

S2 Table. Comparison of WT-EGFR and EGFR L858R total binding energy calculated by Rosetta FlexPepDock and MM-PBSA.

Peptides	Peptide sequences	Rosetta FlexPepDock		MM-PBSA	
		Server (REU)		(kcal/mol)	
		WT-EGFR	EGFR L858R	WT-EGFR	EGFR L858R
MIG6-YY	THYYLLP	-15.695	-16.941	-16.397	-18.706
Peptide 5	STHHYYP	-16.599	-19.640	-4.497	-23.923
Peptide 6	STHHYYL	-17.608	-19.131	-30.592	-9.205
Peptide 10	HTHYLP	-21.908	-20.212	-15.675	-44.791
Peptide 26	KHTHYYD	-16.047	-19.982	-8.544	-25.098
Peptide 27	KRTHYYD	-16.638	-20.093	-45.258	-46.426