Supplementary data

Conformational stability of the epidermal growth factor (EGF) receptor as influenced by glycosylation, dimerization and EGF hormone binding

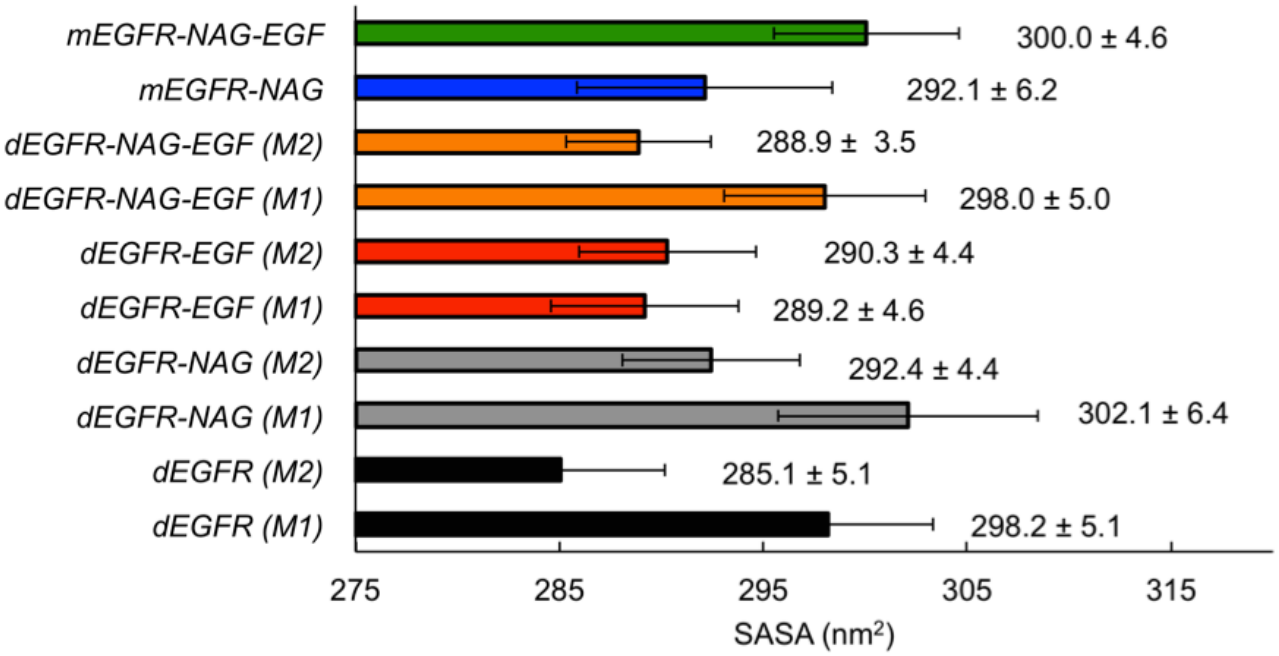

Figure S1. Average solvent accessible surface area (SASA) of each EGFR system. Values at ends of bars are an average of the 50 ns MD simulation (± SD). M1 = Monomer 1; M2 = Monomer 2. *dEGFR* = dimeric EGFR; $dEGFR^{NAG}$ = dimeric, glycosylated EGFR; $dEGFR^{EGF}$ = dimeric, ligand-bound EGFR; $dEGFR^{NAG\text{-}EGF}$ = dimeric, glycosylated, ligand-bound EGFR; $mEGFR^{NAG}$ = monomeric, glycosylated EGFR; and $mEGFR^{NAG\text{-}EGF}$ = monomeric, glycosylated, ligand-bound EGFR.

Table S1. Summary of secondary structural properties of simulated EGFR.

System	Residues	Structural Properties % average (±SD)				SASA at 50 ns (M1, M2)
		α-helix	β-sheet	coil	turn	*nm*
dEGFR	1020	5.6 (0.8)	23.1 (1.2)	32.7 (0.9)	11.1 (1.4)	301.3, 279.9
dEGFR-NAG	1020	3.9 (0.6)	23.2 (2.3)	34.3 (1.3)	11.1 (1.3)	295.5, 283.0
dEGFR-EGF	1020	3.8 (0.6)	22.1 (1.3)	33.3 (1.4)	12.2 (1.2)	293.2, 293.9
dEGFR-NAG-EGF	1020	5.1 (0.8)	20.9 (1.0)	33.6 (0.9)	11.6 (1.1)	296.7, 282.8
mEGFR-NAG	510	3.3 (1.3)	20.1 (1.6)	37.1 (2.3)	10.5 (2.0)	296.0
mEGFR-NAG-EGF	510	5.0 (1.4)	21.3 (1.9)	34.1 (1.3)	10.1 (1.6)	300.5

SASA = solvent accessible surface area, M1 = Monomer 1, and M2 = Monomer 2. *dEGFR* = dimeric EGFR; $dEGFR^{NAG}$ = dimeric, glycosylated EGFR; $dEGFR^{EGF}$ = dimeric, ligand-bound EGFR; $dEGFR^{NAG\text{-}EGF}$ = dimeric, glycosylated, ligand-bound EGFR; $mEGFR^{NAG}$ = monomeric, glycosylated EGFR; and $mEGFR^{NAG\text{-}EGF}$ = monomeric, glycosylated, ligand-bound EGFR.