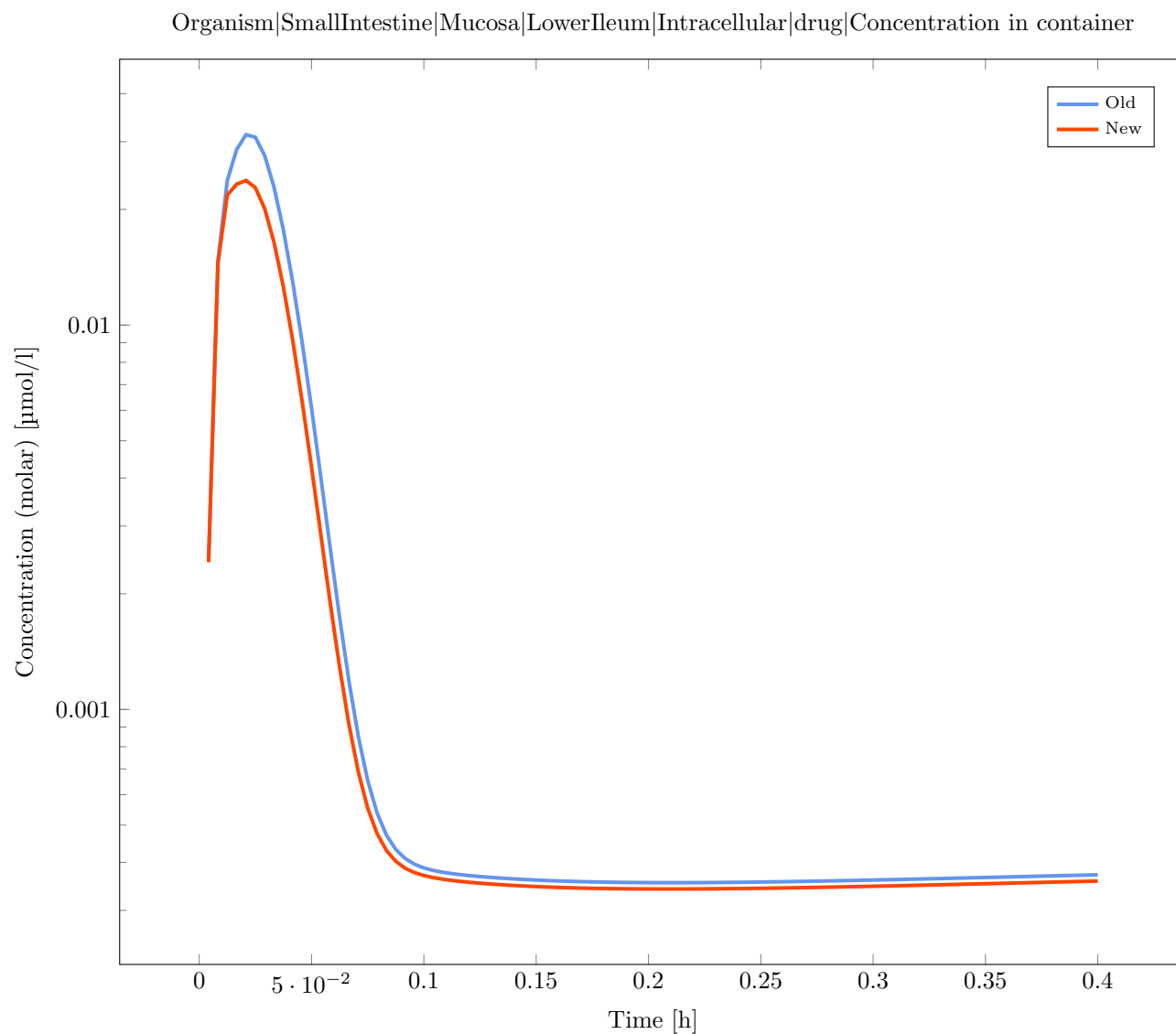
Absolute Tolerance: 1.00E-10

Relative Tolerance: 1.00E-5

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container' is 29.81% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.30

**Figure 1.63**

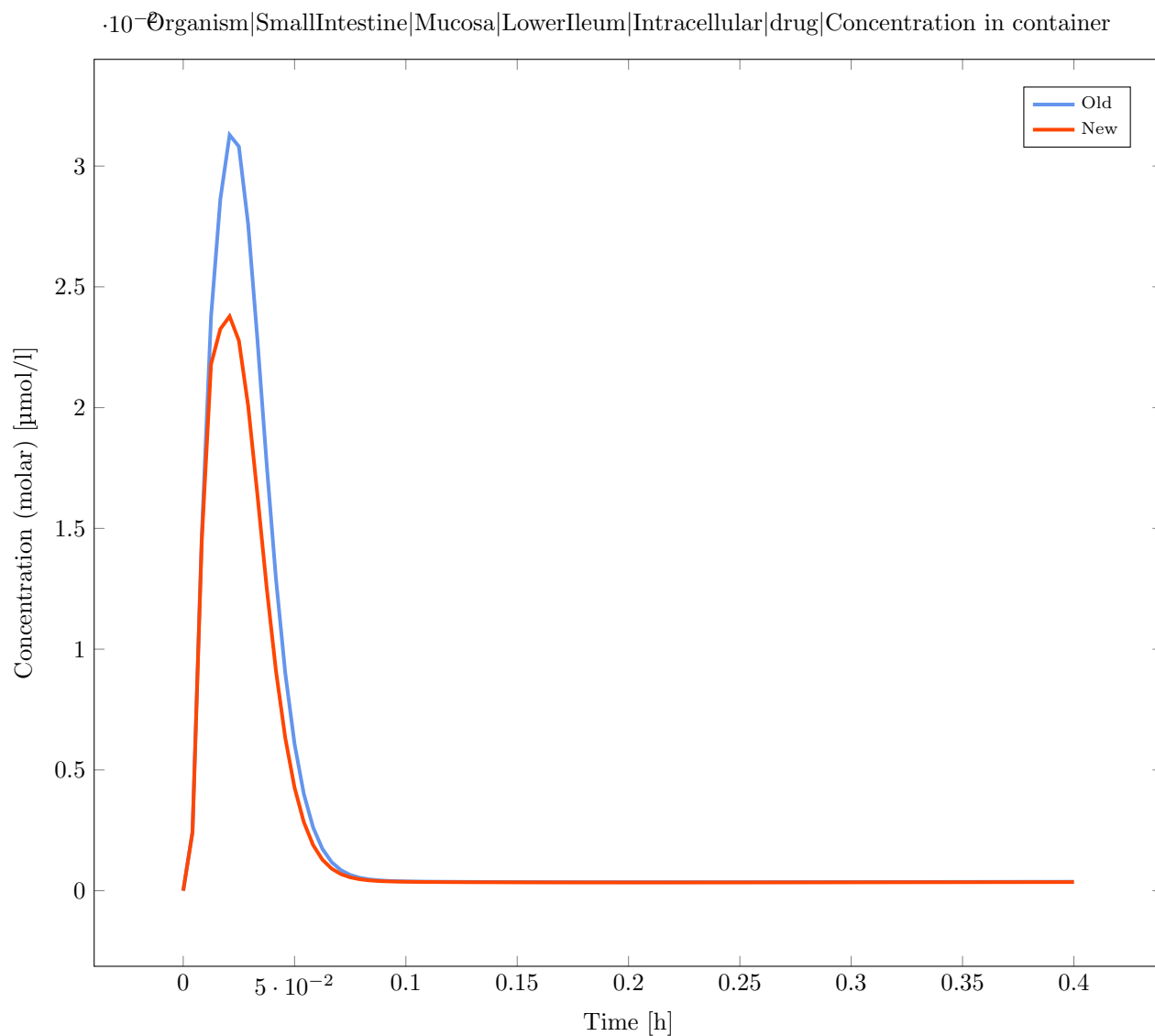
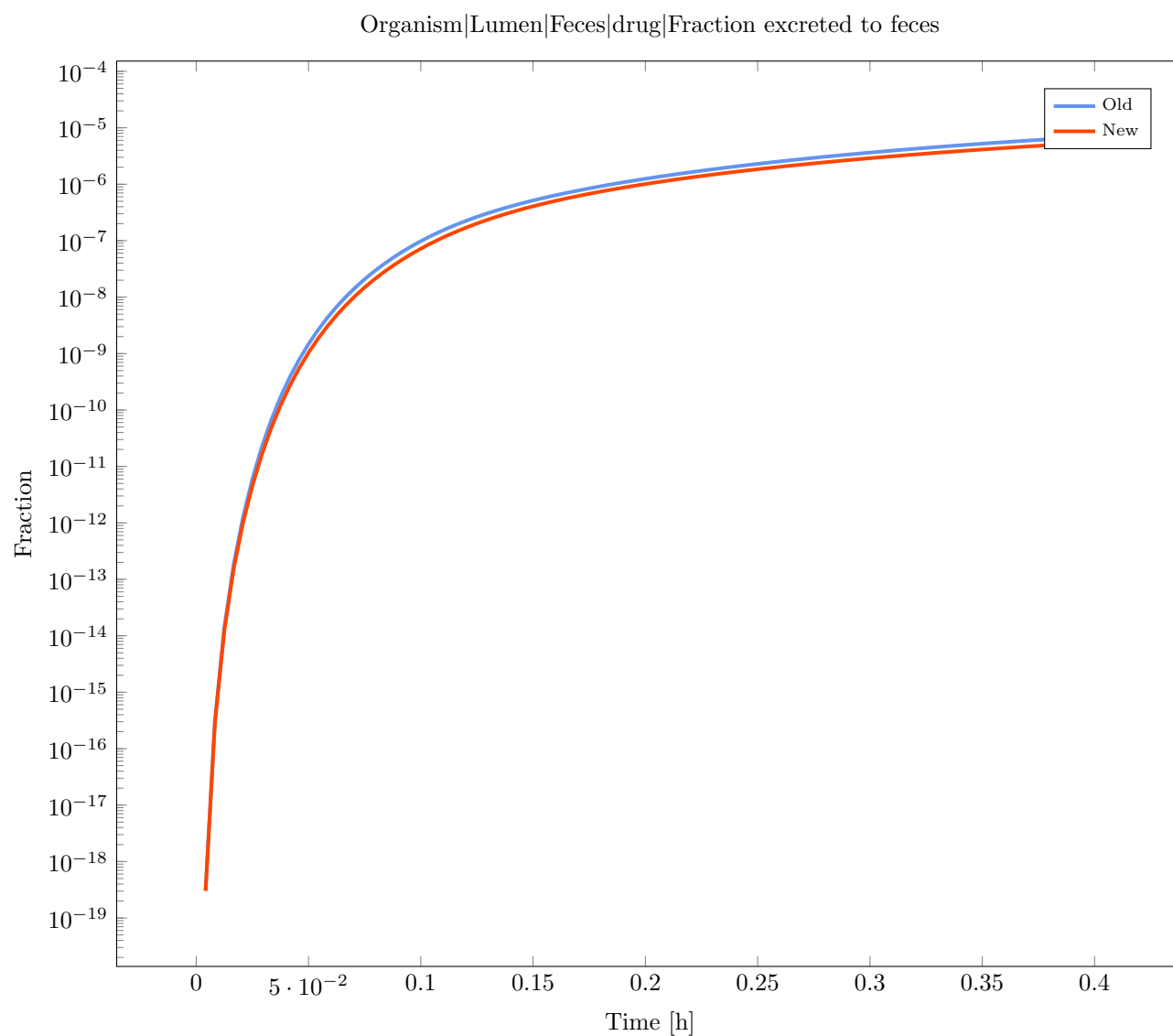


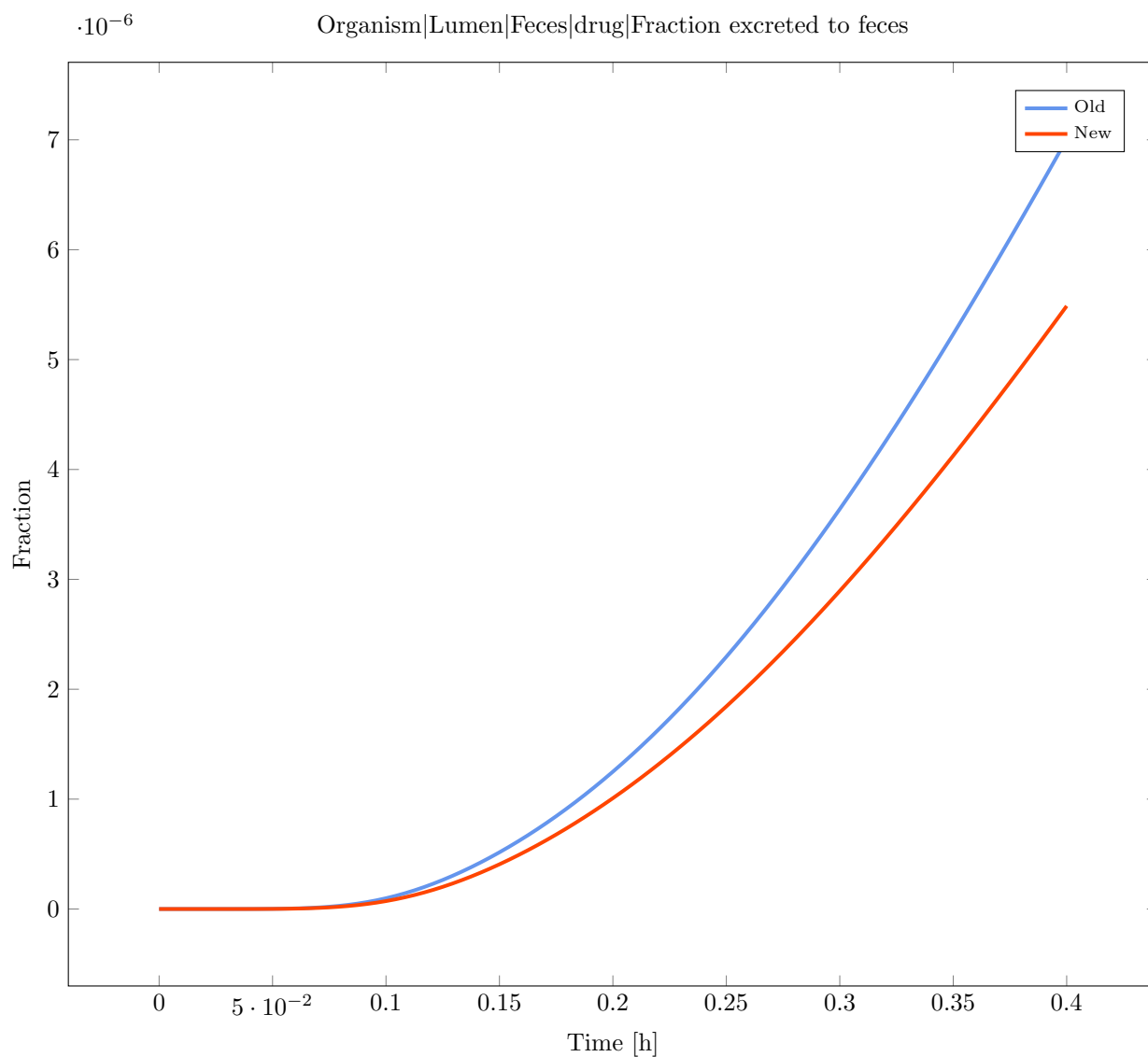
Figure 1.64

Output Path: Organism|Lumen|Feces|drug|Fraction excreted to feces

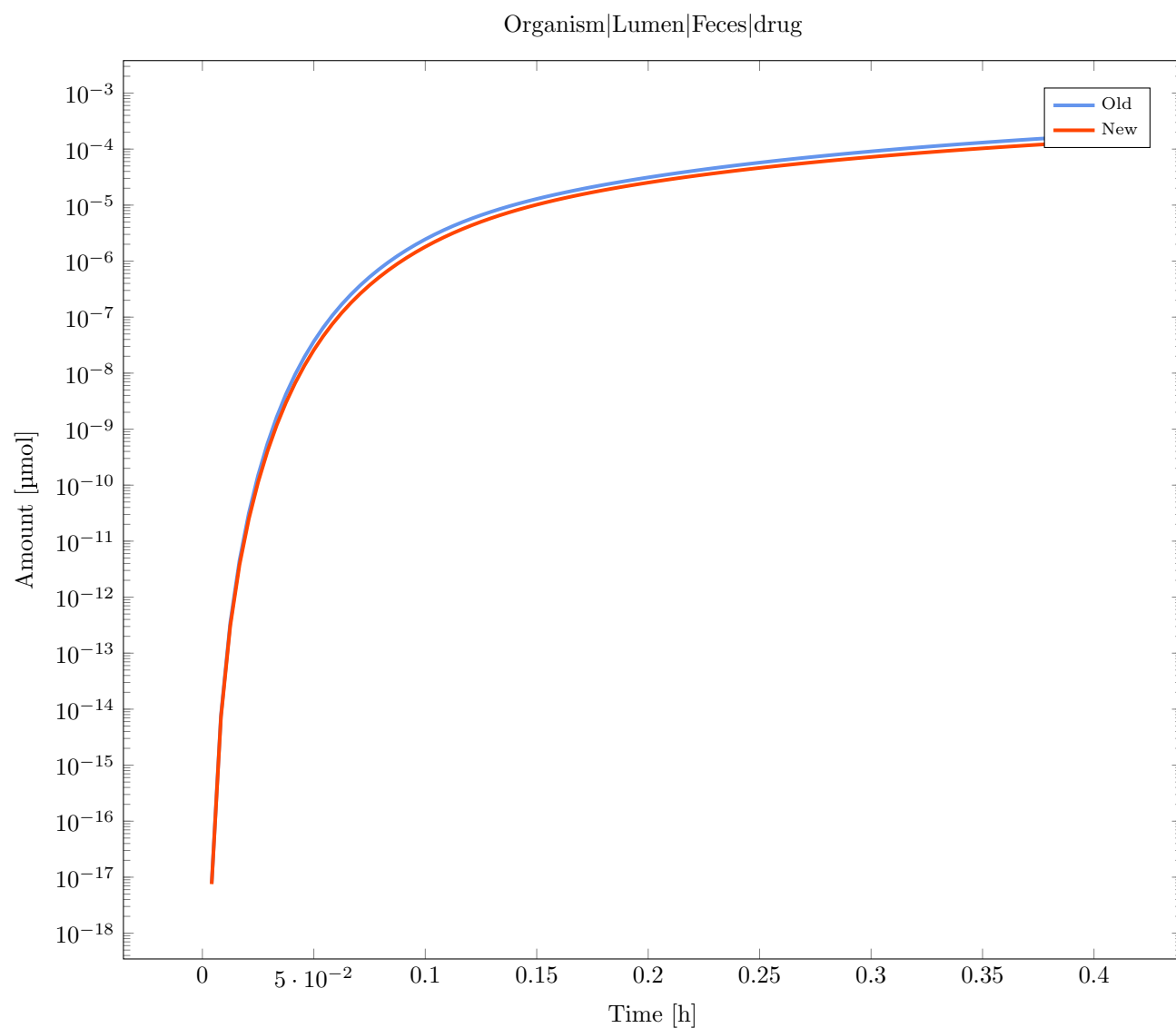
Deviation for 'Organism|Lumen|Feces|drug|Fraction excreted to feces' is 29.80% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.30

**Figure 1.65**

**Figure 1.66****Output Path: Organism|Lumen|Feces|drug**

Deviation for 'Organism|Lumen|Feces|drug' is 29.80% and is greater than the allowed max. tolerance of 3.00%
Deviation: 0.30

**Figure 1.67**

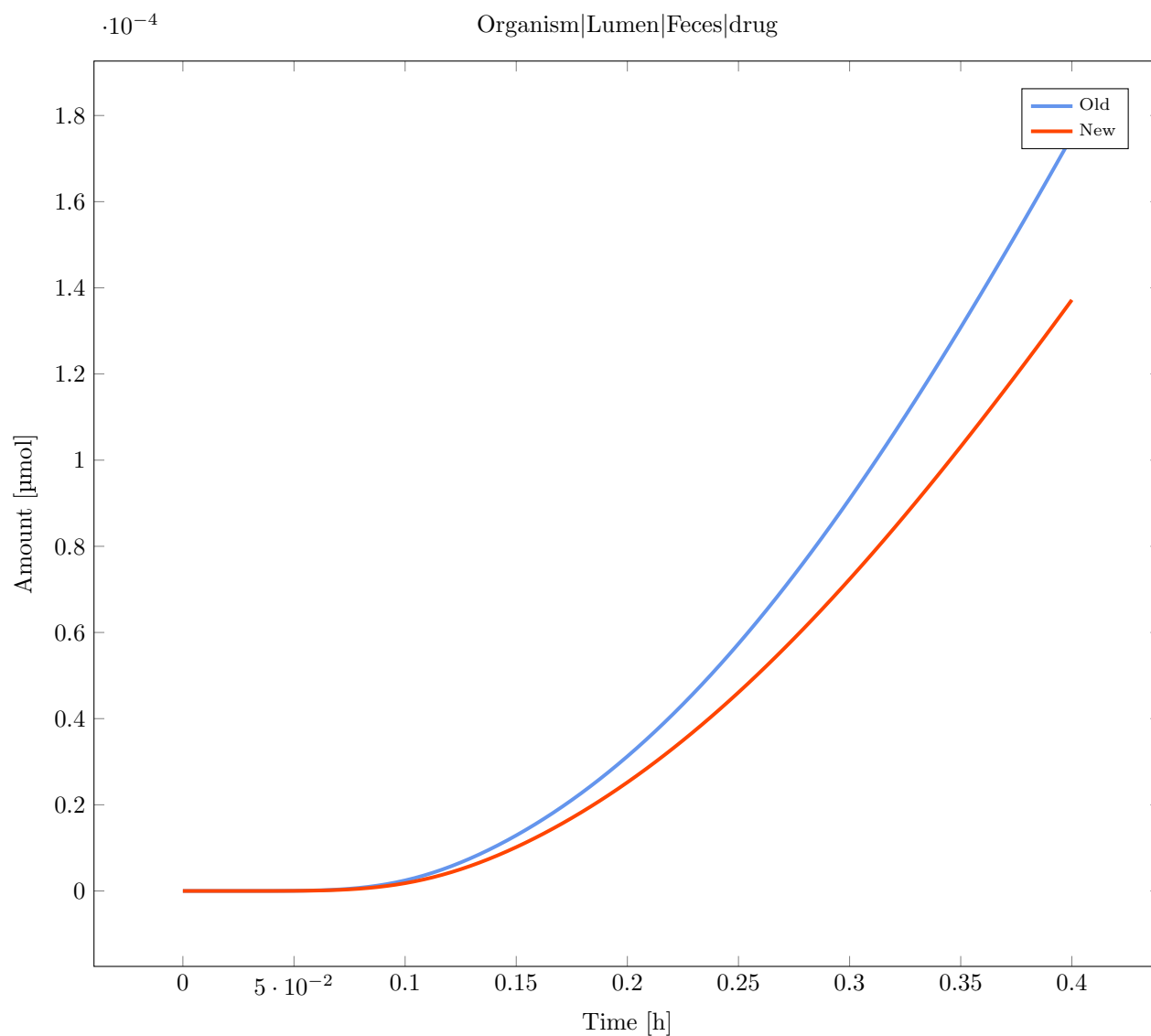
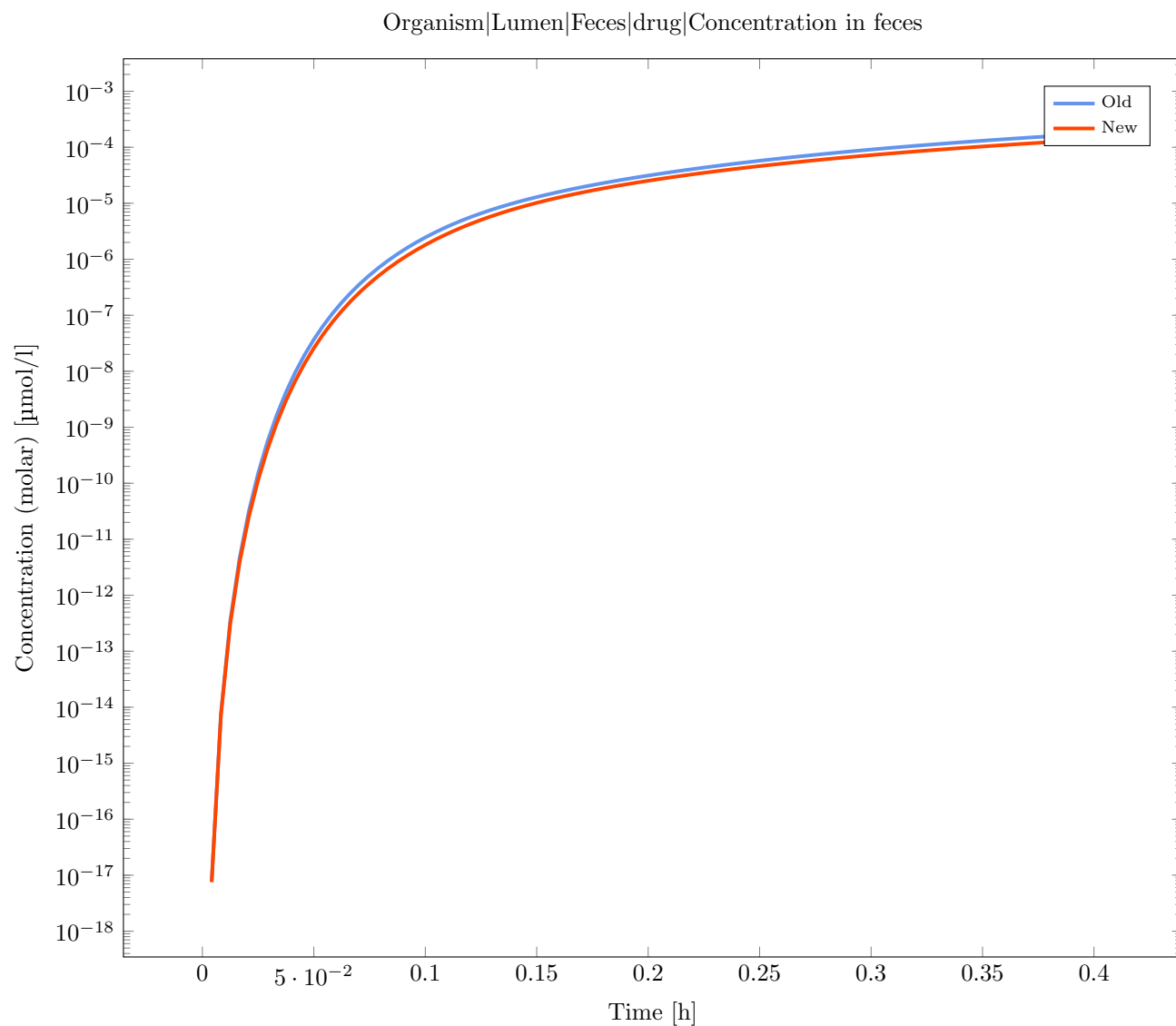


Figure 1.68

Output Path: Organism|Lumen|Feces|drug|Concentration in feces

Deviation for 'Organism|Lumen|Feces|drug|Concentration in feces' is 29.80% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.30

**Figure 1.69**

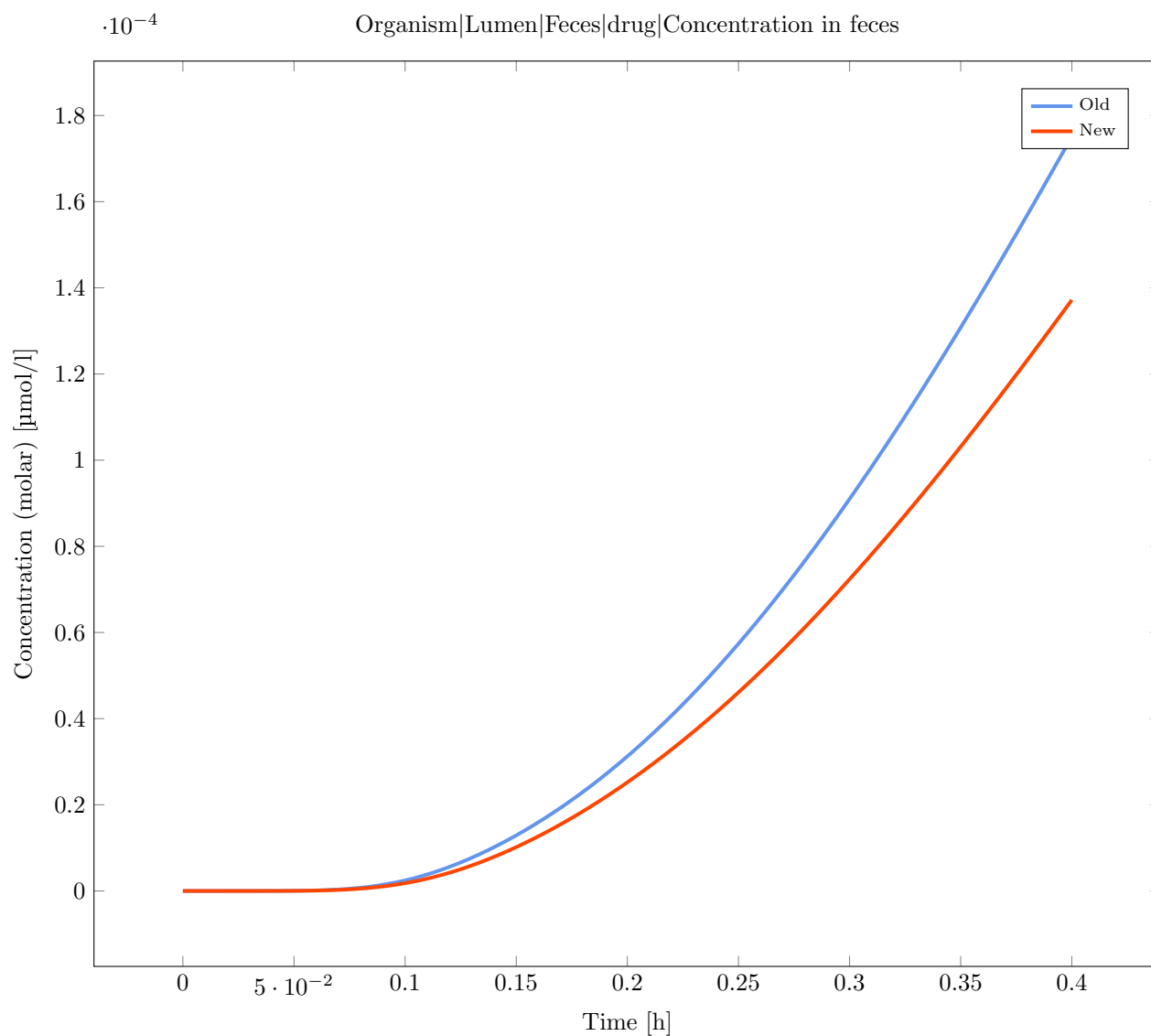
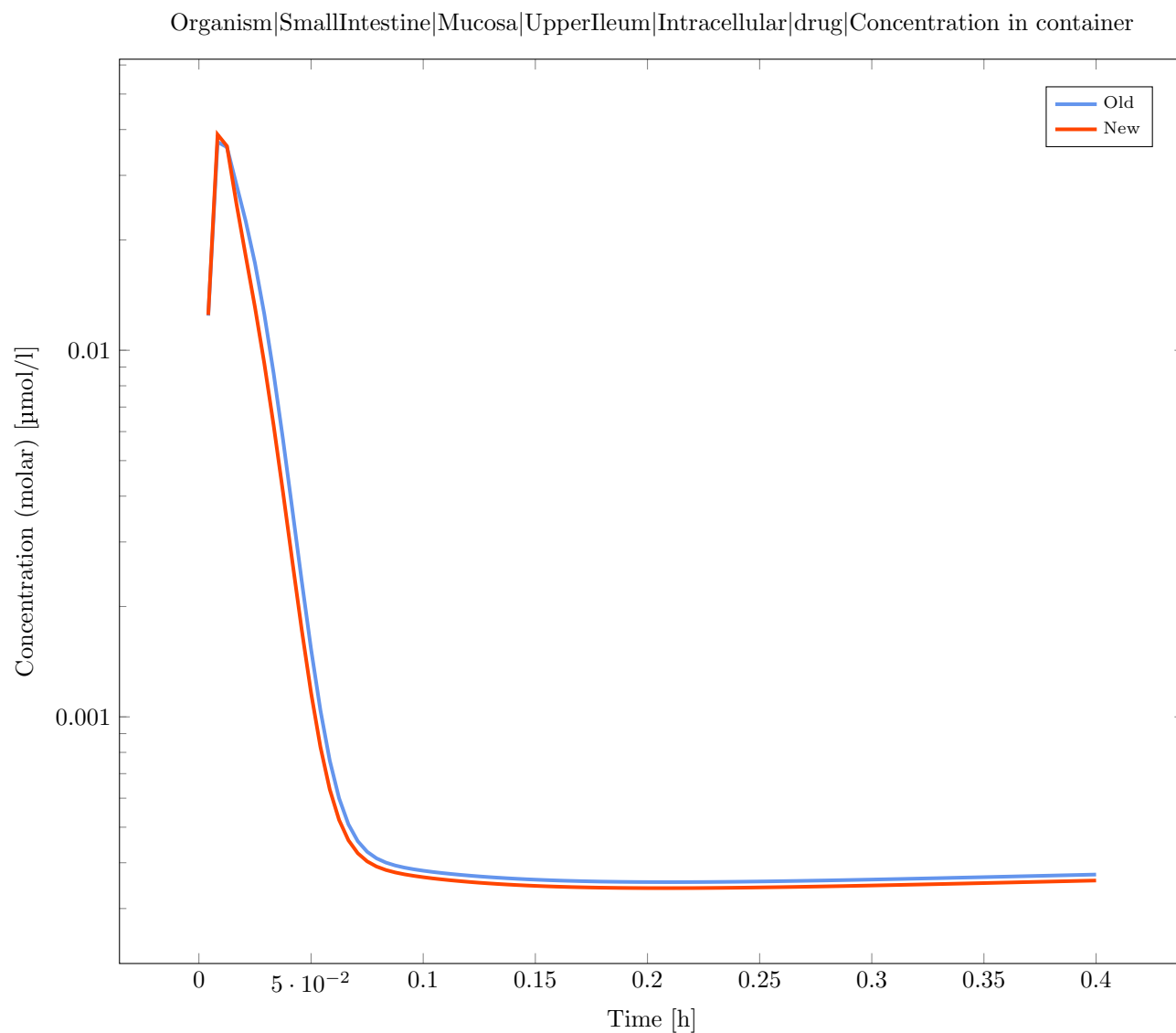


Figure 1.70

Output Path: Organism|SmallIntestine|Mucosa|UpperIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|UpperIleum|Intracellular|drug|Concentration in container' is 28.21% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.28

**Figure 1.71**

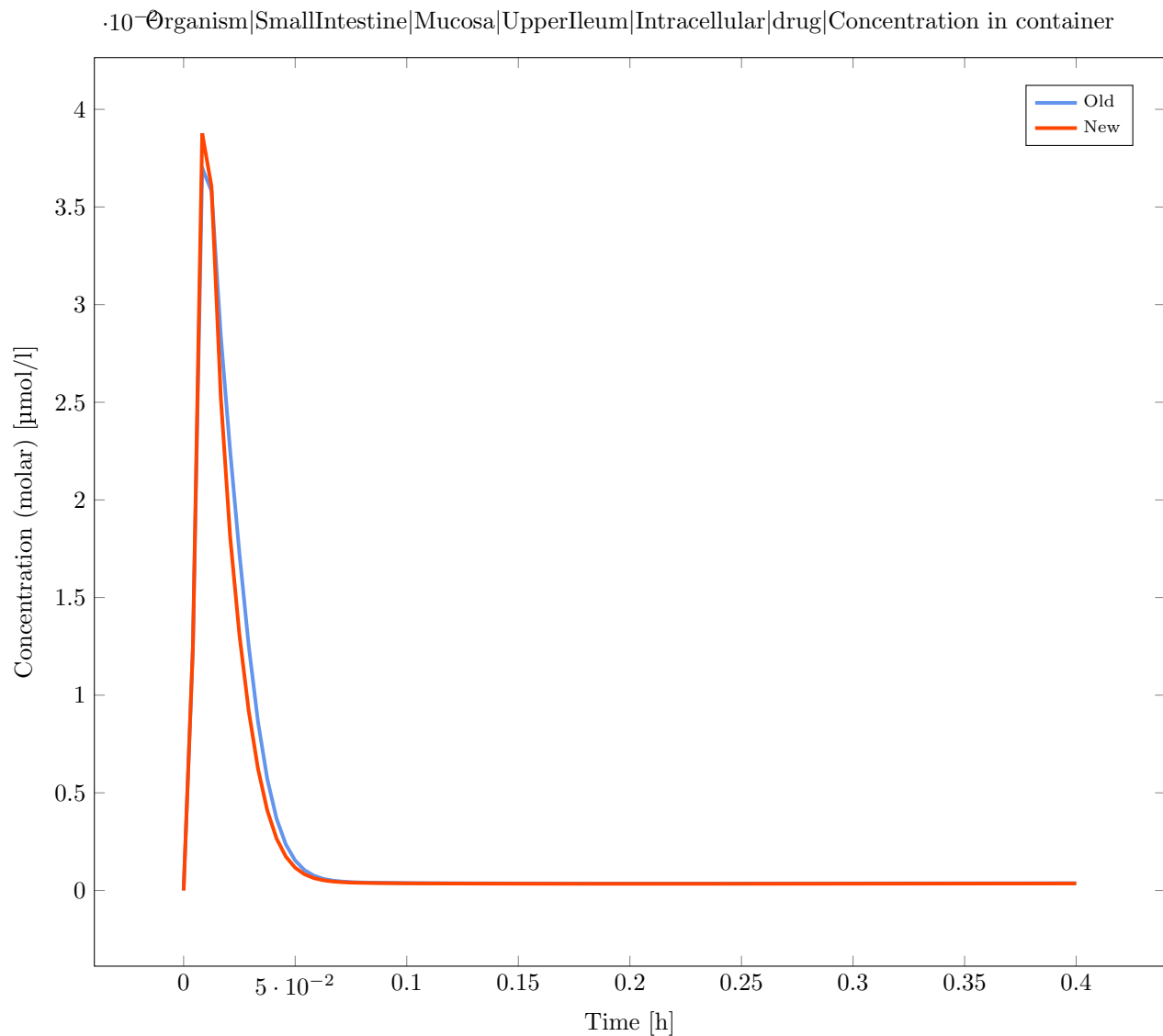


Figure 1.72

Simulation: Human_SingleORAL_PolyParticlesNormal_AsSuspension-Human_SingleORAL_PolyParticlesNormal_AsSuspension_treat_precipated_drug_as_soluble

Result of the validation: **Invalid**

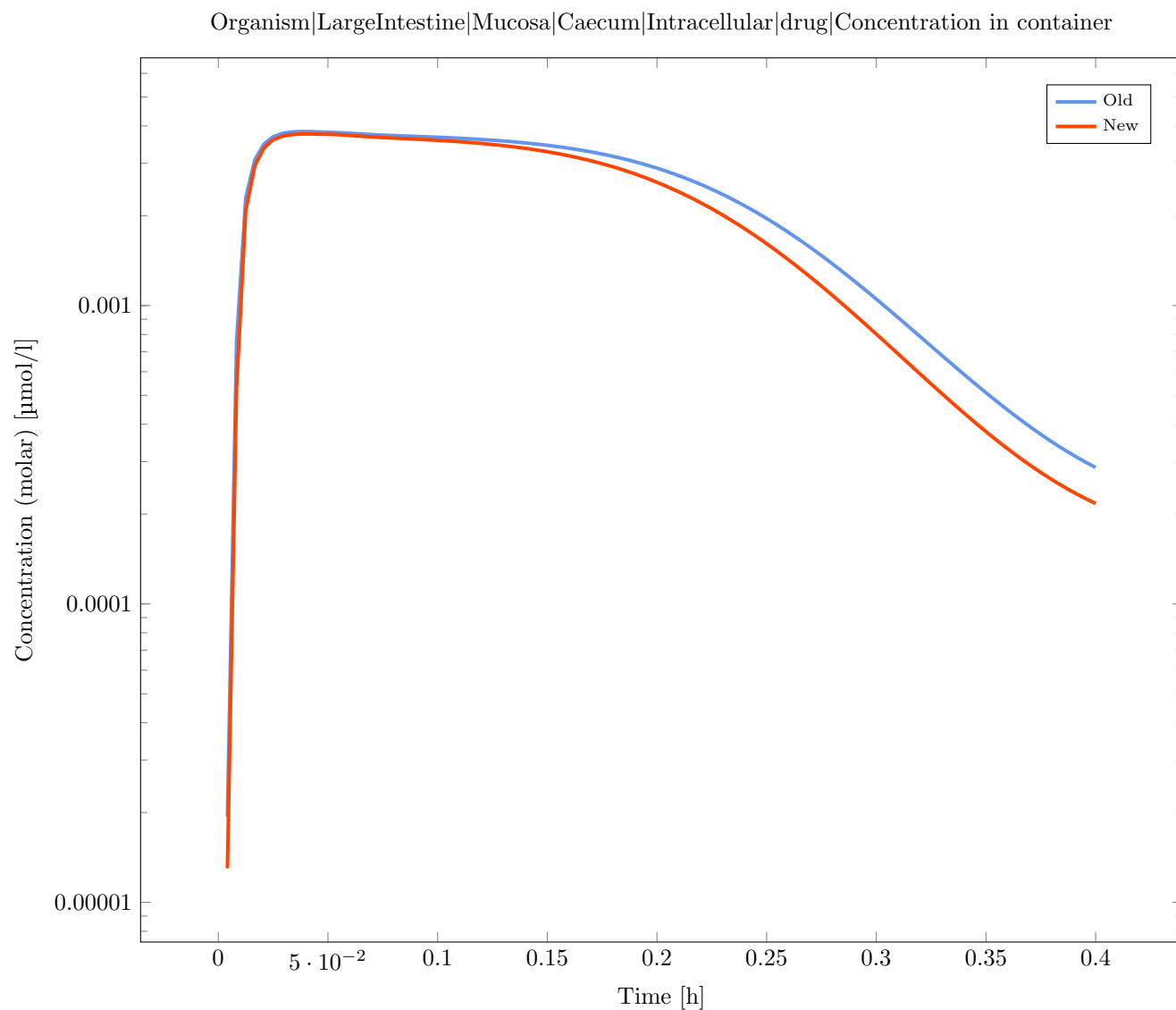
Absolute Tolerance: 1.00E-10

Relative Tolerance: 1.00E-5

Output Path: Organism|LargeIntestine|Mucosa|Caecum|Intracellular|drug|Concentration in container

Deviation for 'Organism|LargeIntestine|Mucosa|Caecum|Intracellular|drug|Concentration in container' is 32.96% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

**Figure 1.73**

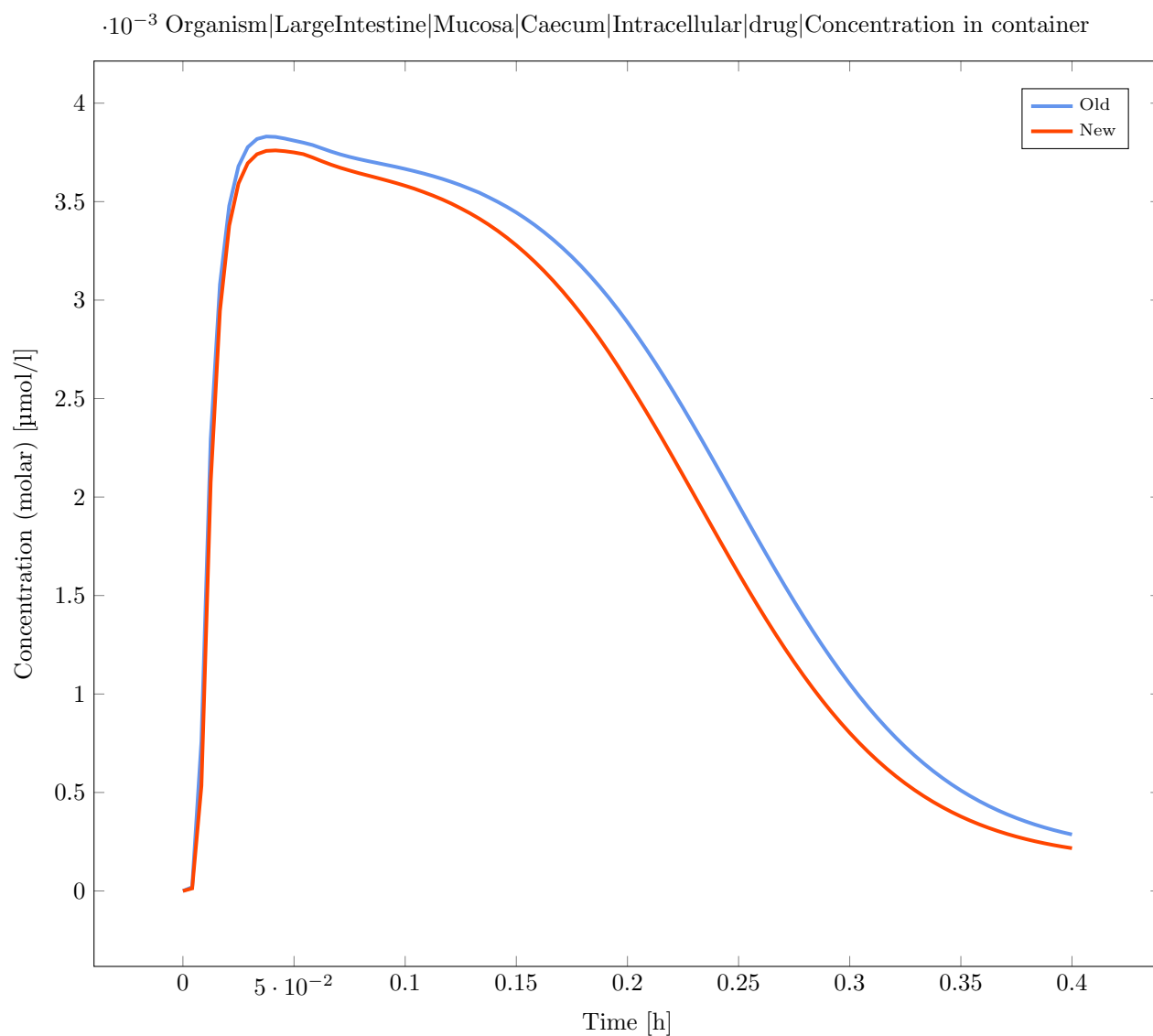


Figure 1.74

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container' is 32.88% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

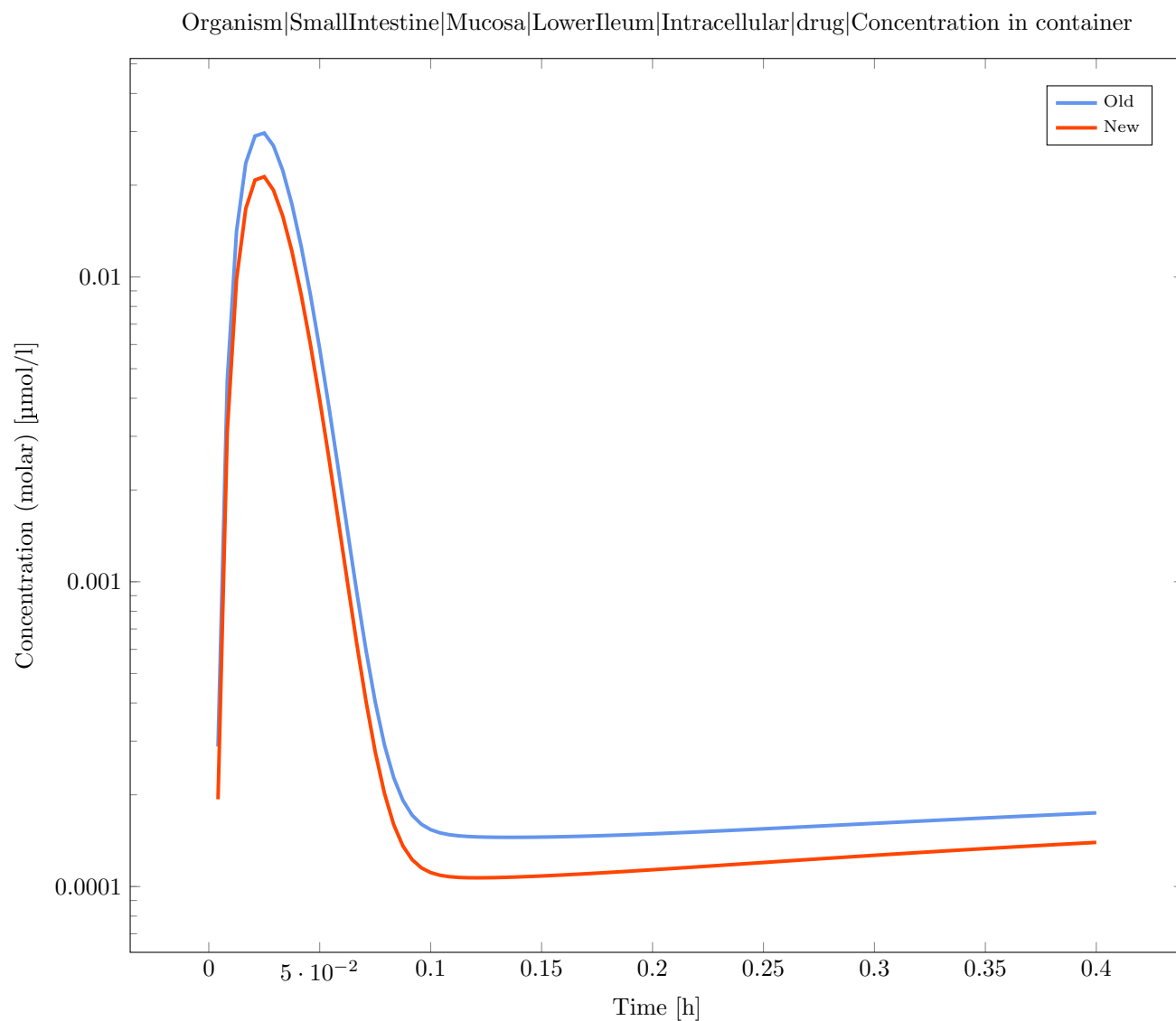


Figure 1.75

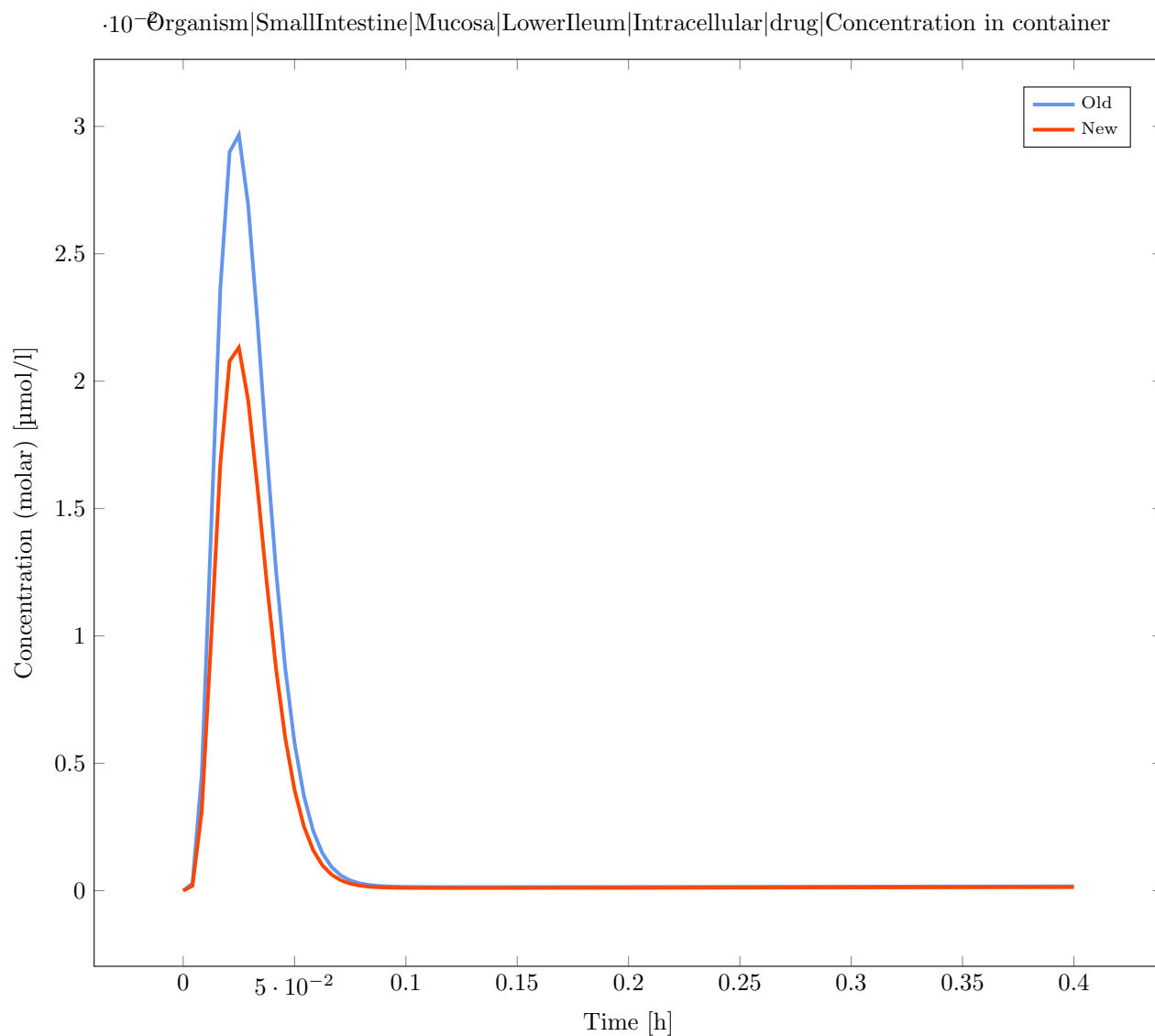


Figure 1.76

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Interstitial|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Interstitial|drug|Concentration in container' is 32.80% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

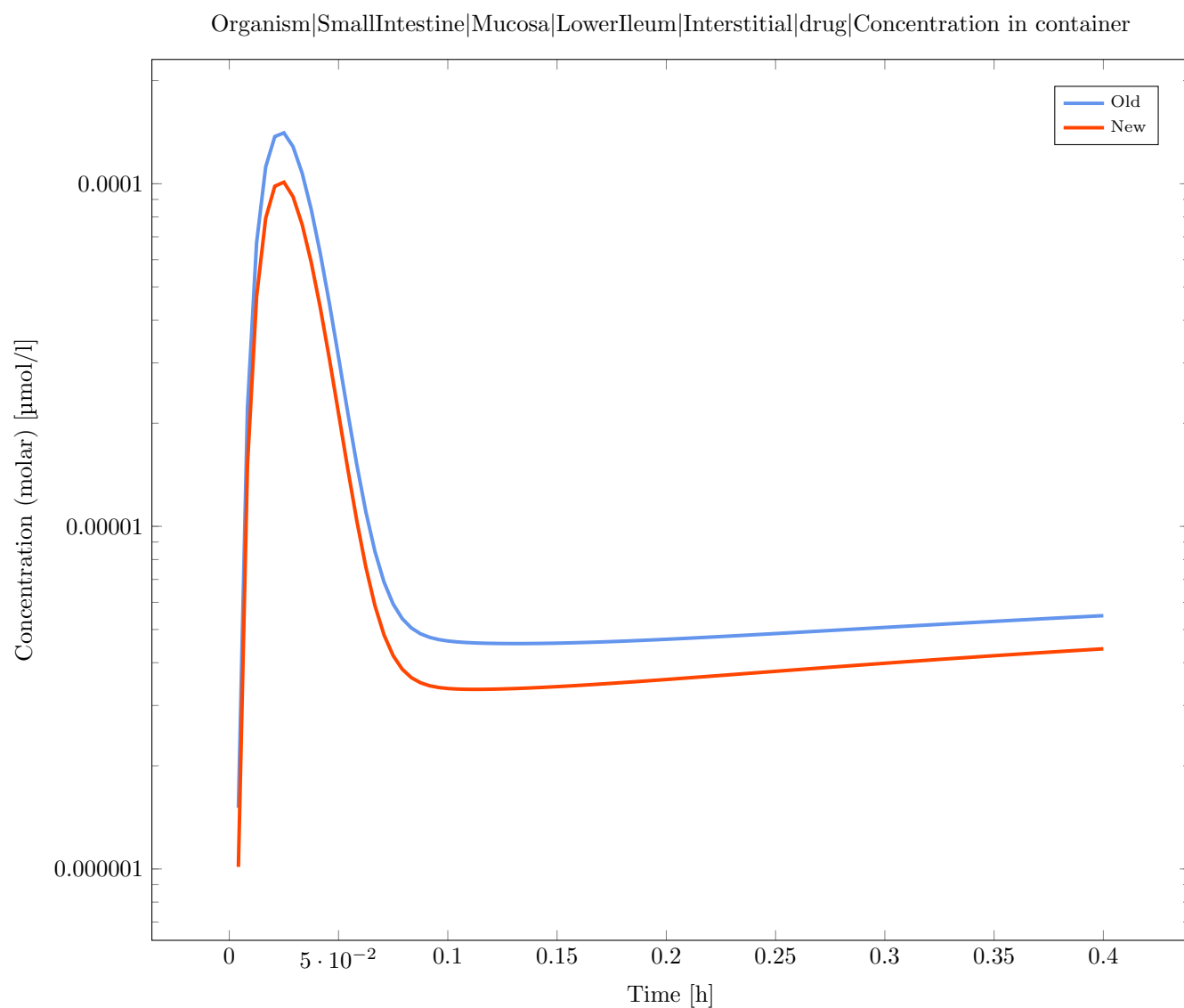


Figure 1.77

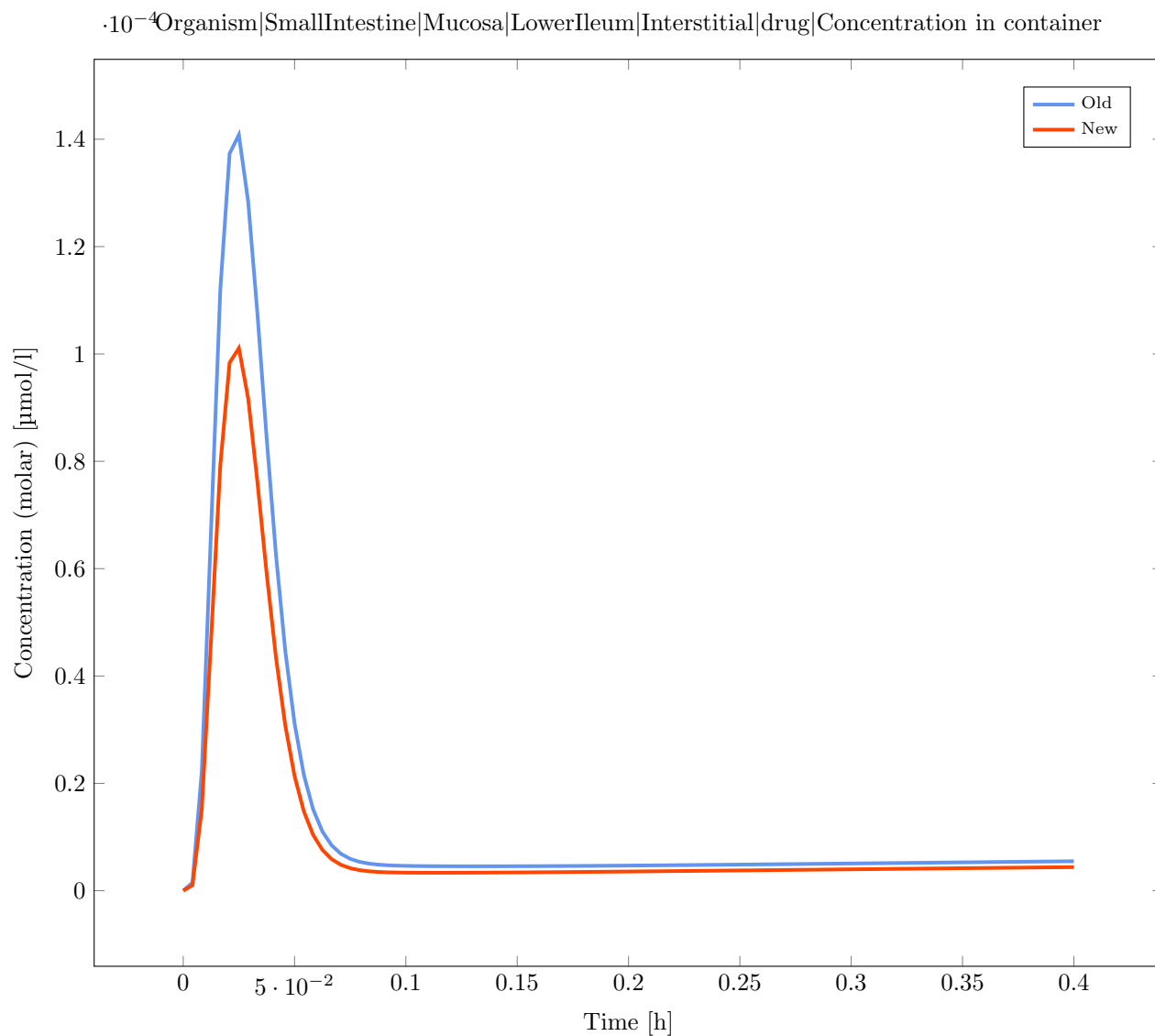


Figure 1.78

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Plasma|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Plasma|drug|Concentration in container' is 32.80% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

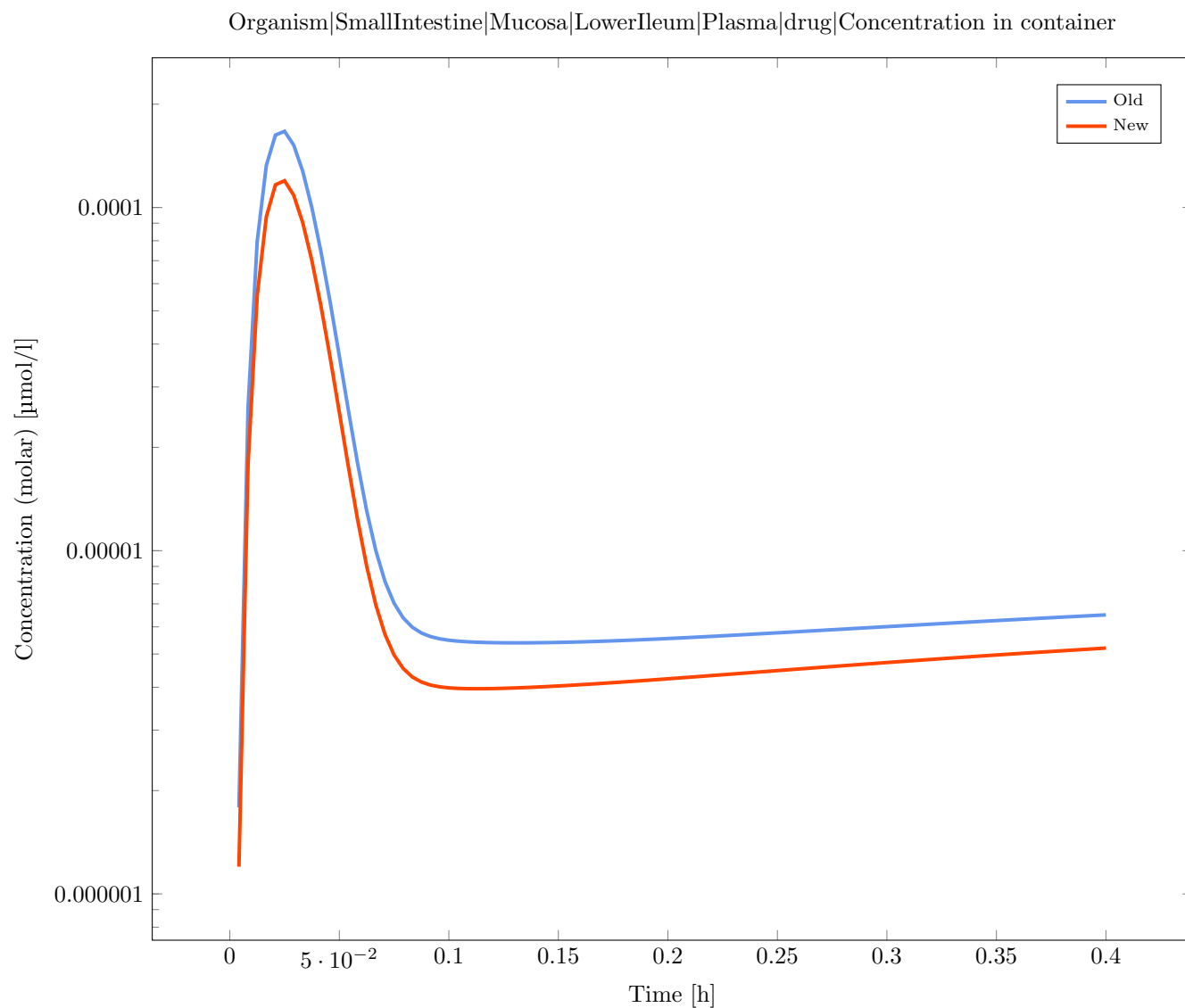


Figure 1.79

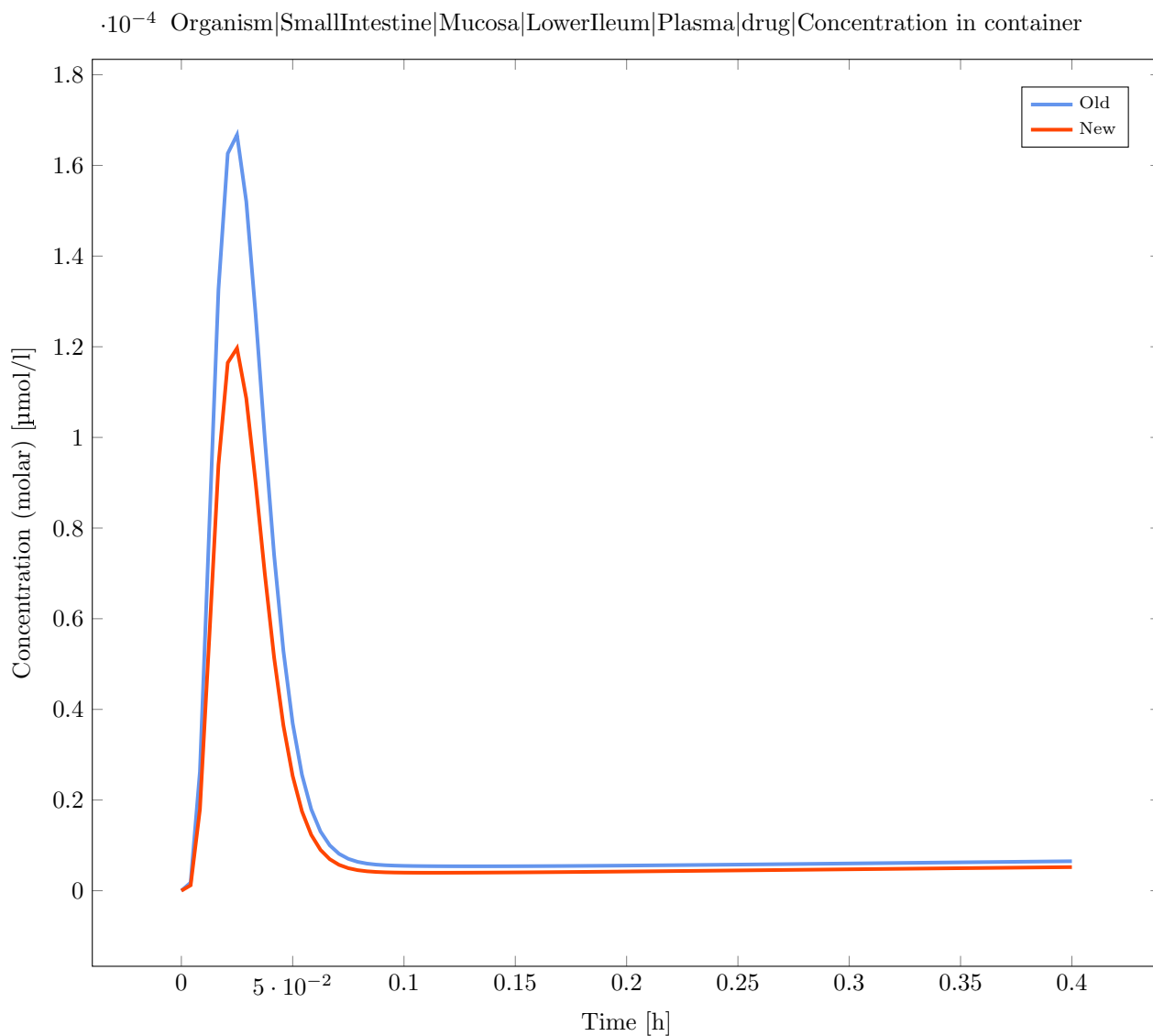
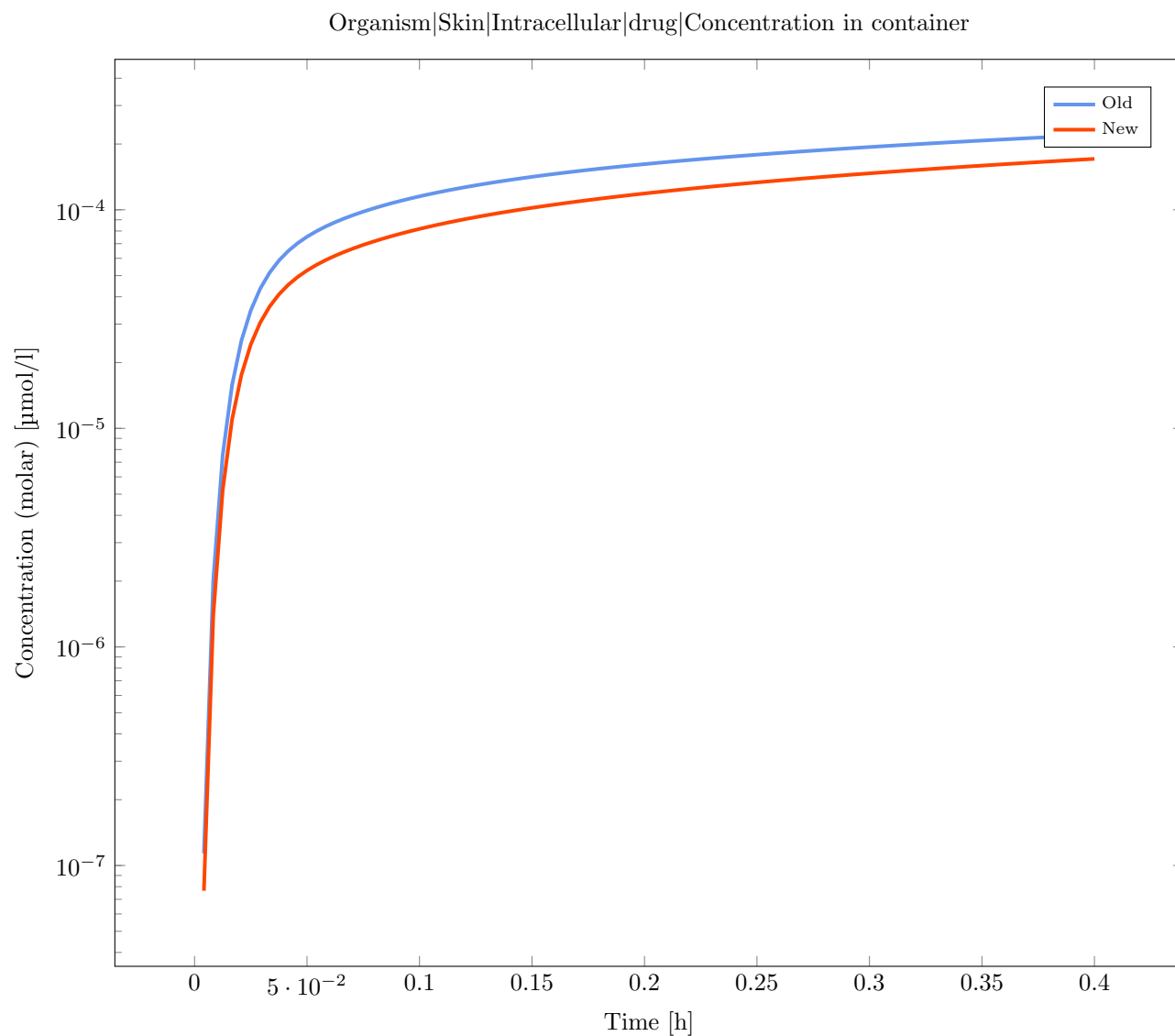


Figure 1.80

Output Path: Organism|Skin|Intracellular|drug|Concentration in container

Deviation for 'Organism|Skin|Intracellular|drug|Concentration in container' is 32.57% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.33

**Figure 1.81**

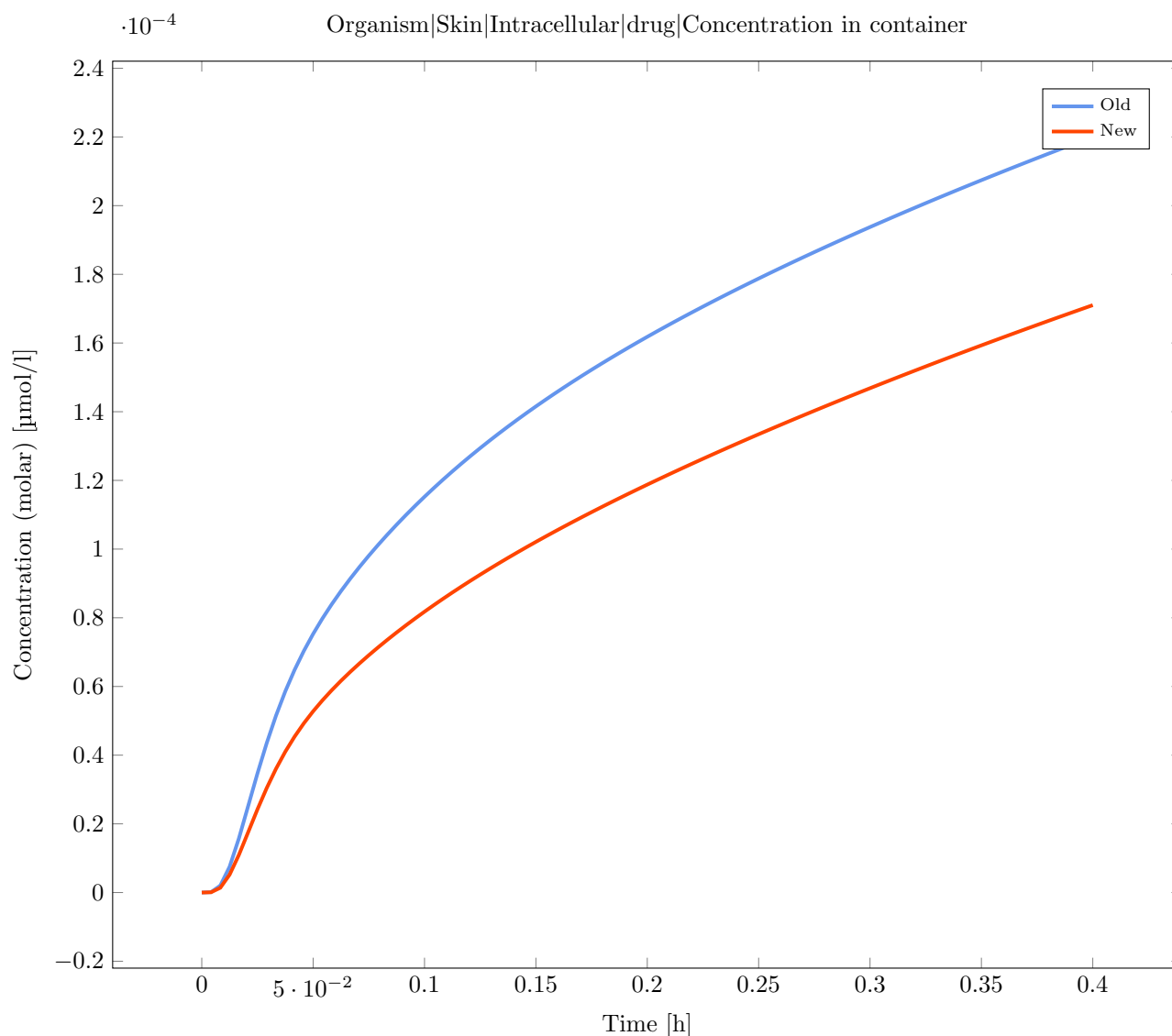


Figure 1.82

Simulation: Human_SingleORAL_Weibull-Human_SingleORAL_Weibull_MW_200_fu_0.2_LogP_5

Result of the validation: **Invalid**

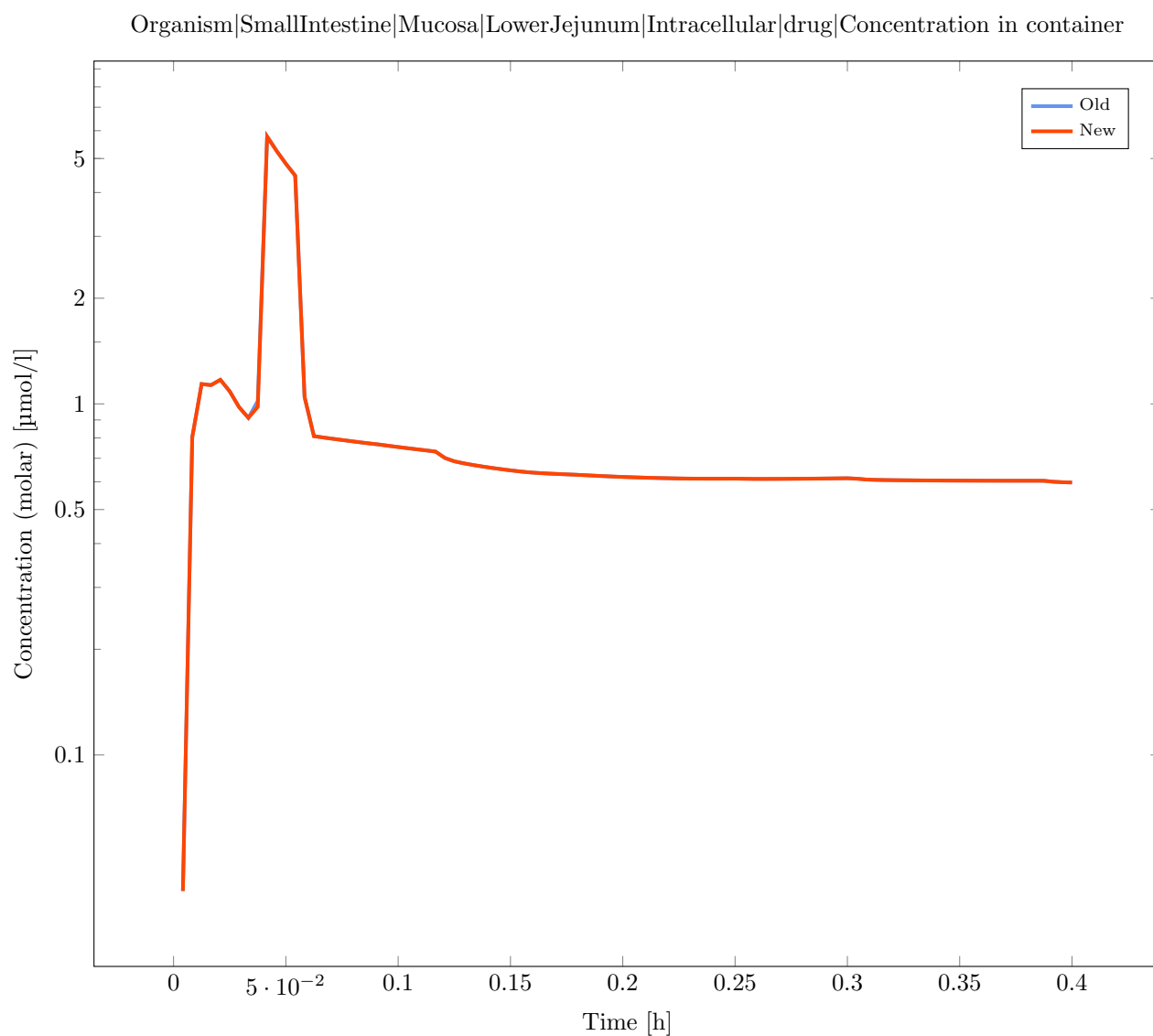
Absolute Tolerance: 1.00E-10

Relative Tolerance: 1.00E-5

Output Path: Organism|SmallIntestine|Mucosa|LowerJejunum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerJejunum|Intracellular|drug|Concentration in container' is 3.89% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.04

**Figure 1.83**

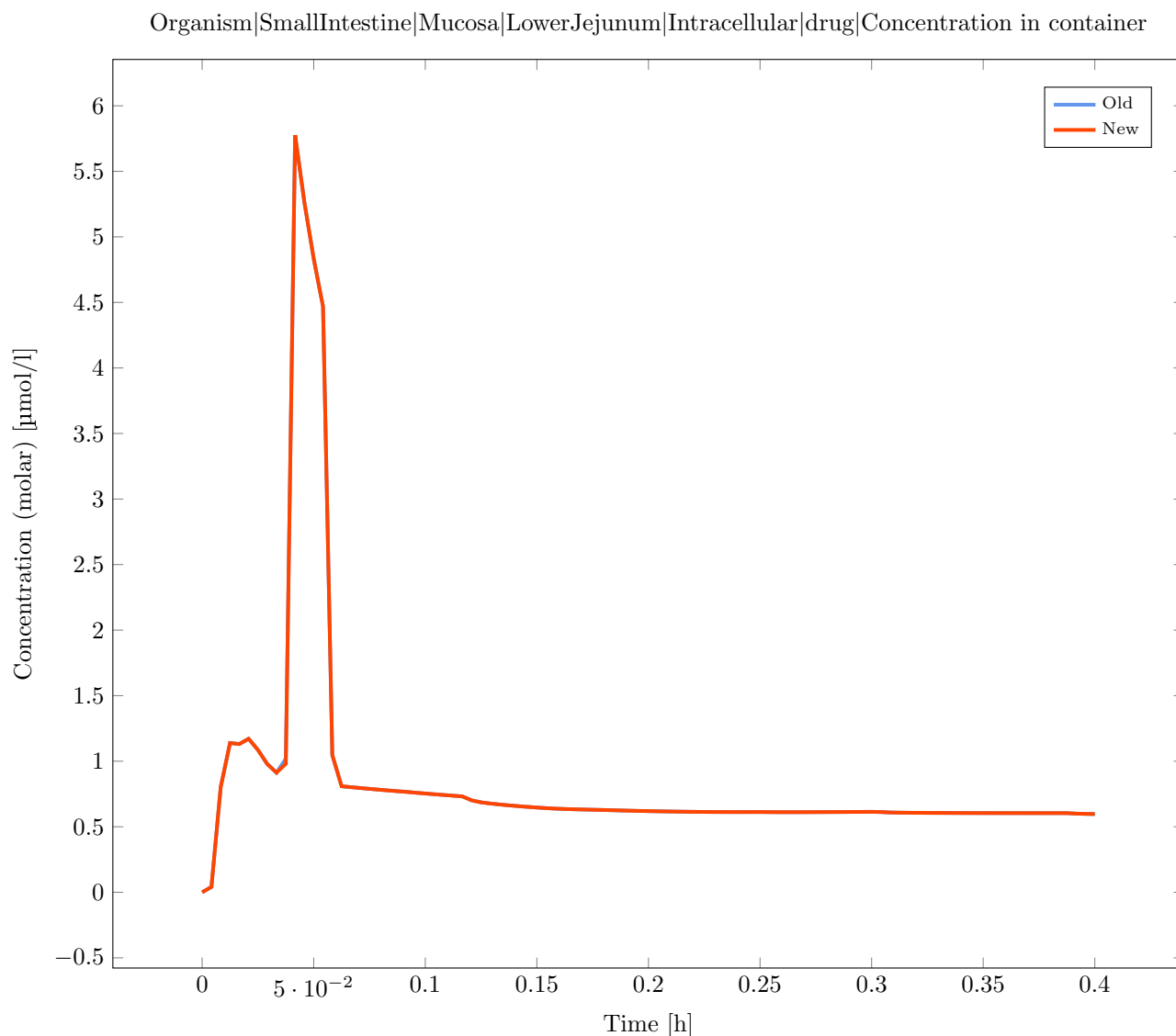
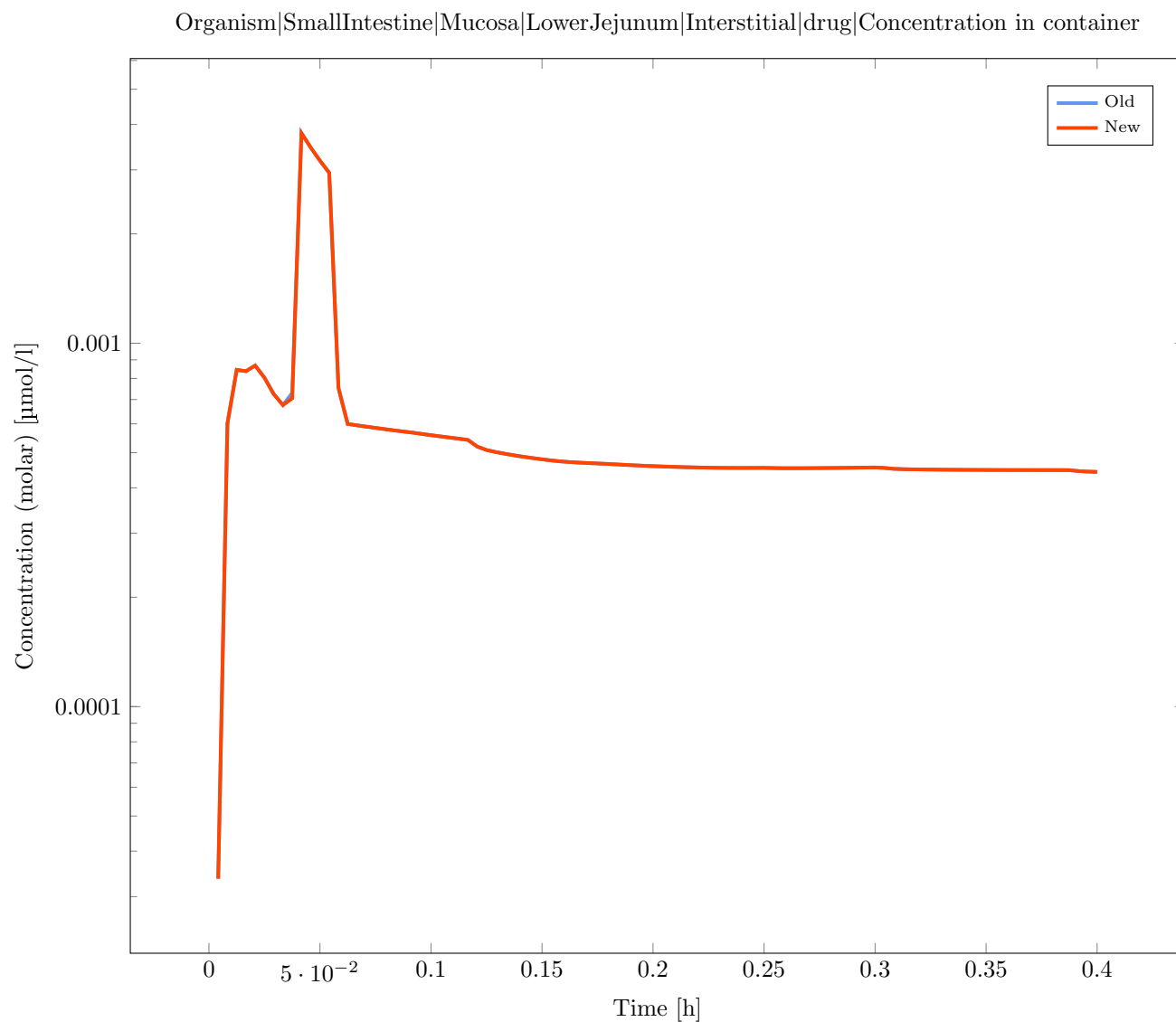


Figure 1.84

Output Path: Organism|SmallIntestine|Mucosa|LowerJejunum|Interstitial|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerJejunum|Interstitial|drug|Concentration in container' is 3.40% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.03

**Figure 1.85**

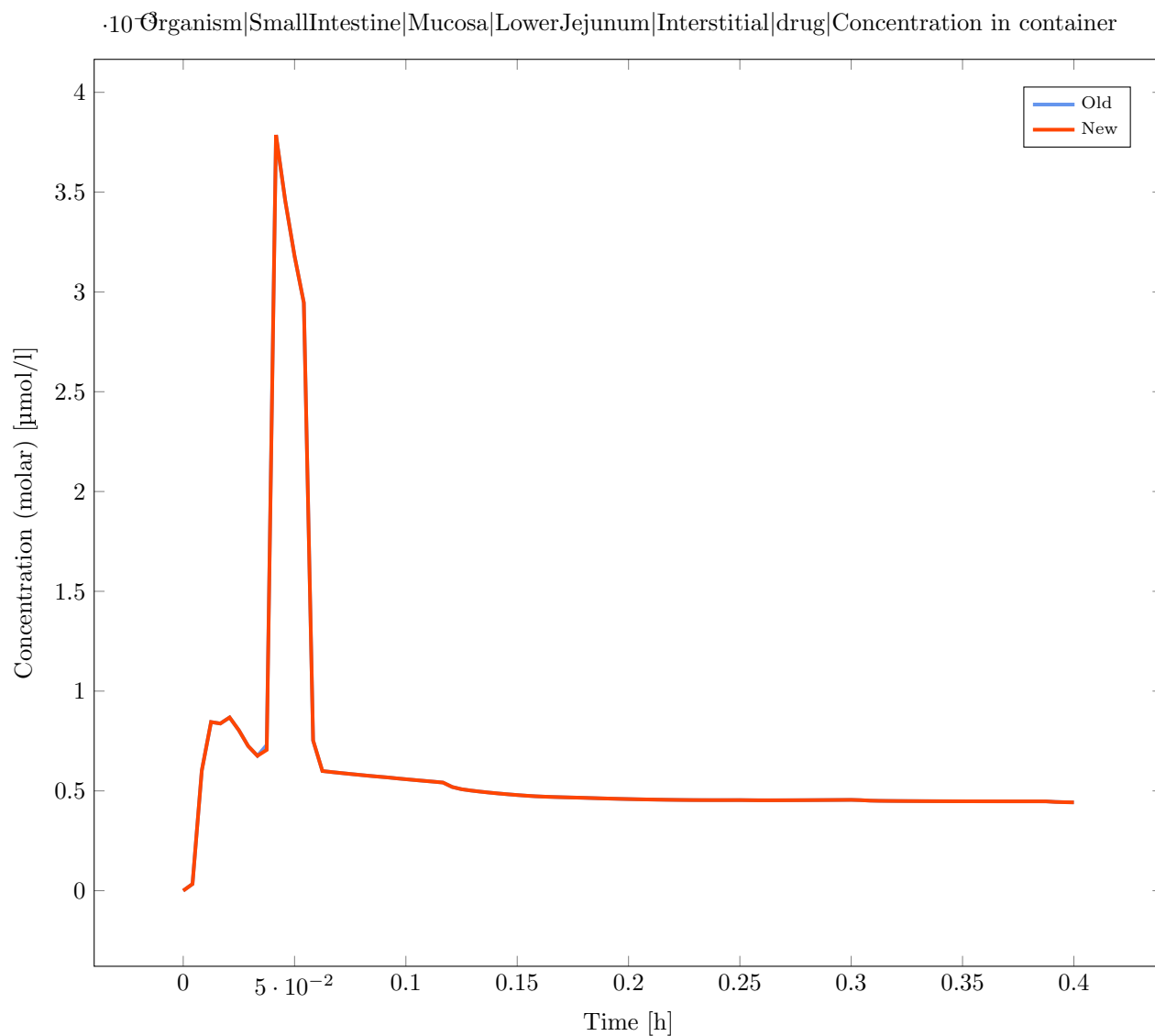


Figure 1.86

Output Path: Organism|SmallIntestine|Mucosa|LowerJejunum|Plasma|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerJejunum|Plasma|drug|Concentration in container' is 3.01% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.03

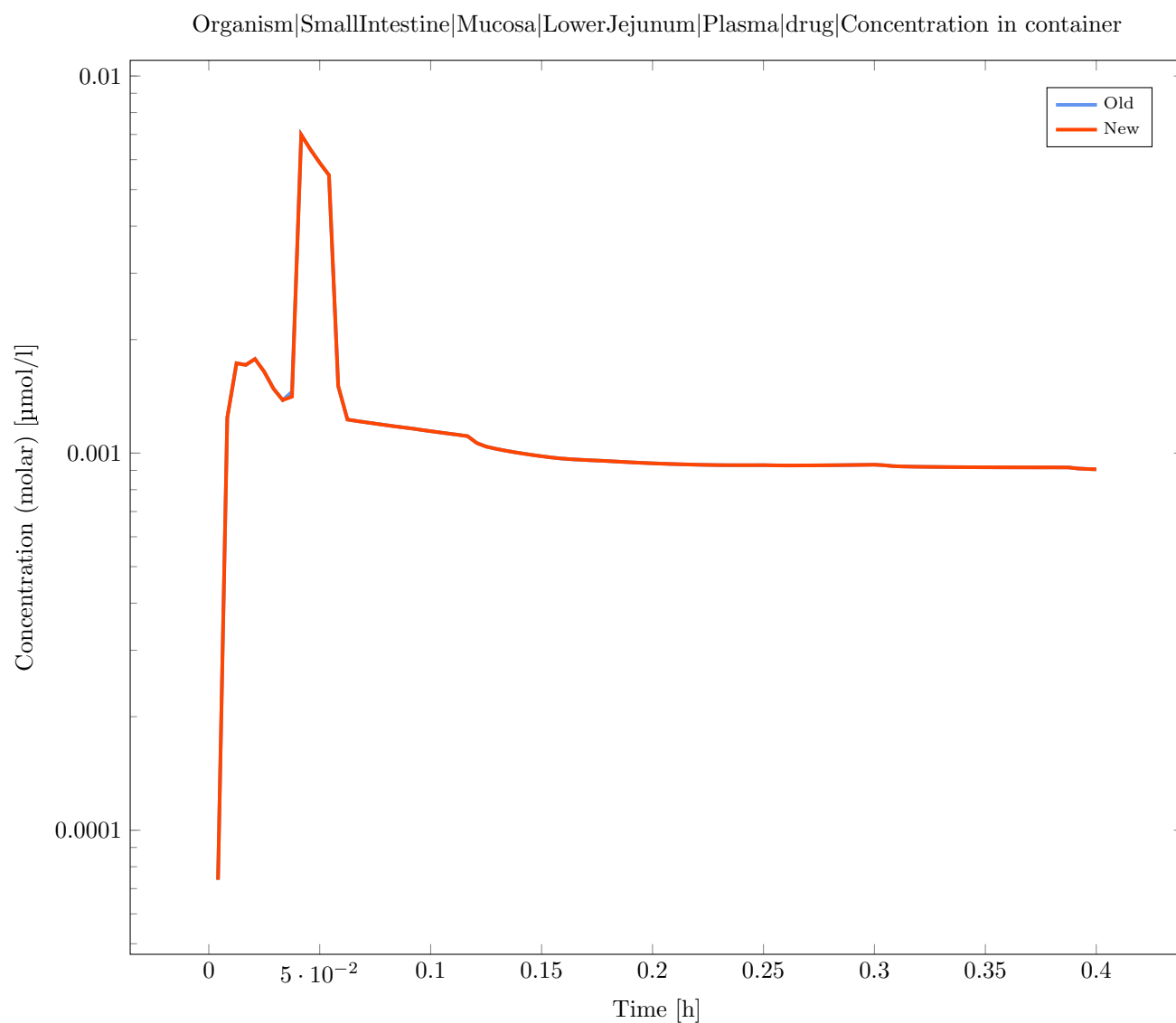


Figure 1.87

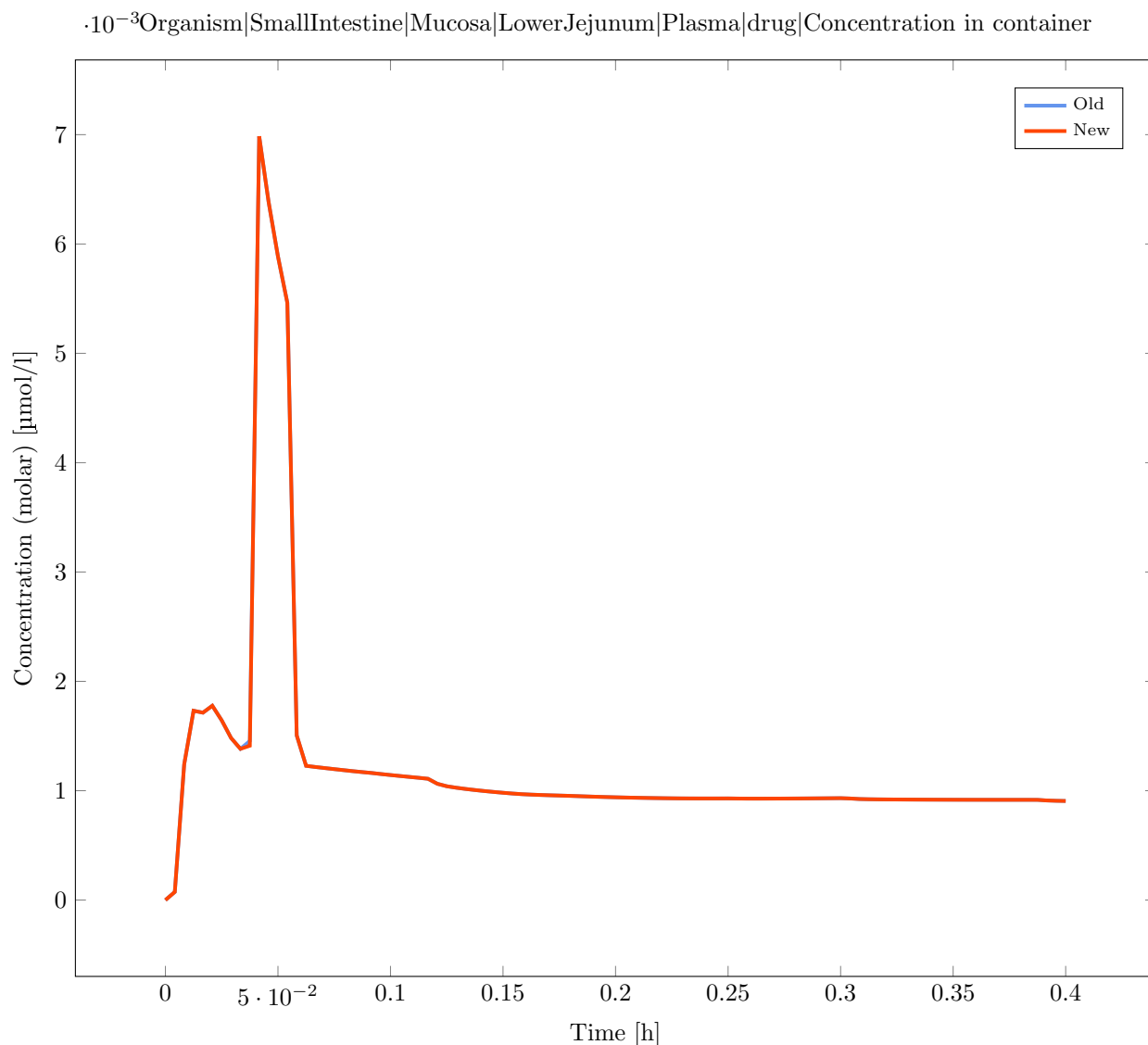


Figure 1.88

Simulation: Rat_MultiORAL_6.6.12_Dissolved-Rat_MultiORAL_6.6.12_Dissolved

Result of the validation: **Invalid**

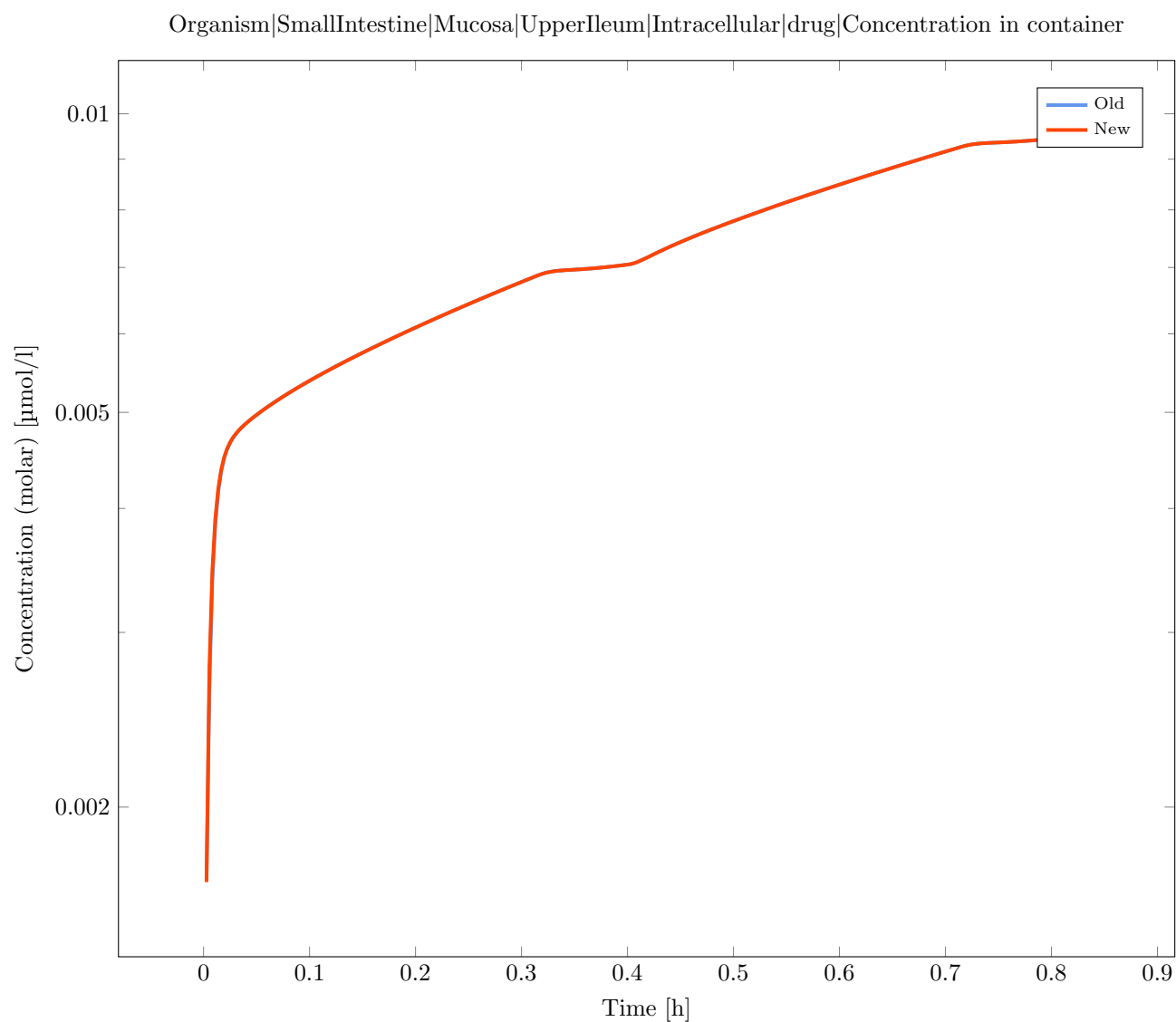
Absolute Tolerance: 1.00E-10

Relative Tolerance: 1.00E-5

Output Path: Organism|SmallIntestine|Mucosa|UpperIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|UpperIleum|Intracellular|drug|Concentration in container' is 4.86% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.05

**Figure 1.89**

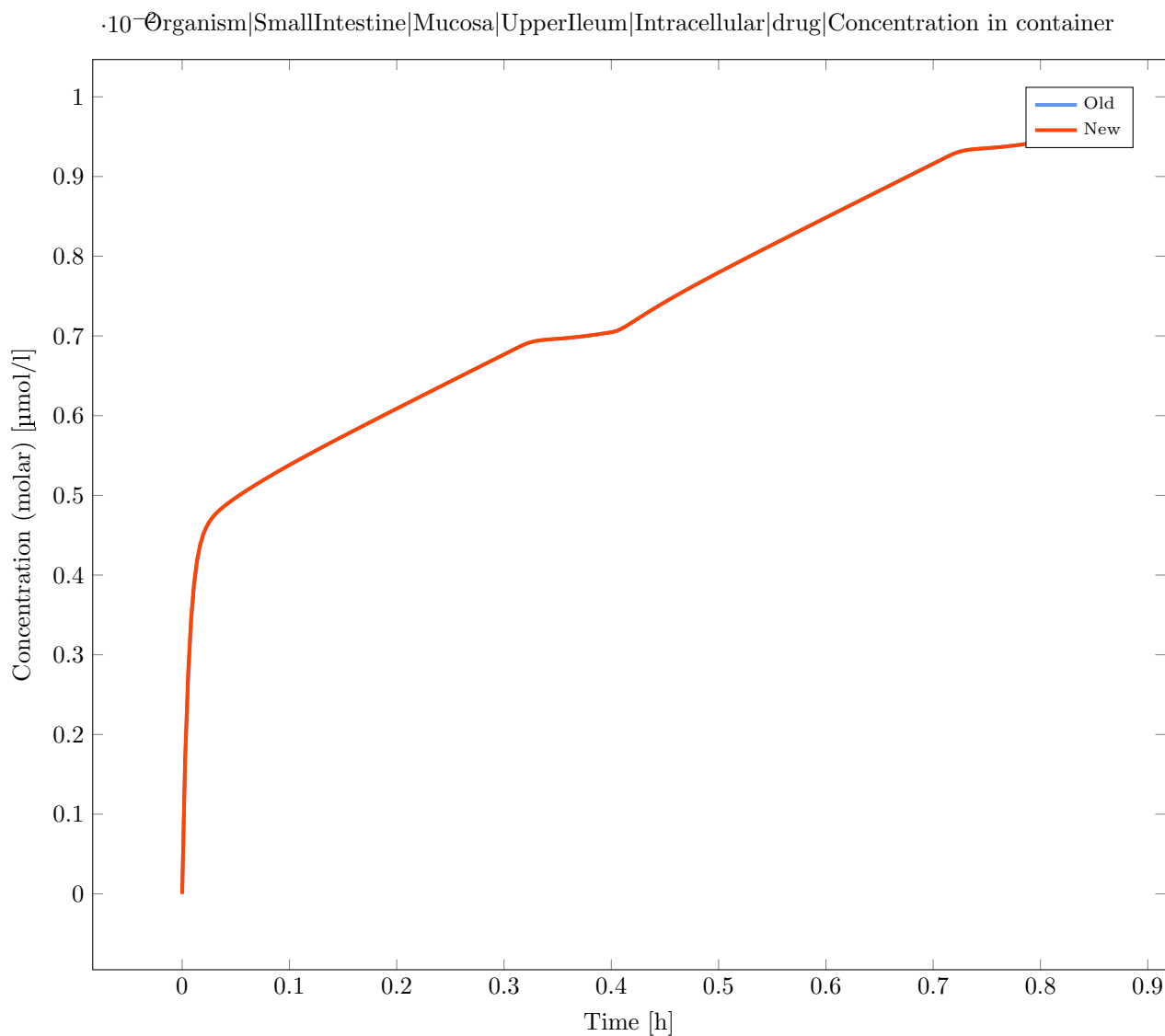
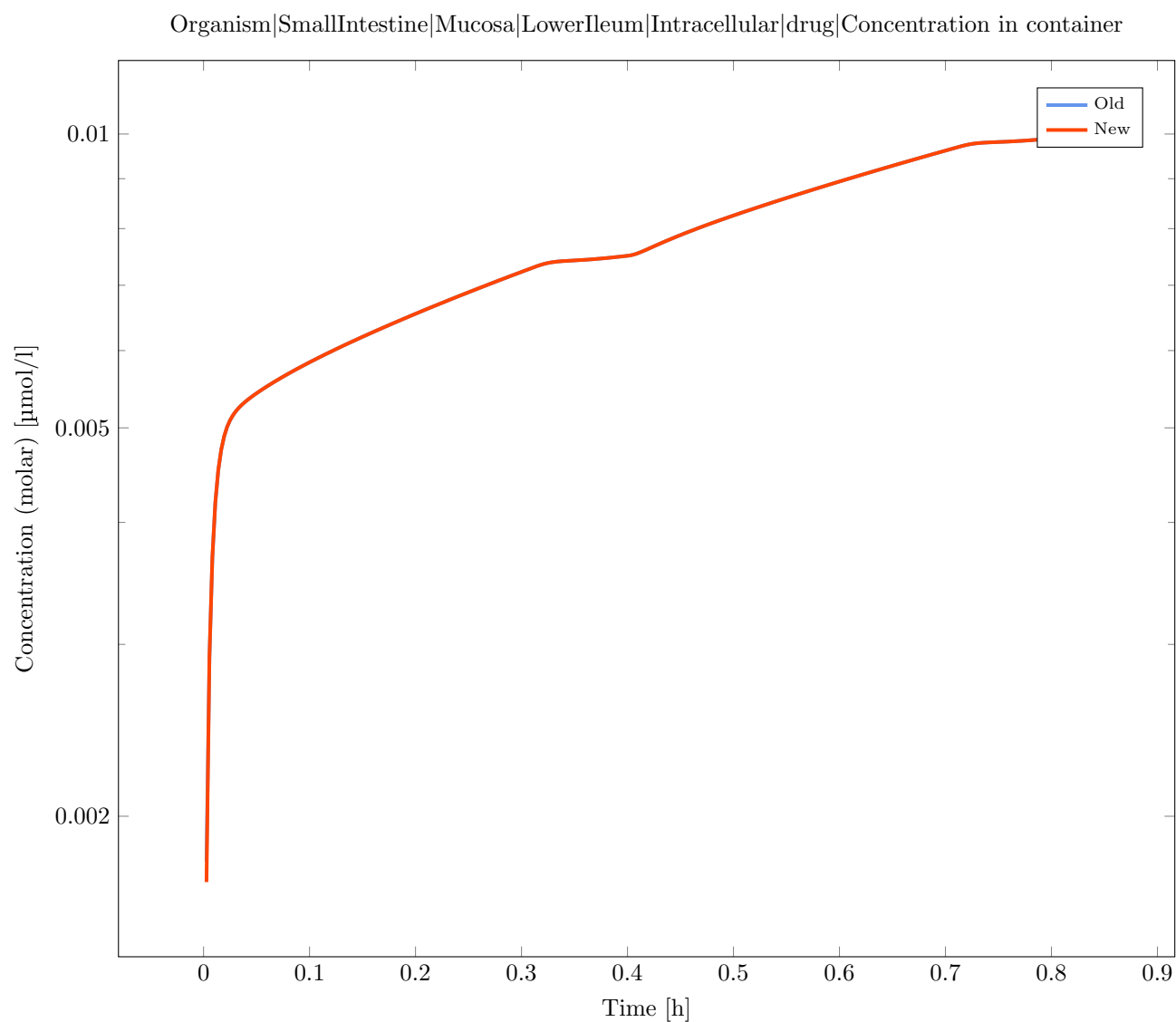


Figure 1.90

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container' is 4.77% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.05

**Figure 1.91**

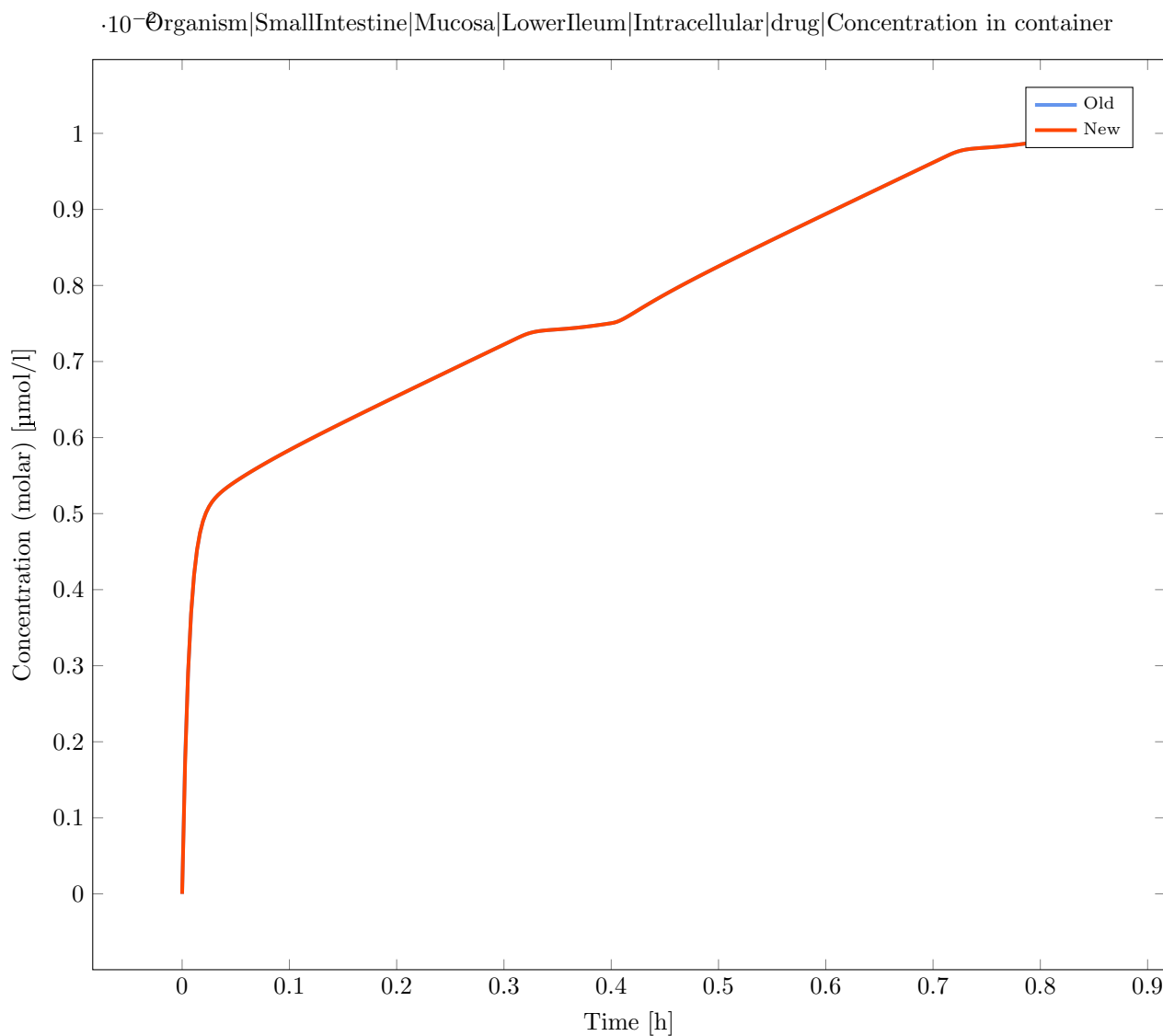
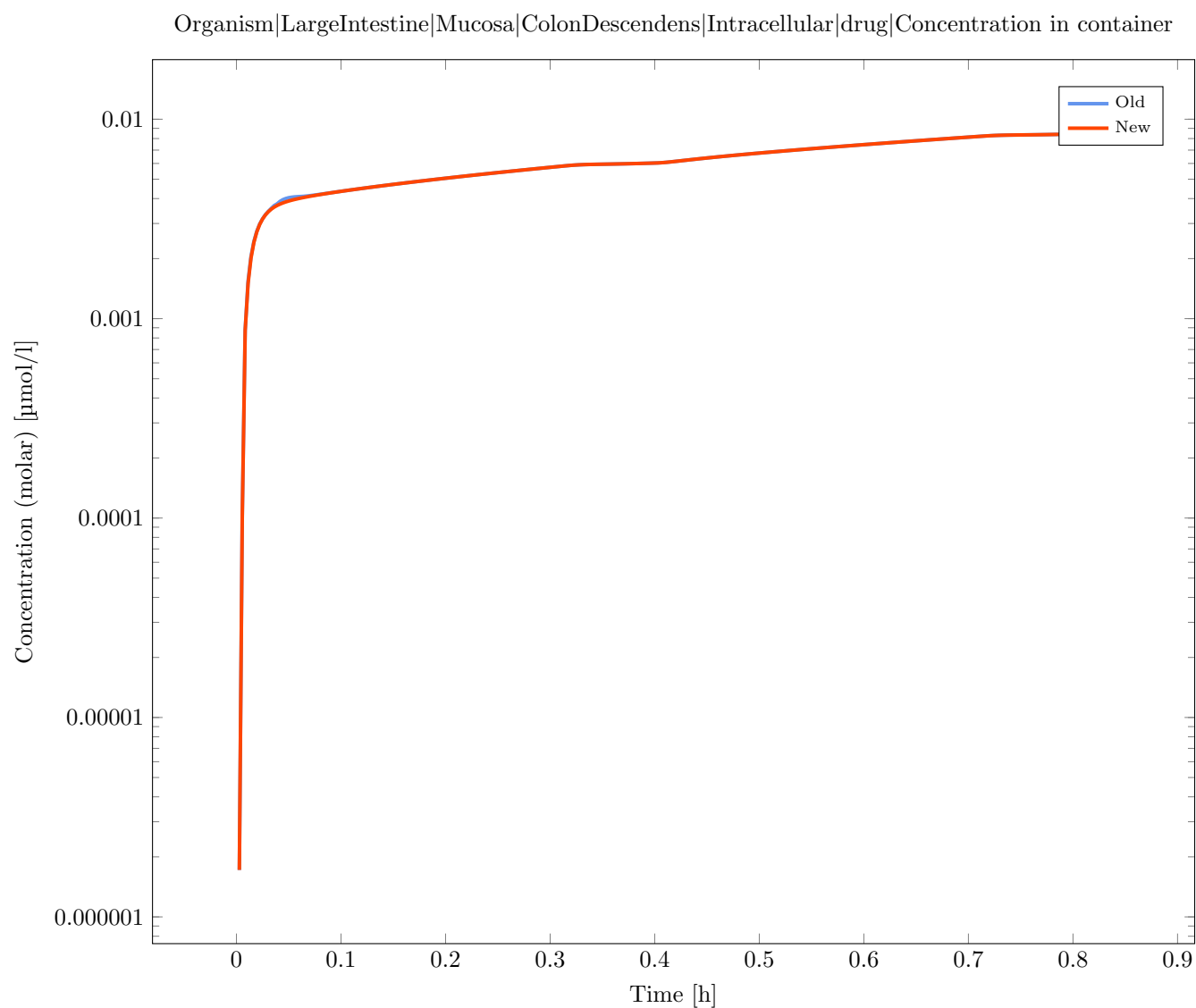


Figure 1.92

Output Path: Organism|LargeIntestine|Mucosa|ColonDescendens|Intracellular|drug|Concentration in container

Deviation for 'Organism|LargeIntestine|Mucosa|ColonDescendens|Intracellular|drug|Concentration in container' is 3.84% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.04

**Figure 1.93**

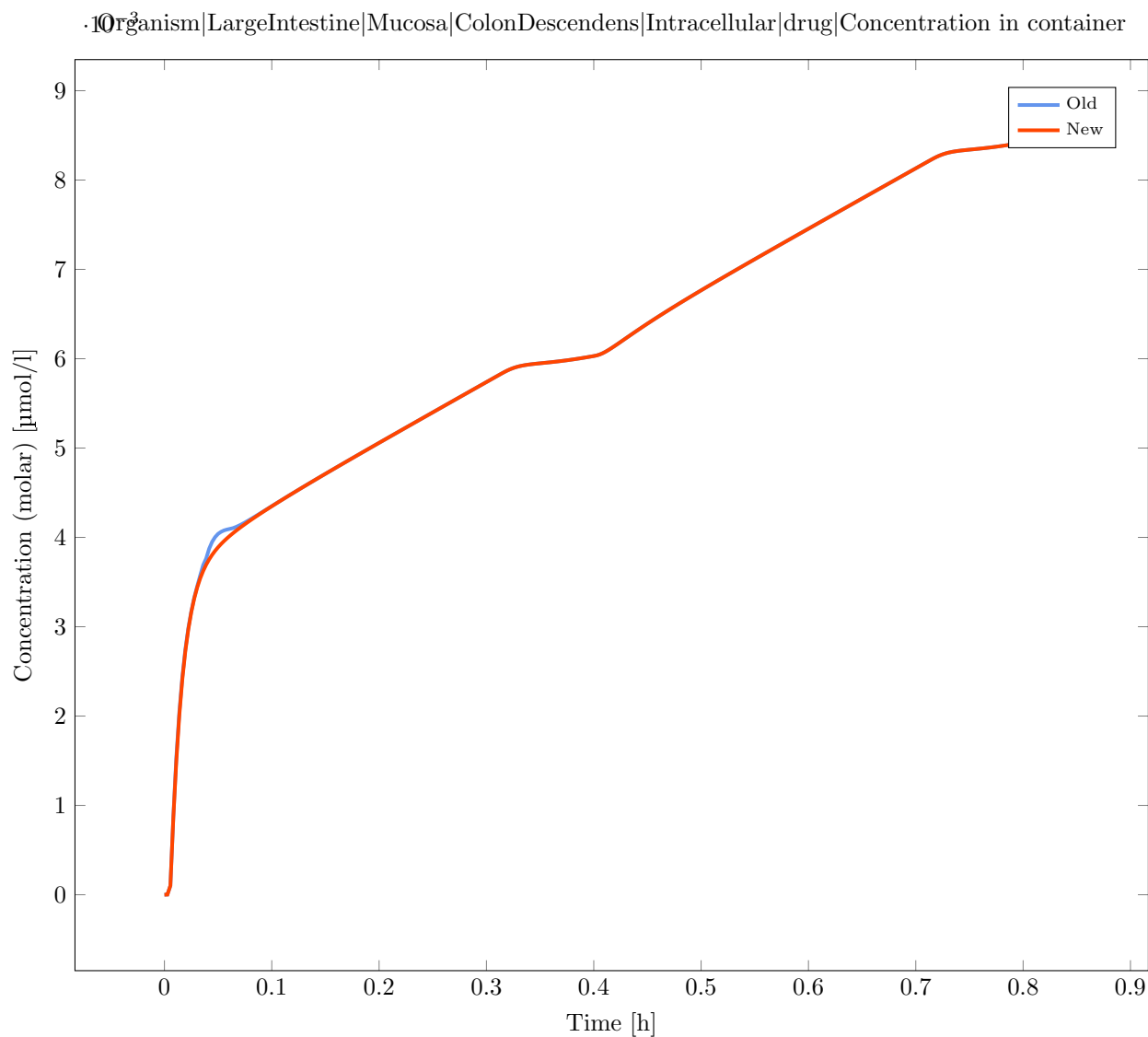


Figure 1.94

Simulation: Rat_MultiORAL_6_6_6_6_Dissolved-Rat_MultiORAL_6_6_6_6_Dissolved

Result of the validation: **Invalid**

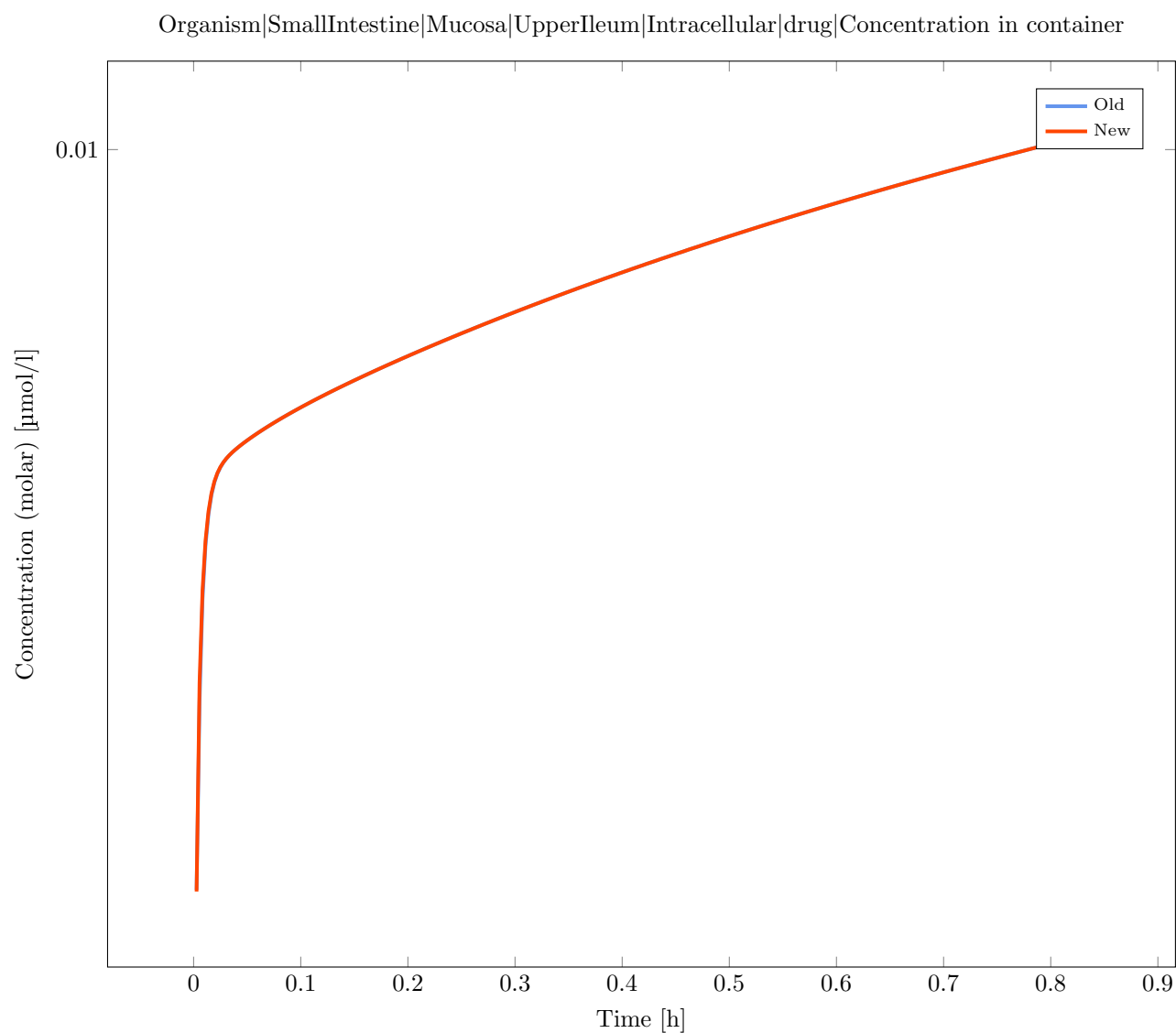
Absolute Tolerance: 1.00E-10

Relative Tolerance: 1.00E-5

Output Path: Organism|SmallIntestine|Mucosa|UpperIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|UpperIleum|Intracellular|drug|Concentration in container' is 4.86% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.05

**Figure 1.95**

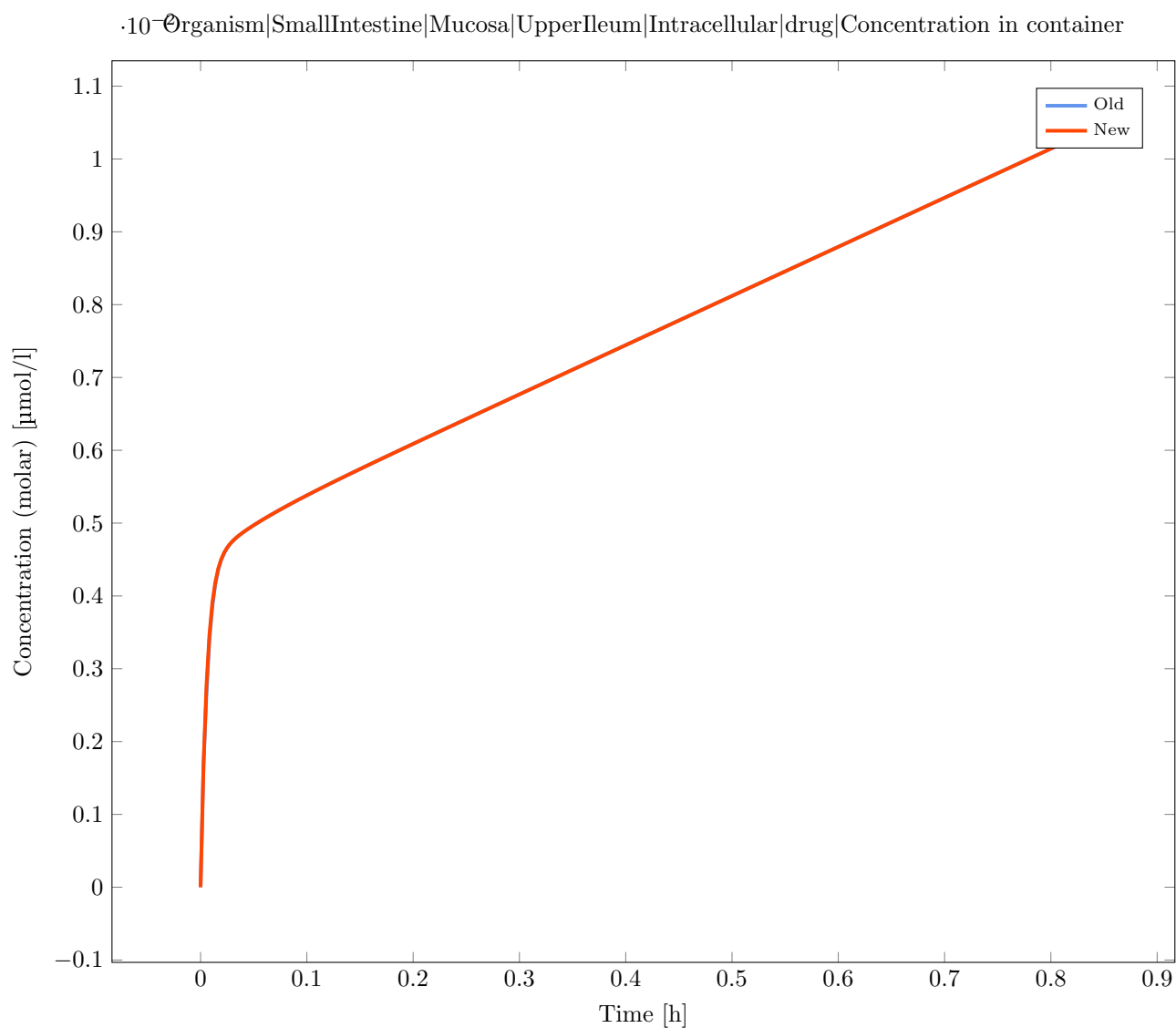
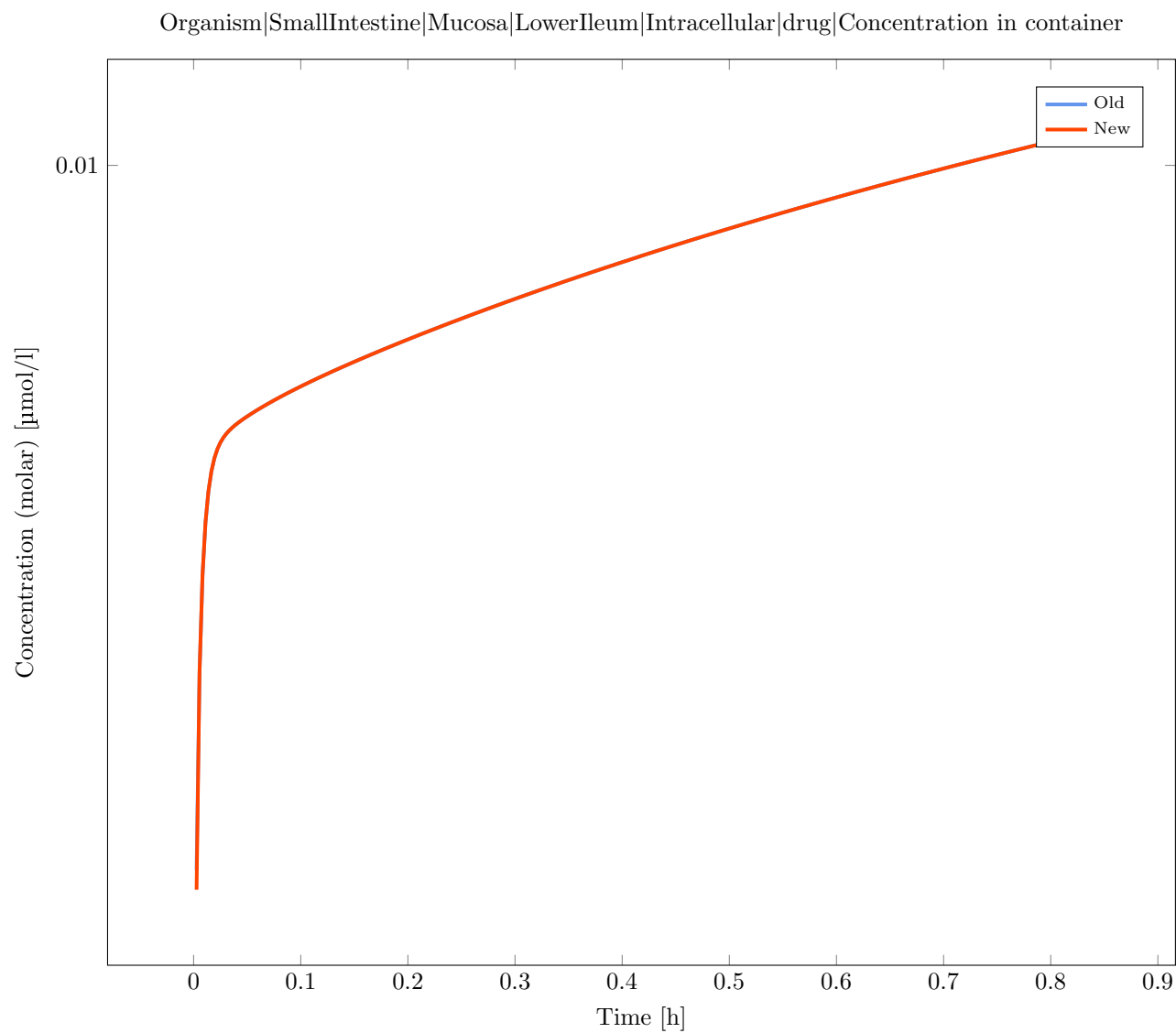


Figure 1.96

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container' is 4.77% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.05

**Figure 1.97**

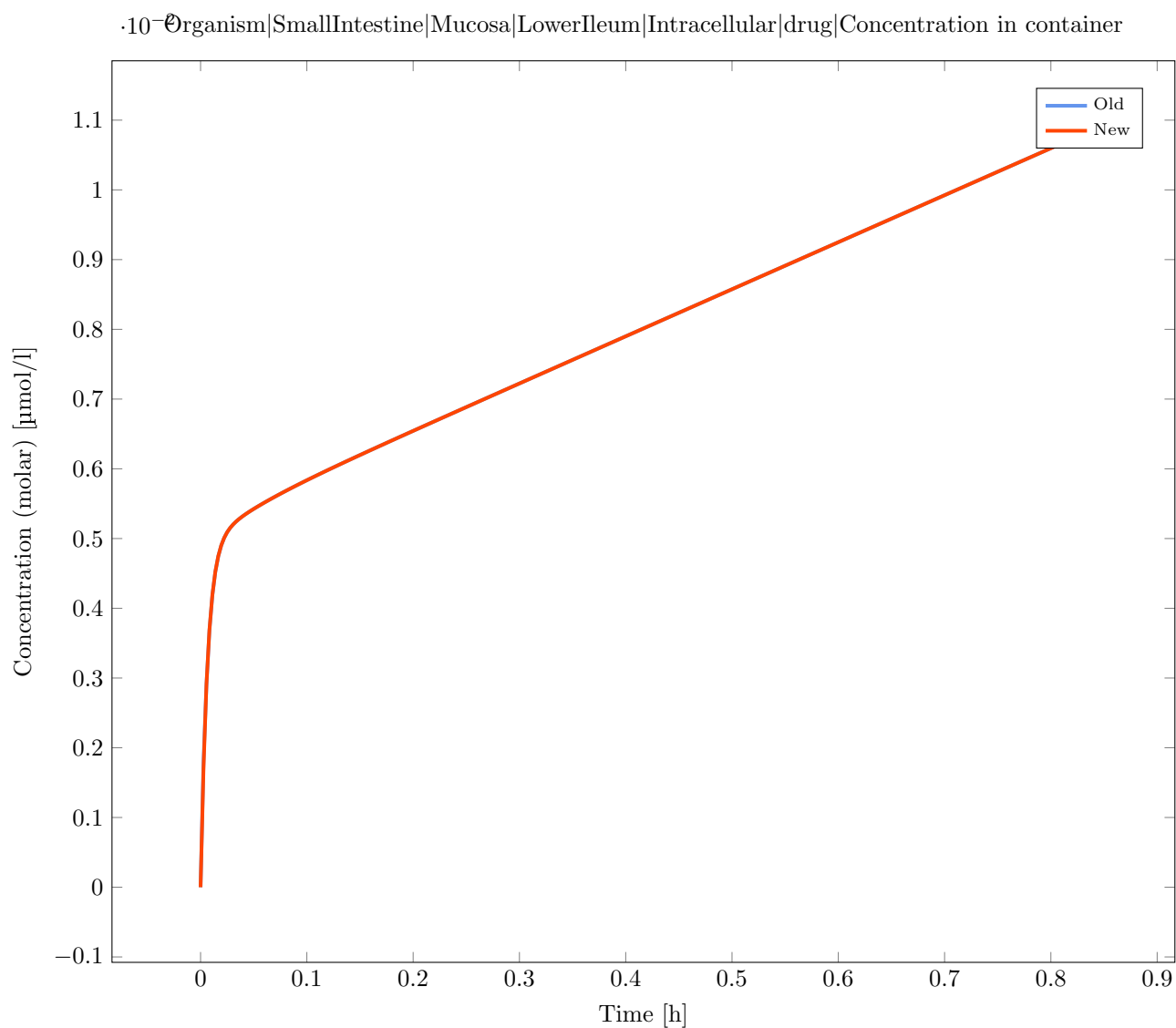
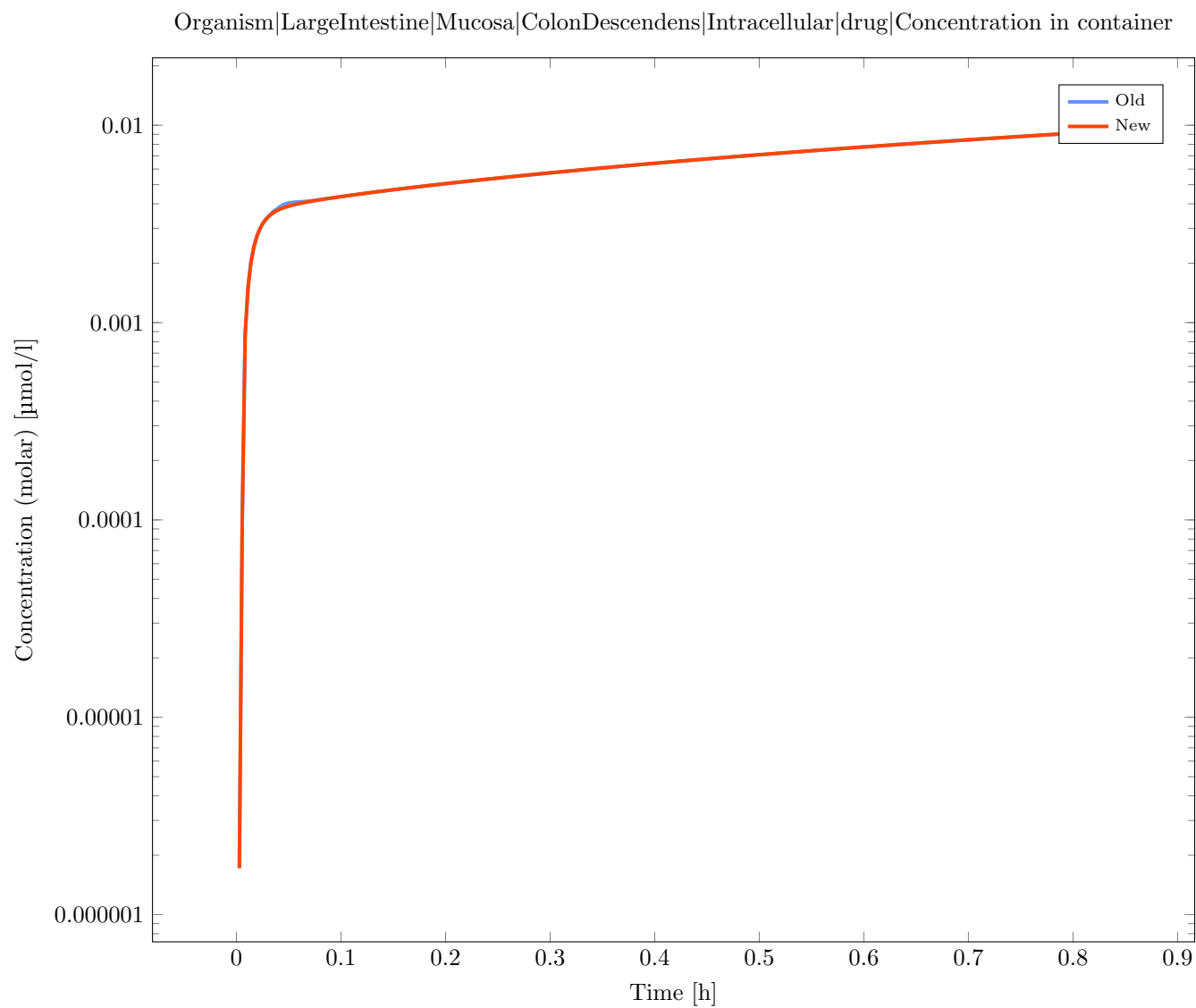


Figure 1.98

Output Path: Organism|LargeIntestine|Mucosa|ColonDescendens|Intracellular|drug|Concentration in container

Deviation for 'Organism|LargeIntestine|Mucosa|ColonDescendens|Intracellular|drug|Concentration in container' is 3.84% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.04

**Figure 1.99**

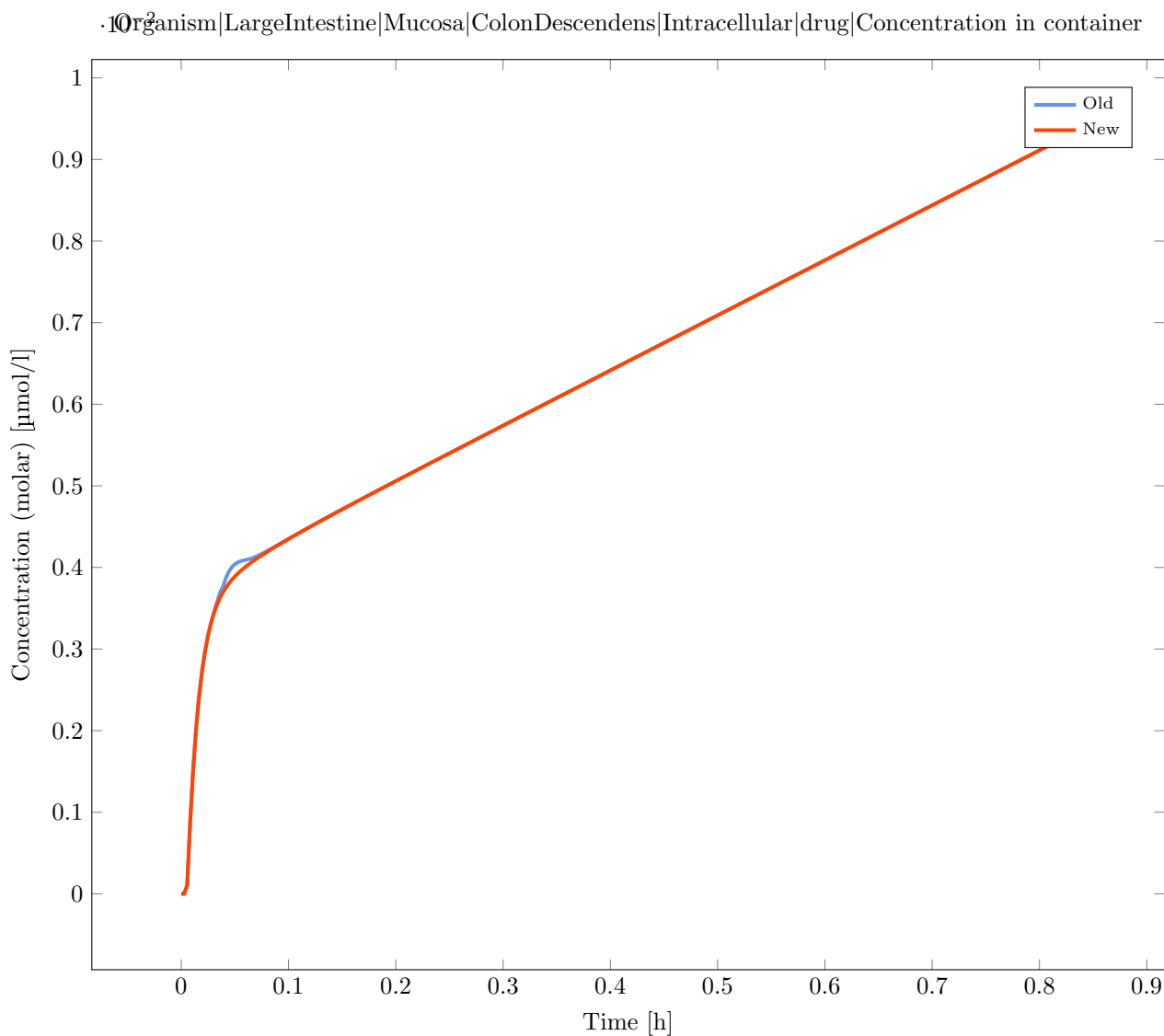


Figure 1.100

Simulation: Rat_MultiORAL_8_8_8_Dissolved-Rat_MultiORAL_8_8_8_Dissolved

Result of the validation: **Invalid**

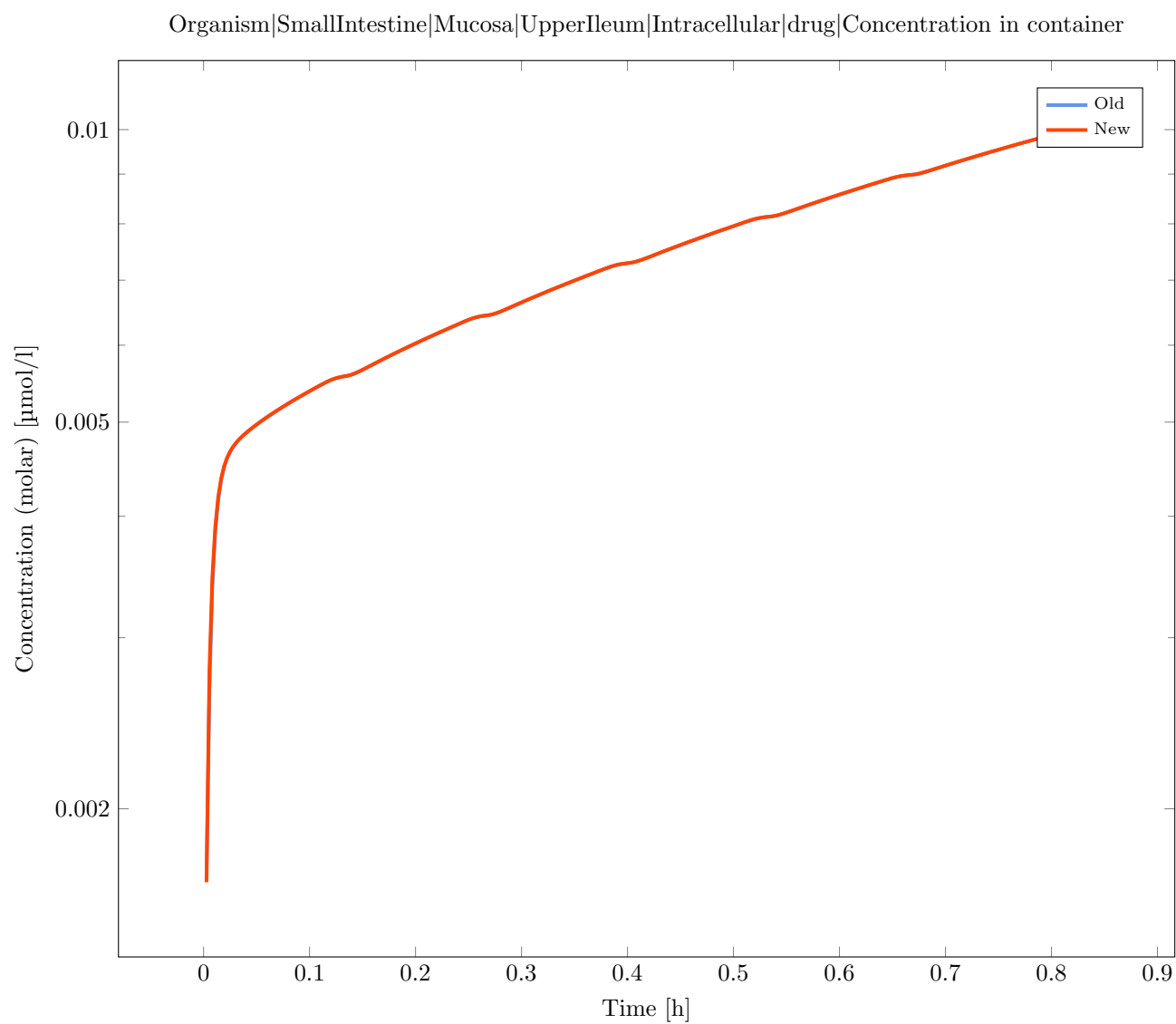
Absolute Tolerance: 1.00E-10

Relative Tolerance: 1.00E-5

Output Path: Organism|SmallIntestine|Mucosa|UpperIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|UpperIleum|Intracellular|drug|Concentration in container' is 4.86% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.05

**Figure 1.101**

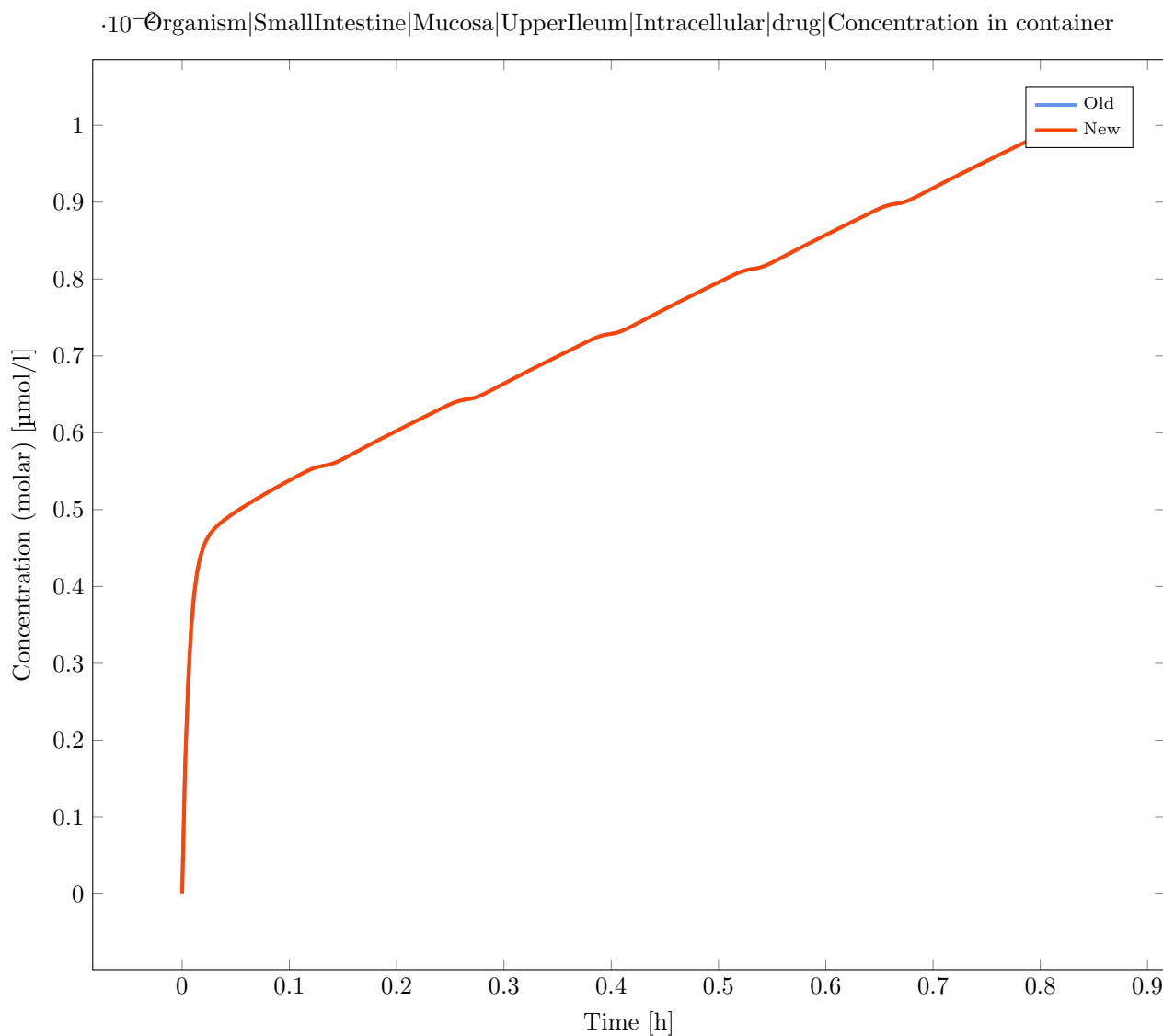
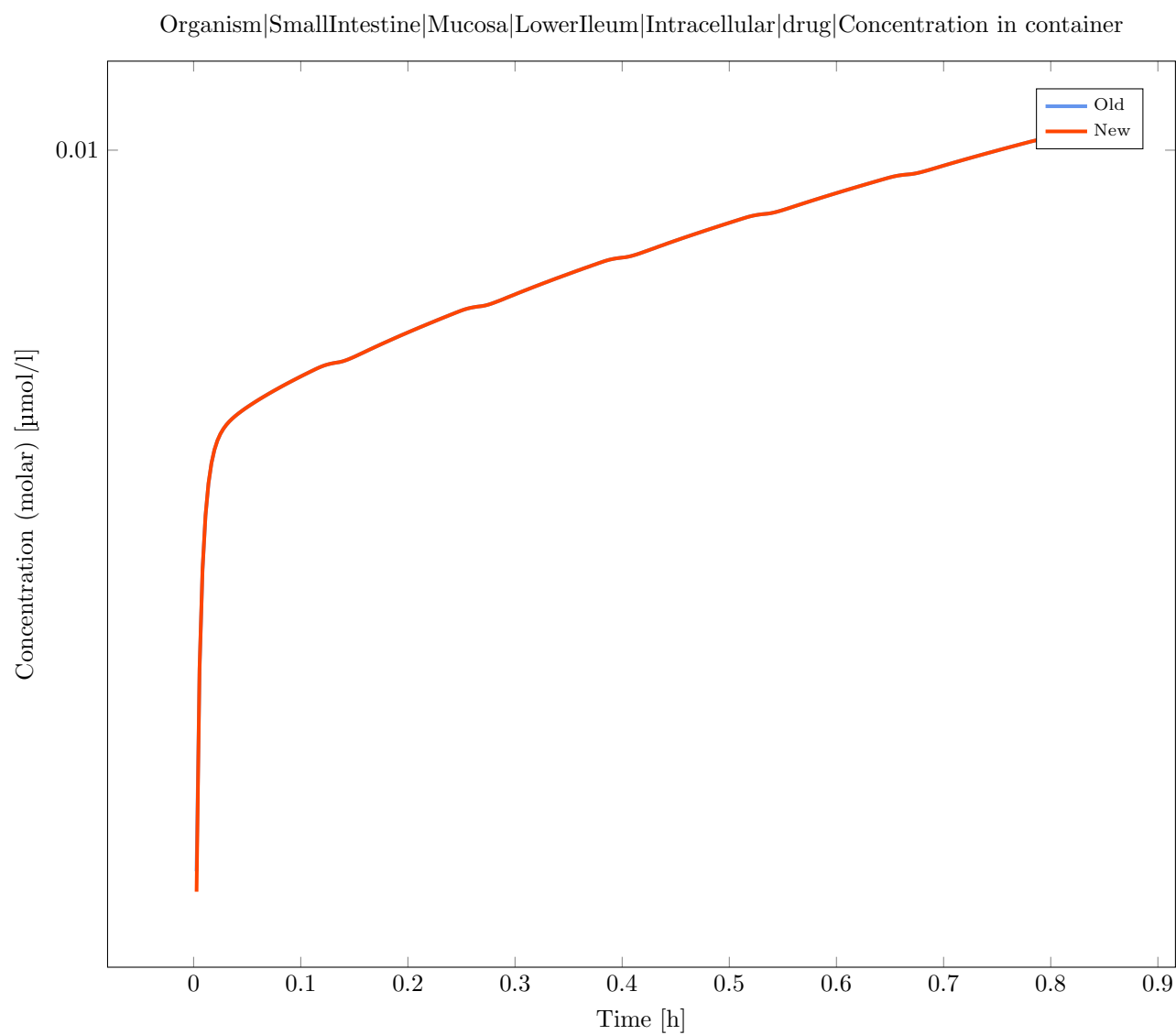


Figure 1.102

Output Path: Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container

Deviation for 'Organism|SmallIntestine|Mucosa|LowerIleum|Intracellular|drug|Concentration in container' is 4.77% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.05

**Figure 1.103**

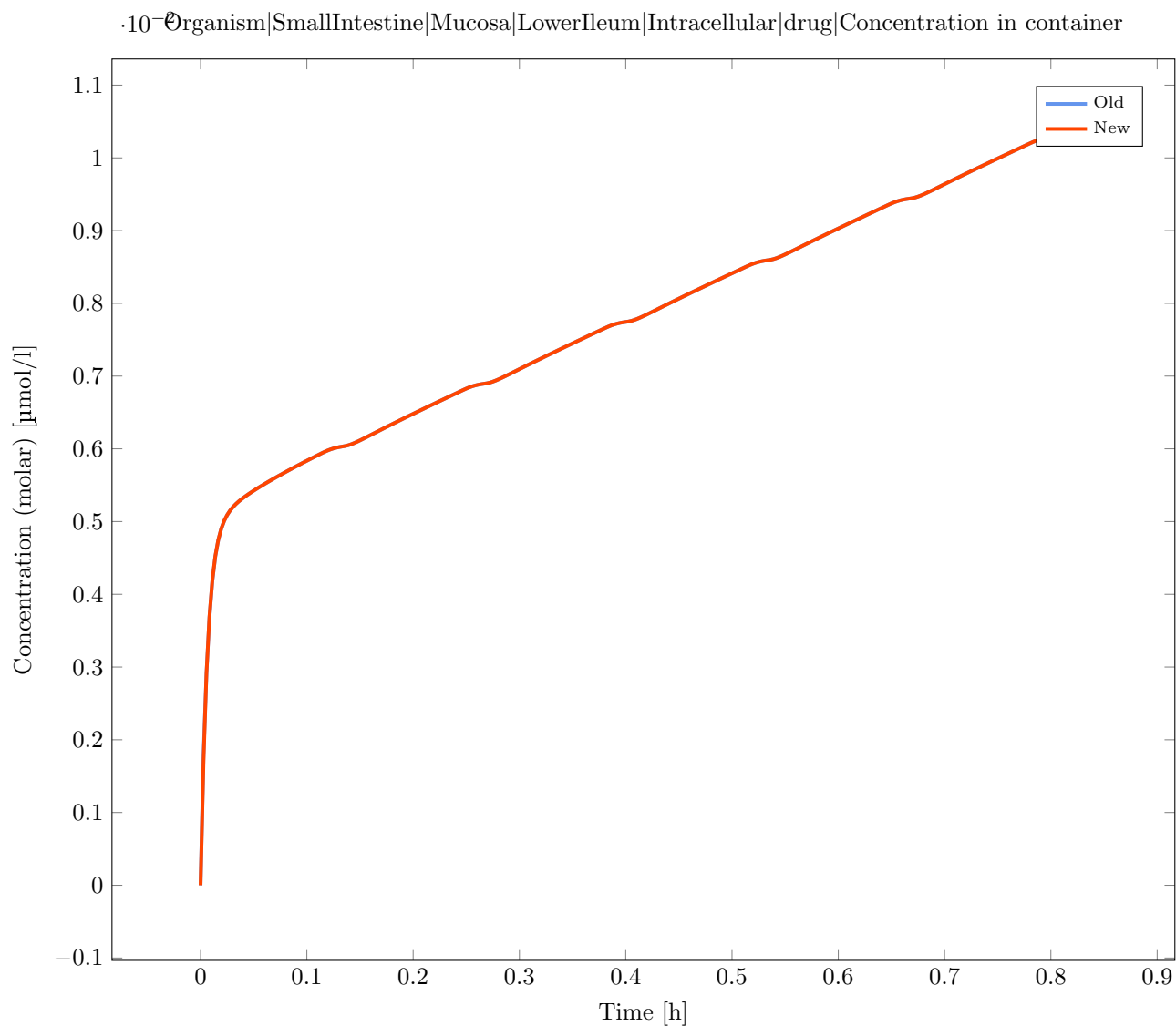


Figure 1.104

Output Path: Organism|LargeIntestine|Mucosa|ColonDescendens|Intracellular|drug|Concentration in container

Deviation for 'Organism|LargeIntestine|Mucosa|ColonDescendens|Intracellular|drug|Concentration in container' is 3.84% and is greater than the allowed max. tolerance of 3.00%

Deviation: 0.04

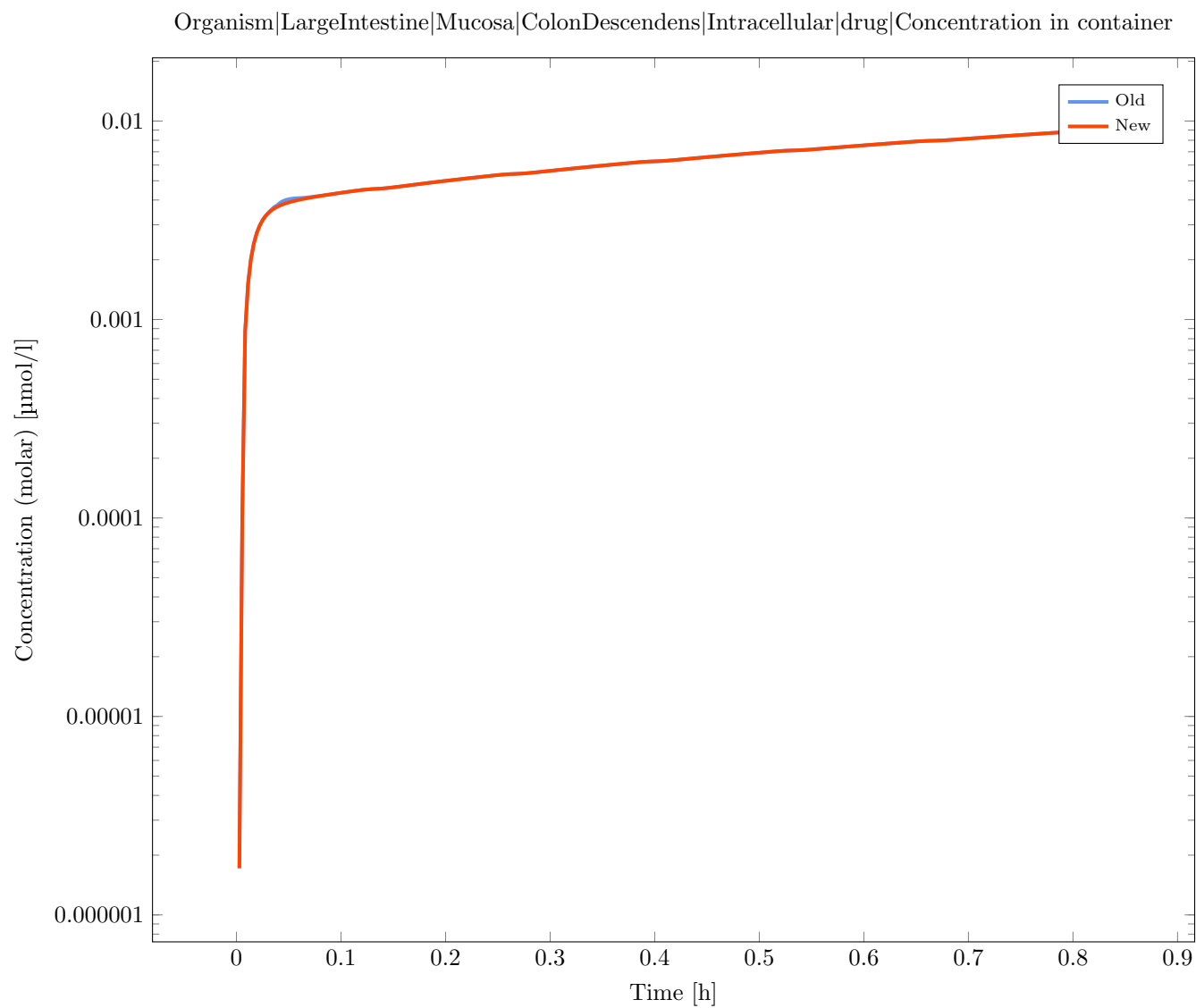


Figure 1.105

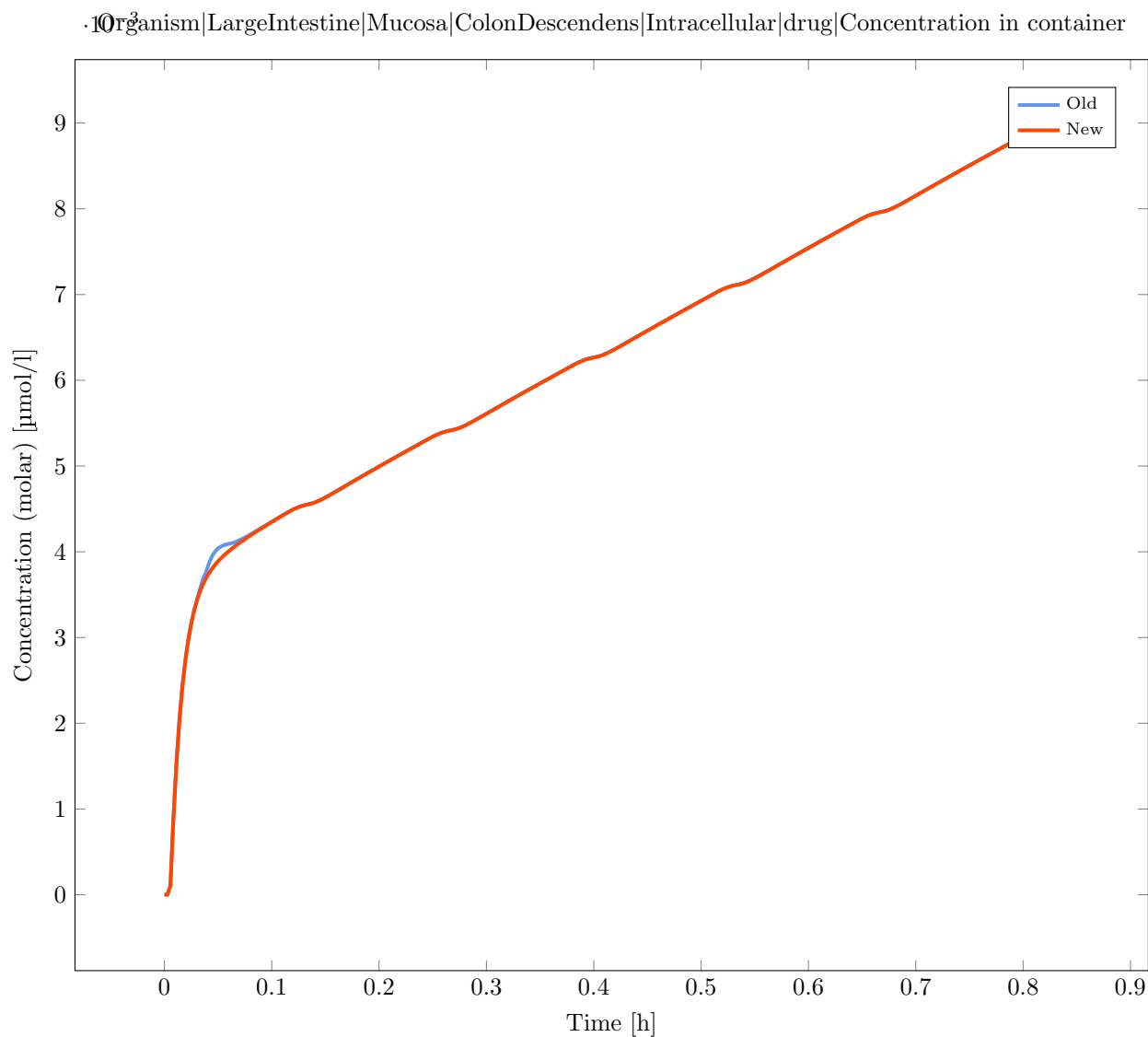


Figure 1.106

1.1.2 Valid Simulations (142/155)

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-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_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_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_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_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: 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