

Supporting Table S5. DUD-E generated decoys binding energies (kcal/mol) obtained by PyRosetta, using 5BR as a target protein

SUBSTRATES	UNPRODUCTIVE POSITION	PRODUCTIVE POSITION
DUD-E 1	18	10
DUD-E 2	Not binding	-2
DUD-E 3	9	2
DUD-E 4	10	-7
DUD-E 5	15	0.1
DUD-E 6	10	-10