

Table S1. Target genes and primer sequences.

Gene	Forward primer	Reverse primer
GAPDH	TGACCCCTTCATTGACCTCA	TGACAAGCTTCCCGTTCTCA
TGIF2	CCCAAGGAGTCGGTGAAGAT	CGGGCATTGATGAACCAGTT
ID1	GCTGTTACTCACGCCTCAAG	CTCCA ACTGAAGGTCCTGA
BMP2	ATTCCCCGTGACCAGACTTT	CCACTTCCACCACGAATCCA

Table SII. Cell inhibition rates of compounds 1-8 and 10.

Compound (5.0 μ M)	Inhibition rate (%)					
	PC3	LNCaP	HeLa	SiHa	K562	HEL
1	22.52 \pm 2.59	10.91 \pm 1.16	49.48 \pm 6.21	43.26 \pm 9.67	14.82 \pm 8.54	8.91 \pm 4.44
2	15.89 \pm 3.45	8.89 \pm 6.45	14.42 \pm 5.65	40.01 \pm 9.12	27.11 \pm 5.51	8.80 \pm 5.89
3	14.45 \pm 2.36	4.45 \pm 4.12	29.34 \pm 7.21	20.46 \pm 3.17	36.89 \pm 2.99	3.96 \pm 2.77
4	20.34 \pm 3.89	28.87 \pm 9.33	30.17 \pm 7.23	10.77 \pm 8.33	16.99 \pm 8.56	14.78 \pm 8.44
5	7.72 \pm 1.17	11.95 \pm 7.45	6.74 \pm 2.76	31.22 \pm 6.97	14.45 \pm 6.22	10.90 \pm 6.10
6	2.77 \pm 2.36	37.08 \pm 3.32	30.12 \pm 3.76	33.98 \pm 6.88	30.76 \pm 9.48	23.70 \pm 4.92
7	8.85 \pm 4.90	11.90 \pm 8.36	6.74 \pm 3.56	31.20 \pm 3.98	34.80 \pm 6.32	12.90 \pm 9.32
8	2.47 \pm 1.32	20.91 \pm 5.52	23.84 \pm 3.52	41.17 \pm 6.37	9.77 \pm 6.21	17.98 \pm 8.39
10	22.93 \pm 7.42	13.65 \pm 9.34	38.45 \pm 3.58	15.90 \pm 2.16	42.55 \pm 7.99	17.87 \pm 8.21

Note: Compound 9 was excluded from testing due to experimental contamination and reportedly low inhibitory activity in literature (90).

Table III. Optimization model results for molecular docking.

Target Symbol	Protein databank ID	Binding Affinity (kcal/mol)
TGIF-2	2DMN	-7.3
ID1	2P57	-6.4
BMP2	4MID	-7.1