

Table S4. Summary of Simulations, Related to Experimental Procedures

Description	Number of atoms (rounded to 1,000)	Duration (μ s)	Membrane size (\AA^2)	Illustration
Simulations of the extracellular domains				
Tethered extracellular monomer	241,000; 251,000	3.6; 2.7	NA	Figure 2
Extended extracellular monomer with EGF	394,000	5.5		Figure 2
Extended extracellular monomer without EGF	395,000	5.4		Figure 2
The 2-ligand extracellular dimer	272,000–391,000	12.8; 6.2		Figure 3, S1
The 2-ligand extracellular dimer (CHARMM22*)	271,000	10.2; 10.5; 8.7		Figure S1
The 1-ligand extracellular dimer	272,000	14.1; 10.7		Figure 3, S1
The 1-ligand extracellular dimer (CHARMM22*)	271,000	15.0; 10.5; 10.8		Figure S1
The ligand-free extracellular dimer	272,000	11.0		Figure 3, S1
The ligand-free extracellular dimer (CHARMM22*)	271,000	16.6; 7.5		Figure S1
Simulations of the transmembrane segments				
The N-terminal transmembrane dimer	38,000	100.2; 51.2	68 × 68	Figure 4
The C-terminal transmembrane dimer	35,000–38,000	30.4; 14.5; 10.7; 33.4	68 × 68	Figure 4
The N-terminal transmembrane dimer (I640E)	36,000	38.6	68 × 68	Figure 4
The N-terminal transmembrane dimer (T624L, G625L, G628L, A629L)	36,000	19.2; 18.5; 18.5; 18.1	68 × 68	Figure S2
The N-terminal transmembrane dimer (T624I/G625I/G628I/A629I)	36,000	5.2; 1.3	68 × 68	Figure S2
The C-terminal transmembrane dimer (I640E)	36,000	19.0; 33.9	68 × 68	Figure 4
Self-assembly simulation with 4 transmembrane helices	37,000	201.2	68 × 68	Figure 4
Self-assembly simulation with 9 transmembrane helices	37,000	103.1	68 × 68	Figure 4
The HER2 N-terminal transmembrane dimer	33,000	134.6	68 × 68	Figure S2
The HER2 C-terminal transmembrane dimer	34,000	120.8	68 × 68	Figure S2

Simulations of the TM–JM–A construct				
The N-terminal transmembrane dimer and the JM-A dimer	45,000	125.0; 40.3	70 × 70	Figure 5, S3
The N-terminal transmembrane dimer and the JM-A dimer (in DMPC bilayer)	46,000	19.0; 14.5, 14.3; 103.0	70 × 70	Figure 5, S3
The left-handed transmembrane dimer and the JM-A dimer (in DMPC bilayer)	46,000	5.1; 10.1	70 × 70	Figure S3
The C-terminal transmembrane dimer and the JM-A dimer	39,000	30.4; 6.4	70 × 70	Figure 5, S3
The TM–JM–A monomer	48,000	18.8; 10.3	68 × 68	Figure 5, S3
Simulations of the TM–JM–KD construct				
The TM–JM–KD, monomer	121,000	2.7	94 × 94	Figure 7, S4
The TM–JM–KD, active dimer	244,000	21.7	138 × 138	Figure 7, S4
The TM–JM–KD, inactive dimer	229,000	26.7; 11.5	138 × 138	Figure 7, S4
The TM–JM–KD, inactive dimer (7.5% POPS)	204,000	10.2	138 × 138	Figure 7, S4
The TM–JM–KD, inactive dimer (2.5% POPS)	246,000	16.6	138 × 138	Figure 7, S4
The TM–JM–KD, inactive dimer (without POPS)	263,000	8.7	138 × 138	Figure 7, S4
Simulations of the monomer and dimers of the near-complete EGFR				
Monomer	229,000	4.7	116 × 116	Figure 6
Inactive dimer	422,000	4.1; 1.5; 2.1	148 × 148	Figure 6
Active dimer	554,000	4.7	150 × 150	Figure 6