

BS148 reduces the aggressiveness of metastatic melanoma via Sigma-2 receptor targeting

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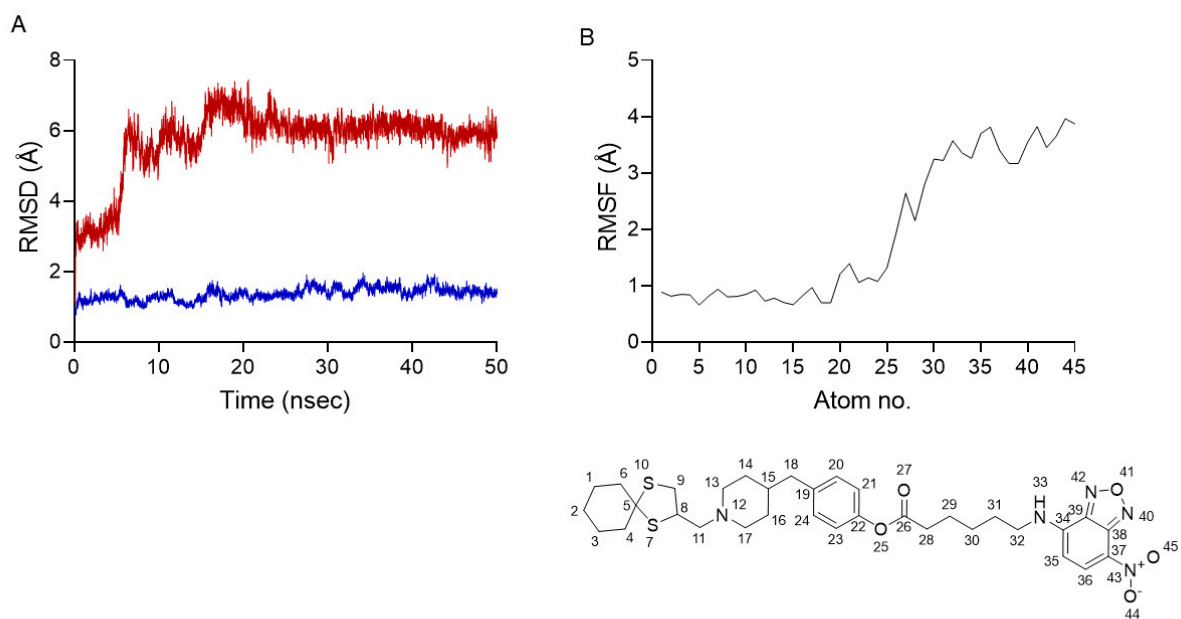


Figure S1. Fig. 2 of main text - Molecular Dynamics - (A) Backbone (blue line) and ligand (red line) RMSD over a period of 50 ns of MD simulation of BS148-fluo-protein complex. (B) RMSF values for BS148-fluo ligand; the atom numbering on the ligand structure is indicated.

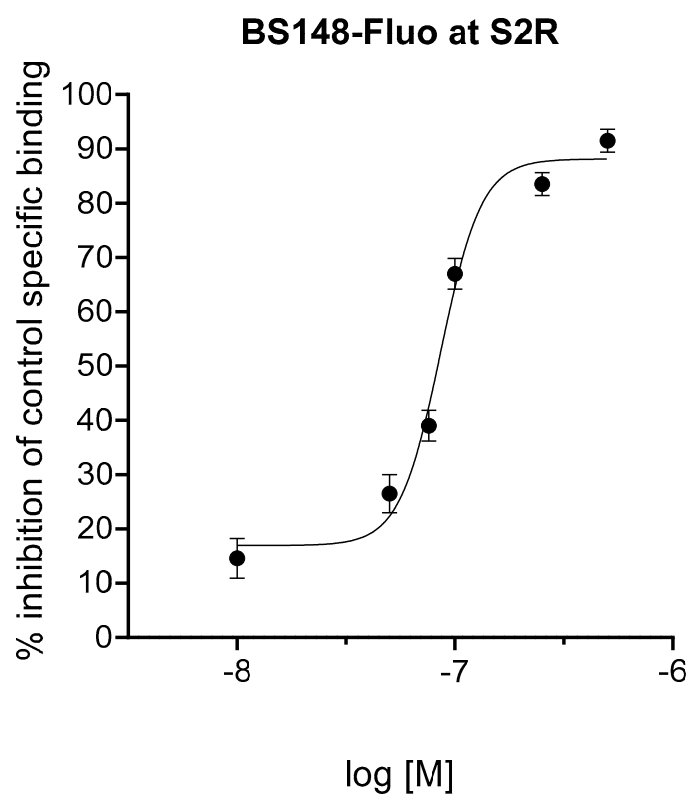


Figure S2. Dose-response curve for BS148-fluo at S2R.

SUPPORTING INFORMATION

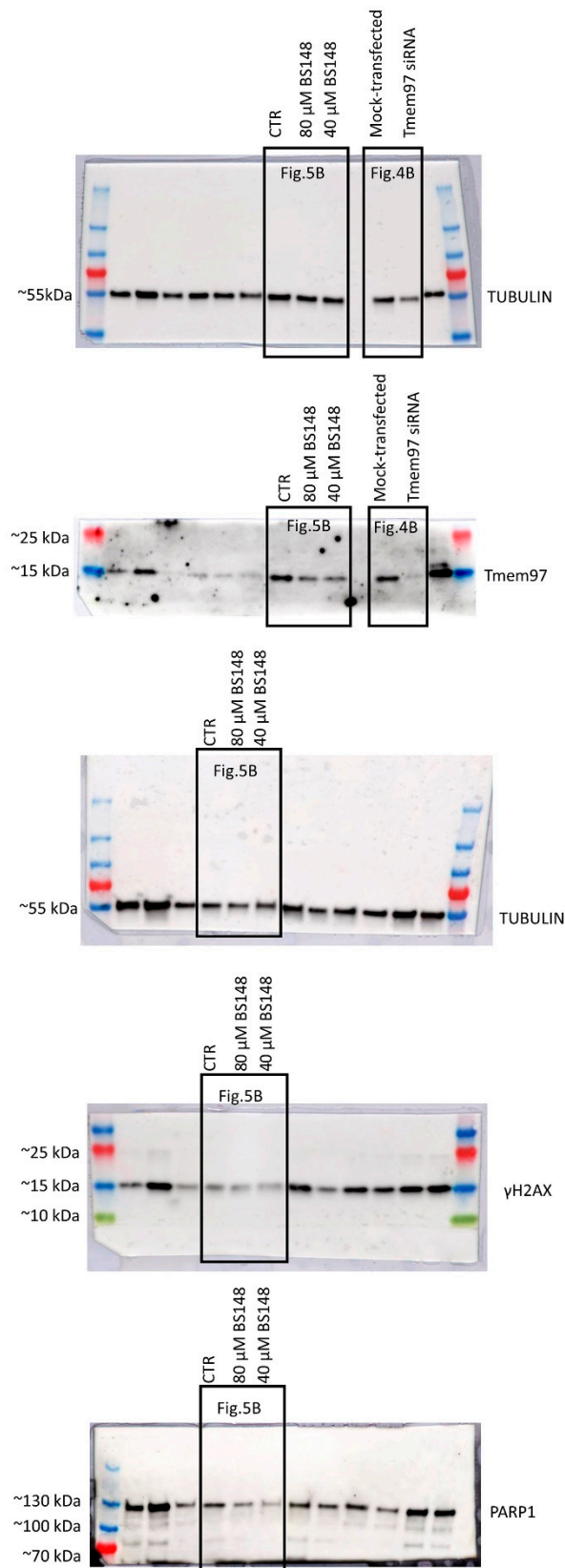


Figure S3. Fig. 4B and 5B of main text - original images – Western Blot

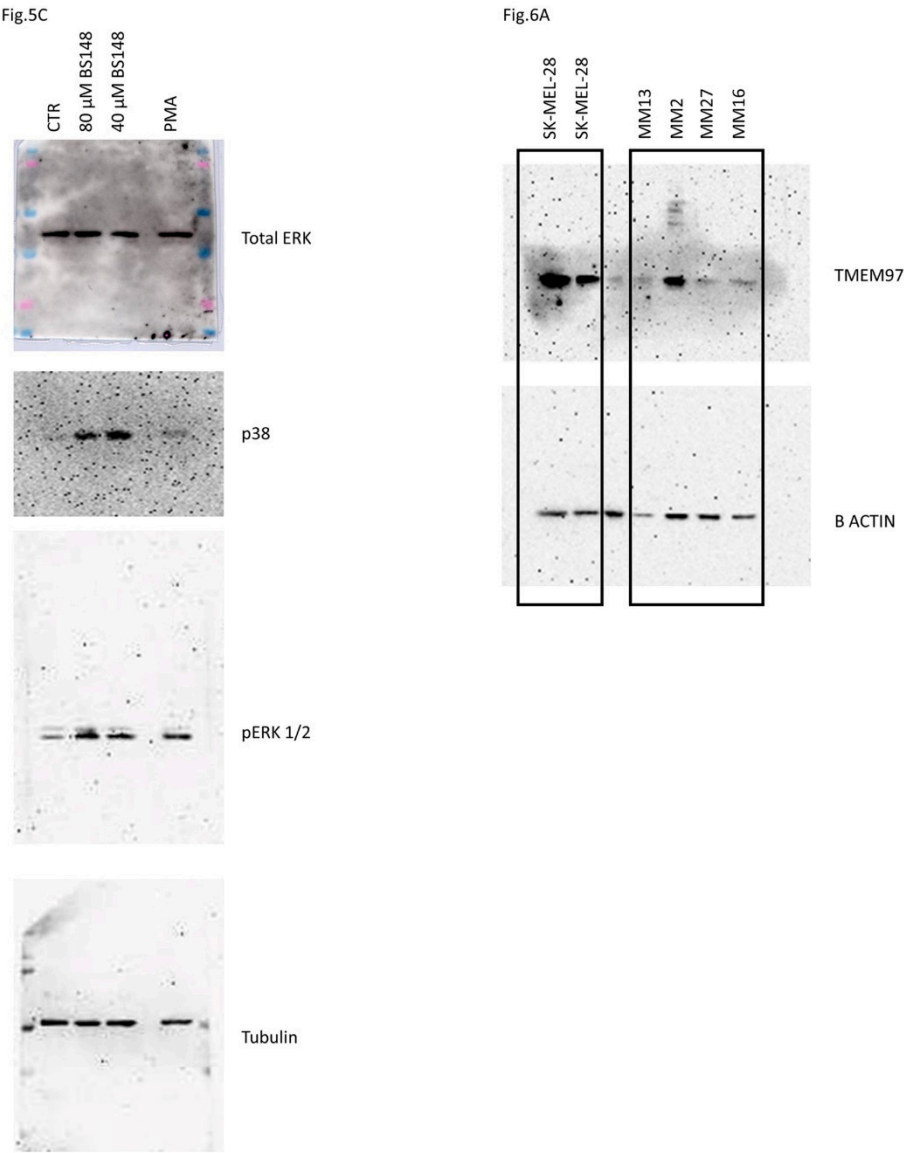


Figure S4. Fig. 5C and 6A of main text - original images – Western Blot

SUPPORTING INFORMATION

Figure 4A			Figure 4C			Figure 5A			Figure 6B				
t-test			two-way ANOVA (multiple comparisons)			Ordinary one-way ANOVA (multiple comparisons)			Ordinary one-way ANOVA (multiple comparisons)				
Samples	Summary	P Value	Samples	Summary	P Value	Samples	Summary	Adj. P Value		24h	Summary	Adj. P Value	
SIGMA1R vs TMEM97	**	0.0062	0 μM siRNA mock vs. 60 μM siRNA mock	**	0.0018	40μM BS148 vs. CTR	**	0.0020	MM13	Conc.(μM)	*	0.0440	
			0 μM siRNA mock vs. 80 μM siRNA mock	***	0.0003	80μM BS148 vs. CTR	***	0.0007		0 vs. 80	**	0.0091	
			0 μM siRNA mock vs. 100 μM siRNA mock	***	0.0003	siTMEM97 vs. CTR	**	0.0025		0 vs. 100	**	0.0028	
			60 μM siRNA mock vs. 60 μM siRNA TMEM97	**	0.0047	40μM BS148 vs. CTR	****	< 0.0001	MM27	0 vs. 40	*	0.0151	
			80 μM siRNA mock vs. 80 μM siRNA TMEM97	*	0.0236	80μM BS148 vs. CTR	****	< 0.0001		0 vs. 80	****	<0.0001	
			100 μM siRNA mock vs. 100 μM siRNA TMEM97	*	0.0239	siTMEM97 vs. CTR	****	< 0.0001		0 vs. 100	****	<0.0001	
						FDF1	40μM BS148 vs. CTR	ns	0.2241	MM16	0 vs. 40	ns	0.3092
							80μM BS148 vs. CTR	ns	0.0633		0 vs. 80	*	0.0310
							siTMEM97 vs. CTR	ns	0.2241		0 vs. 100	*	0.0127
						FDP5	40μM BS148 vs. CTR	**	0.0018	MM2	0 vs. 40	ns	0.2197
							80μM BS148 vs. CTR	***	0.0004		0 vs. 80	**	0.0024
							siTMEM97 vs. CTR	**	0.0018		0 vs. 100	***	0.0002
						ATF4	40μM BS148 vs. CTR	ns	0.3863				
							80μM BS148 vs. CTR	**	0.0023		48h		
							siTMEM97 vs. CTR	ns	0.3863		Summary	Adj. P Value	
						CHOP	40μM BS148 vs. CTR	ns	0.683	MM13	0 vs. 40	ns	0.1424
							80μM BS148 vs. CTR	***	0.0004		0 vs. 80	***	0.0008
							siTMEM97 vs. CTR	*	0.0105		0 vs. 100	****	<0.0001
						XBP1s	40μM BS148 vs. CTR	ns	0.5878	MM27	0 vs. 40	ns	0.1154
							80μM BS148 vs. CTR	*	0.0189		0 vs. 80	**	0.0013
							siTMEM97 vs. CTR	*	0.0263		0 vs. 100	***	0.0006
						BIP	40μM BS148 vs. CTR	ns	0.9797	MM16	0 vs. 40	ns	0.9924
							80μM BS148 vs. CTR	ns	0.9674		0 vs. 80	***	0.0002
							siTMEM97 vs. CTR	ns	0.9797		0 vs. 100	****	<0.0001
										MM2	0 vs. 40	**	0.0030
											0 vs. 80	****	<0.0001
											0 vs. 100	****	<0.0001

Table S1. Fig. 4A, 4C, 5A and 6B of the main text - calculated p-values (Prism software). (* p < 0.05; ** p < 0.01; *** p < 0.001; **** p < 0.0001; ns, not significant).