

SUPPORTING INFORMATION

In-silico Dynamic Analysis of Cytotoxic Drug Administration to Solid Tumours: Effect of Binding Affinity and Vessel Permeability

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Biochemical and drug delivery model parameters

List of model parameters associated with the *Biochemical Solver Module* and the *Drug Delivery Solver Module* (see Fig 1). Cells marked with an asterisk denote shared values for both tissue types, while “NA” denotes non-applicable.

Parameter	Description	Host	Tumour	Source
λ_ϵ [d ⁻¹]	ECM remodelling rate	8.64e-4	8.64e-1	adapted from [1]
δ_ϵ [d ⁻¹]	ECM degradation rate from MDEs	7.465	NA	[2]
δ_d [d ⁻¹]	ECM degradation rate from drug	0.	8.64e-2	this work
$\bar{\epsilon}$ [-]	ECM remodelling threshold	0.33	*	[2]
$\bar{\epsilon}_d$ [-]	ECM depletion threshold (due to drug), see Eq (13)	NA	0.1	this work
$\bar{\epsilon}_i$ [-]	see Eq (13)	NA	0.01	this work
a_d [-]	see Eq (13)	NA	2.5	this work
s_c [nm]	size of drug molecule, see Eq (9)	1.		
τ_c [h]	half-life of the drug	4.		this work
k_{on} [s ⁻¹]	drug association (affinity) rate	0.	0.005, 0.05, 0.5, 5.	adapted from [3]
k_{off} [s ⁻¹]	drug disassociation rate	0.	1.e-4	[3]
k_{int} [s ⁻¹]	drug internalisation rate	0.	5.e-5	[3]
δ_b [s ⁻¹]	internalised drug decay rate	0.	0.0864e-5	this work

References

1. Wood LB, Ge R, Kamm RD, Asada HH. Nascent vessel elongation rate is inversely related to diameter in in vitro angiogenesis. *Integrative Biology*. 2012;4:3579–3600.
2. Vavourakis V, Wijeratne PA, Shipley R, Loizidou M, Stylianopoulos T, Hawkes DJ. A Validated Multiscale In-Silico Model for Mechano-sensitive Tumour Angiogenesis and Growth. *PLOS Computational Biology*. 2017;13(1):e1005259. doi:10.1371/journal.pcbi.1005259.
3. Stylianopoulos T, Jain RK. Combining two strategies to improve perfusion and drug delivery in solid tumors. *Proceedings of the National Academy of Sciences of the United States of America*. 2013;110(46):18632–18637. doi:10.1073/pnas.1318415110.