

Table S1: List of parameter values relating to ABT-737 pharmacokinetics and pharmacodynamics.

Parameter	Value	Source
$\tau_A$	1 day	[1]
$\alpha_{perit}$	$11.56 \times 10^3$ nM	[2]
$\mu_A$	6 per day	see text
$\lambda_A$	3.37 per day	[2]
$K_{CP}^A$	2.40 per day	see text
$K_{PC}^A$	$3 \times 10^{-3}$ per day	see text
$K_A$	3.36 per day	see text
$k_a^A$	172.80 per day per nM	[3,4] <sup>1</sup>
$k_d^A$	172.80 per day	[4] <sup>2</sup>
$k_a^X$	172.80 per day per nM	[3]
$k_d^X$	1728 per day	[3]
$\beta$	75 nM	[3]
$\chi$	83.33 nM	[3]

### References

- [1] Witham J, Valenti MR, De-Haven-Brandon AK, Vidot S, Eccles SA, et al. (2007) The Bcl-2/Bcl-xL family inhibitor ABT-737 sensitizes ovarian cancer cells to carboplatin. Clin Cancer Res 13: 7191-7198.
- [2] Tse C, Shoemaker AR, Adickes J, Anderson MG, Chen J, et al. (2005) ABT-263: a potent and orally bioavailable Bcl-2 family inhibitor. Cancer Res 68: 3421-3428.
- [3] Hua F, Cornejo MG, Cardone MH, Stokes CL, Lauffenburger DA (2005) Effects of Bcl-2 levels on Fas signaling-induced caspase-3 activation: molecular genetic tests of computational model predictions. J Immunol 175: 985-995.
- [4] Oltersdorf T, Elmore SW, Shoemaker AR, Armstrong RC, Augeri DJ, et al. (2005) An inhibitor of Bcl-2 family proteins induces regression of solid tumours. Nature 435: 677-681.

<sup>1</sup>It is assumed that rate of the forward reaction of ABT-737 with Bcl-2/xL is similar to that of Bax binding to Bcl-2.

<sup>2</sup>The dissociation constant for ABT-737 binding Bcl-2/xL is  $\sim 1$  nM.