

Variable	Name
1compartment	One compartment model (O’Flaherty 1981), shown in Figure 1.
3compartment	Three compartment model (Jamei <i>et al.</i> 2009), shown in Figure 1.
3compartmentss	Three compartment steady state model (Wetmore <i>et al.</i> 2012; Wetmore 2015).
BW	Body weight.
C_{ss}	Average plasma concentration of a chemical at steady state.
Cl_{int}	<i>In vitro</i> intrinsic hepatic clearance.
$Cl_{metabolism}$	Whole liver hepatic clearance, scaled from Cl_{int} .
$Cl_{well-stirred}$	Hepatic clearance modeled with well-stirred approximation using $Cl_{metabolism}$.
f_{ub}	Fraction unbound, <i>in vitro</i> ratio of unbound to total concentration in plasma.
httk	High-throughput toxicokinetics.
k_{elim}	Elimination rate.
k_{gutabs}	Gut absorption rate, default of $1 h^{-1}$.
logP	Logarithm (base 10) of octanol to water partition coefficient.
pbtk	Physiologically based toxicokinetic model, shown in Figure 1.
PM	Poor metabolizers.
$Q_{cardiac}$	Cardiac output, blood flow through the heart and lungs.
Q_{gfr}	Glomerular filtration rate.
Q_{rest}	The difference between $Q_{cardiac}$ and the flow to the liver, kidney, and gut.
Q_{tissue}	Blood flow to a tissue.
QSAR	Quantitative structure-activity relationship.
$R_{blood2plasma}$	Ratio of the blood concentration of a chemical to the plasma concentration.
SBML	Systems biology markup language.
SMILES	Simplified molecular-input line-entry system.
V_{dist}	Volume of distribution, the weighted sum of all partition coefficients.

Table 1: List of abbreviations.