

**Table S1.** Summary of the ITC data for the binding interactions using Hsp90, FKBP51 and LA1011.

Cell component and concentration	Injectant and concentration	<i>K<sub>d</sub></i>	N	Comment
30 $\mu$ M Hsp90	400 $\mu$ M FKBP51	-	-	One site fit. Overall, a poor fit
30 $\mu$ M Hsp90	400 $\mu$ M FKBP51	$K_d = 0.5 \pm 0.1 \mu\text{M}$ $K_d = 32.4 \pm 6.3 \mu\text{M}$	-	Two site fit
30 $\mu$ M Hsp90	400 $\mu$ M FKBP51- $\Delta$ 7He	$K_d = 11.6 \pm 1.1 \mu\text{M}$	1.25	-
30 $\mu$ M Hsp90	1 mM LA1011	$K_d = 13.1 \pm 1.7 \mu\text{M}$	0.5 (fixed)	-
30 $\mu$ M Hsp90 60 $\mu$ M FKBP51	1 mM LA1011	$K_d = 108 \pm 3.0 \mu\text{M}$	0.5 (fixed)	-
30 $\mu$ M Hsp90 60 $\mu$ M FKBP51- $\Delta$ 7He	1 mM LA1011	$K_d = 17.9 \pm 1.27 \mu\text{M}$	0.5 (fixed)	-
30 $\mu$ M Hsp90 1 mM LA1011	400 $\mu$ M FKBP51	$K_d = 2.1 \pm 0.2 \mu\text{M}$	1.0	One site fit
30 $\mu$ M Hsp90 1 mM LA1011	400 $\mu$ M FKBP51	$K_d = 5.2 \pm 2.7 \mu\text{M}$ $K_d = 2.7 \pm 1.9 \mu\text{M}$	-	Two site fit