Substrate	

Compound Name	Morphine
Version number	Not applicable
Compound Type	Small Molecule
PhysChem and Blood Binding	
Mol Weight (g/mol)	285.340
log P	0.770
Compound Type	Ampholyte
pKa 1	9.630
pKa 2	7.930
BP Input	User Input
B/P	1.080
Haematocrit	45.000
fu Input	User
fu	0.620
Reference Binding Component	HSA
Protein Reference Conc (g/L)	45.000
Distribution	
Distribution Model	Full PBPK Model
Replacement Organ?	No
Organ Replaced	n/a
User-defined Additional Organ	No
Type	n/a
Vss mode	Predicted
Prediction Method	Method 2
Concentration-dependent volume	No
log Po:w	0.770
logP vo:w	Predicted
logP vo:w value	-0.491
Compound Type	Ampholyte
pKa 1	9.630
pKa 2	7.930
B/P	1.080
Haematocrit	45.000
fu	0.620
Adipose Input Type	Predicted
Adipose Value	1.079
Bone Input Type	Predicted
Bone Value	2.092
Brain Input Type	Predicted
Brain Value	1.517
Gut Input Type	Predicted
Gut Value	7.228
Heart Input Type	Predicted

Heart Value	7.737
Kidney Input Type	Predicted
Kidney Value	4.187
Liver Input Type	Predicted
Liver Value	12.417
Lung Input Type	Predicted
Lung Value	1.970
Muscle Input Type	Predicted
Muscle Value	6.597
Skin Input Type	Predicted
Skin Value	3.521
Spleen Input Type	Predicted
Spleen Value	7.273
Pancreas Input Type	Predicted
Pancreas Value	4.771
Kp Scalar Value	1.000
Elimination	
Clearance Type	Enzyme Kinetics
Pathway 1	6MG
Enzyme	UGT2B7
Vmax	1917.000
Km	115.800
fu mic	1.000
Pathway 1	3MG
Enzyme	UGT2B7
Vmax	9250.000
Km	115.800
fu mic	1.000
CL R (L/h)	8.000
Transport	
Organ/Tissue	Liver
CL_{PD}(mL/min/10^6 cells)	0.003
fuIW Type	Predicted
fuEW Type	Predicted
Organ/Tissue	Liver
Transporter	SLC22A1 (OCT1)
Location	Sinusoidal
Function	Influx
Jmax (pmol/min/10^6 cells)	29.000
Km (µM)	3.400
System	User
RAF/REF	5.100