

Supplemental Table 1 Comparison of predictors in the training and testing datasets.

	Training set	Testing set	p-value
<i>Simulated concentrations at 24h (SC_{24h}) (mg/L)</i>	2.1 [0.3-10.1]	2.1 [0.3-9.5]	NS
<i>Predicted concentrations at 24h (EC_{24h}) (mg/L)</i>	1.9 [0.3-7.2]	1.8 [0.3-6.8]	NS
<i>Difference between SC_{24h} and EC_{24h} (mg/L)</i>	0.2 [-0.2-2.9]	0.2 [-0.2-2.7]	NS
<i>Ratio between SC_{24h} and EC_{24h}</i>	0.9 [0.7-1.6]	0.9 [0.7-1.5]	NS
<i>Relative ratio between SC_{24h} and EC_{24h}</i>	0.1 [-0.6-0.3]	0.1 [-0.5-0.3]	NS
<i>Clearance (CL) (L/h)</i>	3.8 [1.1-14.8]	3.9 [1.1-14.5]	NS
<i>Peripheric volume (V₂) (L)</i>	501.0 [89.6-1022.2]	493.0 [95.0-1026.6]	NS
<i>Eta of MAP-BE CL (ETA 1)</i>	0.1 [-1.1-1.4]	0.1 [-1.0-1.3]	NS
<i>Eta of MAP-BE V₂ (ETA 2)</i>	-2.6x10 ⁻⁴ [-0.1-0.2]	-2.0x10 ⁻⁵ [-0.1-0.2]	NS
<i>Body Mass Index (BMI) (kg/m²)</i>	26.2 [14.9-39.7]	26.6 [15.2-39.7]	NS
<i>Sex (%)</i>	M: 50.8%	M: 46.8%	NS

ETA is the relative deviation of PK parameters from the typical value of that parameter. The quantitative data were presented in median [min-max]. The Wilcoxon test was performed to compare the 2 sets. EC_{24h} is the predicted concentrations at 24h, SC_{24h} is the simulated concentrations at 24h. NS: not significant (with a threshold of 0.05).