

Steady State Inhibition Metric (SSIM) =
$$\frac{C_{ss}}{C_{ss} + IC_{50}}$$

	In vitro	In vivo	In vivo	In vivo
Tissue	-	Circulation	Circulation	Tissue
Ligand	no	no	yes	no
IC ₅₀	K_{ss}	$K_{ss} \cdot T_{fold}$	$K_{ss} \cdot T_{fold} \cdot L_{fold}$	$\frac{K_{ss} \cdot T_{fold}}{B}$
Model	<div><div><div><div>D</div><div>+</div><div>T</div><div>↔</div><div>DT</div></div></div><div><div><div>Dose_{iv}</div><div>↓</div><div>D</div></div><div>+</div><div><div>↓</div><div>T</div></div><div>↔</div><div><div>↓</div><div>DT</div></div><div><div>D₂</div><div>↕</div><div>D</div></div></div><div><div><div>Dose_{iv}</div><div>↓</div><div>D</div></div><div>+</div><div><div>↓</div><div>T</div></div><div>+</div><div><div>↓</div><div>L</div></div><div>↕</div><div><div>↕</div><div>DT</div><div>↕</div><div>TL</div></div><div><div>D₂</div><div>↕</div><div>D</div></div></div><div><div><div>Dose_{iv}</div><div>↓</div><div>D₃</div></div><div>+</div><div><div>↕</div><div>M₃</div><div>↕</div><div>S₃</div><div>↕</div><div>S₁</div><div>↕</div><div>M₁</div></div><div>+</div><div><div>↕</div><div>DM₃</div><div>↕</div><div>DS₃</div><div>↕</div><div>DS₁</div><div>↕</div><div>DM₁</div></div><div><div>D₂</div><div>↕</div><div>D₁</div></div></div></div>			
<div>D = Drug T = Target L = Ligand M = Membrane-bound target S = Soluble target (shed)</div>		<div>1 = central compartment 2 = peripheral compartment 3 = tissue compartment T_{fold} = fold-increase in total target after binding drug L_{fold} = fold-increase in ligand after drug binds target B = tissue biodistribution coefficient</div>		

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T = Target
L = Ligand
M = Membrane-bound target
S = Soluble target (shed)

1 = central compartment
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T_{fold} = fold-increase in total target after binding drug
L_{fold} = fold-increase in ligand after drug binds target
B = tissue biodistribution coefficient