Supplementary Material for Integrin Mechanosensing relies on Pivot-clip Mechanism to Reinforce Cell Adhesion

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Table S1: Steered Molecular Dynamics Parameters

Parameter	**Setting**
Time step	2fs
Number of steps (Time) for 1nm/ns	10000000 (20ns)
Number of steps (Time) for 10nm/ns	1500000 (3ns)
Integrator	Leapfrog algorithm
Constraint Algorithm	LINear Constraint Solver (LINCS)
Constraints	H-bonds constrained
Cutoff scheme	Verlet (Buffered neighbor searching)
Short-range neighbor list cutoff	1.4nm
Short-range electrostatic cutoff	1.4nm
Short-range van der Waals cutoff	1.4nm
Electrostatics	Fast smooth Particle-Mesh Ewald (SPME)
Interpolation order	Cubic
Grid spacing for fast Fourier Transform	0.12nm
Temperature coupling	Nosé-Hoover
Reference temperature	310K
Temperature time constant	1.0ps
Temperature coupled groups	Protein and non-protein
Pressure coupling	Off
Dispersion correction	long range dispersion corrections for energy and pressure
Velocity generation	Off
Harmonic potential	Umbrella
Force constant	50 kJ/mol-nm^2
Pull direction	y-direction (vertical)
Pull rate for 1nm/ns	0.001nm/ps = 1nm/ns
Pull rate for 10nm/ns	0.010nm/ps = 10nm/ns

Table S2: Time resolved Force Distribution Analysis Parameter Settings

Parameter	**Setting**
Pairwise forces	Summed
Pairwise groups	Protein
Residue based calculation	Punctual Stress
Pairwise force type	Coulombic interactions only

Table S3: Catch bond parameters for whole-cell finite element model

Variable	**Wildtype**	**R1374/9A**
K_{on}	$0.1\ s^{-1}$	$0.02\ s^{-1}$
K_a	$0.4\ s^{-1}$	$0.8\ s^{-1}$
K_b	$4E-7s^{-1}$	$8E-7s^{-1}$
F_a	$-25pN$	
F_b	$-15pN$	

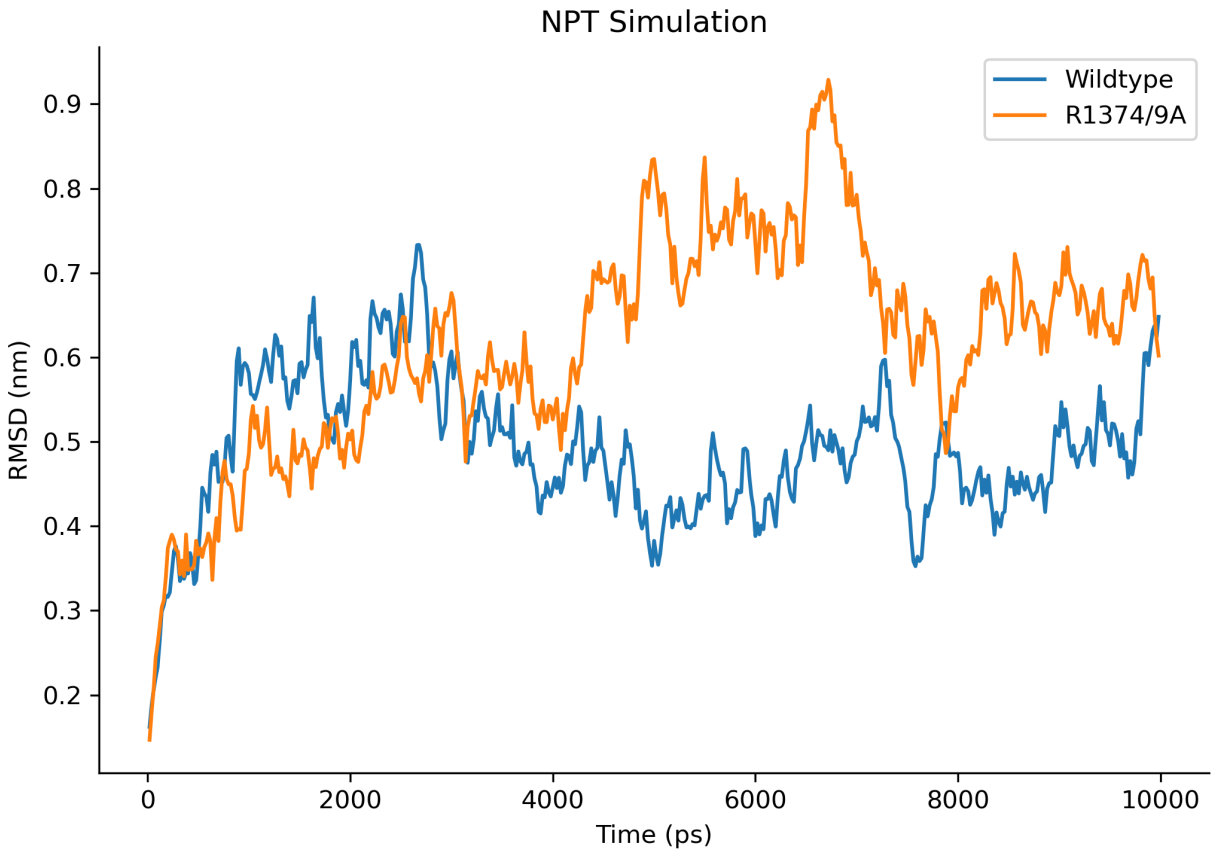

Figure S1: Root-mean-square deviation (RMSD) of wildtype and mutant during NPT simulation

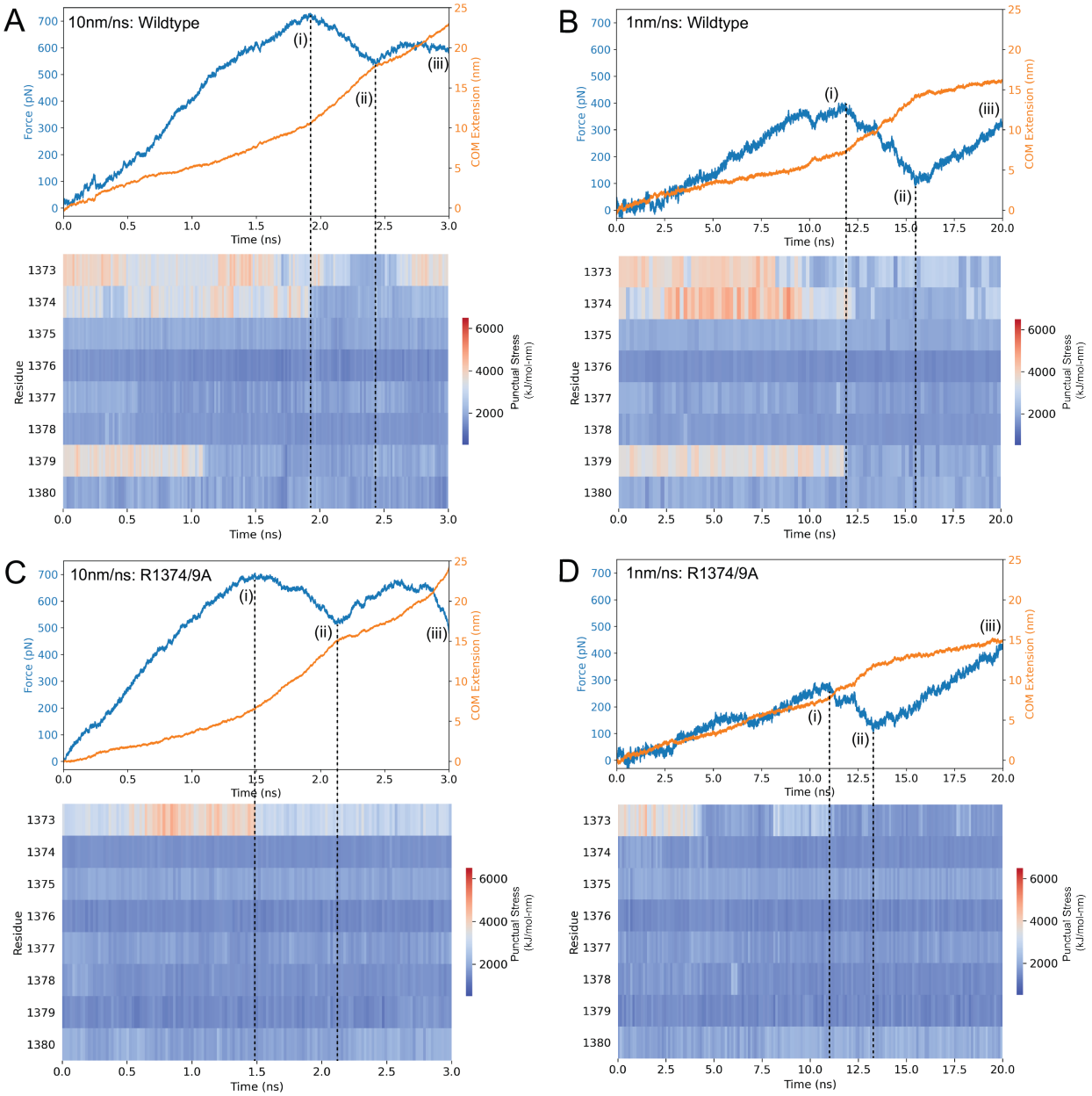

Figure S2: Force and COM extension over time plotted over punctual stress at the synergy site [1373-1380] for A) 10nm/ns wildtype $\alpha_5\beta_1$-FN, B) 1nm/ns wildtype $\alpha_5\beta_1$-FN, C) 10nm/ns R1374/9A $\alpha_5\beta_1$-FN, and D) 1nm/ns R1374/9A $\alpha_5\beta_1$-FN. Positions (i), (ii), and (iii) correspond to the time at the peak force, local minimum, and final frame, respectively.