Supplement - A comprehensive framework for physiologically based pharmacokinetic modelling in Matlab®

Table S1: Parameters and their abbreviation and units used to build a PBPK model.

Parameter	Abbreviation	Unit
concentration of acidic phospholipids	[AP]	-
inhibitor concentration	[Inh]	mg/L
substrate concentration	[Sub]	mg/L
abundance	AB	hepatic enzymes: pmol/mg hepatic transporter: pmol/Mio cells intestinal enzymes: nmol/intestine intestinal transporter: fmol/cm²
time-dependent abundance	ABt	hepatic enzymes: pmol/mg hepatic transporter: pmol/Mio cells intestinal enzymes: nmol/intestine intestinal transporter: fmol/cm²
blood-to-plasma ratio	BP	-
concentration	C	mg/L
clearance	CL	L/h
absorption clearance	CL_{ab}	L/h
intrinsic clearance of an enzymatic / transporter isoform	CL_{int}	µL/min/pmol enzyme / transporter
intrinsic clearance not assigned to a specific enzyme	$CL_{int,hep}$	µL/min/mg protein
cardiac output	CO	L/h
fraction of extracellular water	f_{EW}	-
fraction of intracellular water	f_{IW}	-
fraction of neutral lipids	f_{NL}	-
fraction of neutral phospholipids	f_{NP}	-
fraction unbound	fu	-
fold expansion factor for the villi of the surface area	F*villi*	-
glomerular filtration rate	GFR	mL/min
hematocrit	HCT	-
hepatocytes per gram liver	HPGL	Mio cells / g liver
half maximal inducer concentration	IC_{50}	µM
maximum fold induction	IndMax	-
flux	J	L/h
affinity constant for acidic phospholipids	KaAP	-
apparent inhibition constant	K_{app}	µM
affinity constant for binding proteins	KaPR	-

Parameter	Abbreviation	Unit
degradation rate	k_{deg}	1/h
inhibition constant	K_i	µM
inactivation rate	k_{inact}	1/h
ionized form	K_{io}	-
Michaelis-Menten constant	K_m	µM
partition coefficient of plasma binding proteins	KpPR	-
unbound drug partition coefficient	Kpu	-
length	Le	cm
lymph flow	L	L/h
vegetable oil-water partition coefficient	logD	-
octanol-water partition coefficient	logP	-
total lymph flow	L_{tot}	L/h
microsomal proteins per gram liver	MPPGL	mg / g liver
apparent permeability	P_{app}	10^-6 cm/sec
effective permeability in man	$P_{eff,man}$	10^-4 cm/sec
binding protein concentration	PR	g/L
permeability surface area	PSA	cm²
blood flow	Q	L/h
radius	r	cm
volume	V	L
maximum velocity	V_{max}	pmol/min/pmol enzyme / transporter
volume of distribution at steady state	Vss	L

Table S2: Subscripts and their abbreviation used to build the PBPK model.

Parameter	Abbreviation
arterial blood	ab
additional	ad
adipose	AD
bone	BO
brain	BR
intracellular space	cel
enzyme	E
efflux	ef
gonads	GO
gut	GU
gut	gut
hepatic arterial	ha
heart	HE
hepatic	hep
interstitial space	ine
intracellular water	IW
kidney	KI
liver	LI
lymph-node	LN
lung	LU
muscle	MU
organ	org
pancreas	PA
plasma	PL
portal vein bypass	PVBY
renal	R
red blood cells	RBC
remaining organ	RE
refers to a 30 years old subject arbitrarily chosen to represent a “young” subject	Ref
skin	SK
spleen	SP
transporter	T

Parameter	Abbreviation
thymus	TH
total	tot
uptake	up
vascular space	vas
venous blood	vb