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Supporting Material

Phosphorylation Facilitates Filamin's Integrin Binding Under Force

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Supplementary Material

"Binding of the bacteriophage P22 N-peptide to the boxB RNA motif studied by molecular dynamics simulations "

(Bahadur, Kannan, and Zacharias)

Molecular mechanics/Poisson-Boltzmann (MMPBSA) calculations

Binding free energy were calculated from 2500 snapshots of the last 10 ns of the simulations of complex and isolated partners using the equation (1, 2):

$$\Delta\Delta G_{binding} = \Delta G_{complex} - (\Delta G_{rna} + \Delta G_{peptide})$$

The free energies of complex ($\Delta G_{complex}$), RNA (ΔG_{rna}) and peptide ($\Delta G_{peptide}$) were calculated for the snapshots form the MD trajectories using the equation.

$$\Delta G = \Delta G_{gas} + \Delta G_{solvation}$$

The gas phase energies or molecular mechanics (MM) energies for the complex, RNA and N-peptide were computed using the parm99 force field (3) in AMBER9 (4). The MM energies represent the internal bonded energy (energy of bonds+ angles+dihedrals) as well as the non-bonded van der Waals, and Coulomb energies. An infinite cutoff for all interactions was used. The solvation ($G_{solvation}$) free energy was calculated from the equation:

$$\Delta G_{solvation} = \Delta G_{PB/GB} + \Delta G_{nonpolar}$$

The electrostatic contribution or polar contribution for the solvation free energy was calculated with both the Generalized Born (GB) and finite-difference Poisson-Boltzmann (FDPB) model. In the GB model, the igb=5 option in the Amber was used, and for the FDPB model, we used either the implementation in Amber9 (linearized PB) or the adaptive Poisson-Boltzmann Solver (APBS) to solve the full non-linear PB equation (5).

The solute and solvent were assigned a dielectric constant of 1 and 80, respectively. The mbondi2 set of radii and atomic charges from parm99 were used for all calculations. The nonpolar contribution for the solvation free energy was estimated using the equation,

$$\Delta G_{nonpolar} = \gamma * SASA + b$$

where the solvent accessible surface area (SASA) was calculated with the linear combination of pairwise overlaps (LCOP) method (6). The surface tension proportionality constant γ and the free energy of nonpolar solvation for a point solute *b* were set to 0.0072 kcal·mol^{-1}·Å^{-2} and 6.08 kcal·mol^{-1}, respectively. The radius of the sphere used to calculate SASA was set to 1.4 Å.

For the calculation of the salt dependence nonlinear FDPB calculations at different salt concentrations: 0.001 M, 0.01 M, 0.1 M, 0.2 M, 0.5 M and 1.0 M were performed on snapshots from the last 10 ns of the simulations.

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Figure legends (suppl. Material):

Figure S1. Average calculated B-factor of the RNA nucleotides in bound (continuous line) and free (dashed line) form during the final 10 ns MD simulation.

Figure S2. Cumulative averages of the total calculated MM/PBSA free energies vs. simulation time. Accumulation of averages was taken over the last 10 ns of the MD trajectories.

Figure S3. Schematic view on the N-peptide-RNA association process (lower panel) and the change in various energetic contributions associated with the transiion from unbound to bound conformation of RNA (Receptor) and Peptide (ligand).

Figure S4. Localization of tightly bound water molecules at the peptide-RNA interface. Water molecules are shown as red (oxygen) and white (hydrogen) van der Waals spheres. The RNA molecule is shown in blue while the helical peptide is colored green (van der Waals surface representation). Both views differ by a rotation of 180^{o} with respect to a vertical (z)-axis.

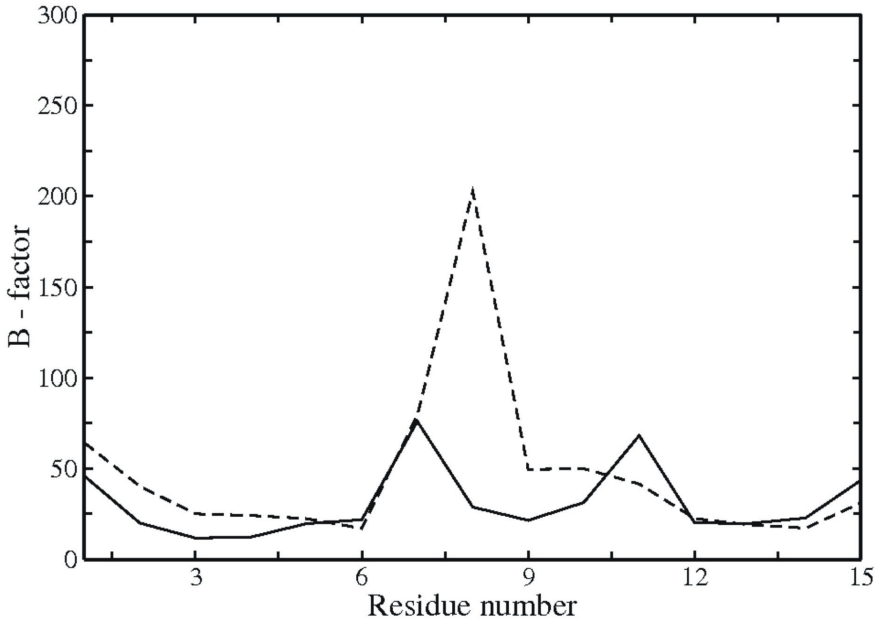

Figure S1

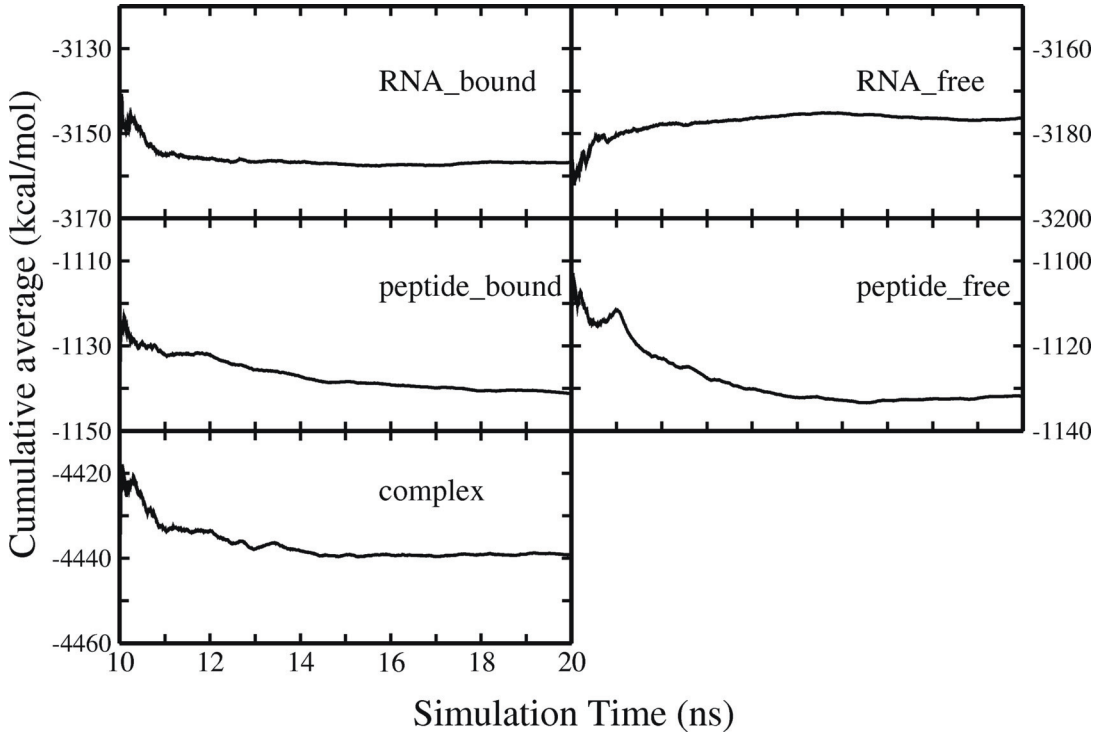
RNA_bound
RNA_free
peptide_bound
peptide_free
complex
Cumulative average (kcal/mol)
Simulation Time (ns)
-3130
-3150
-3170
-3160
-3180
-3200
-1110
-1130
-1150
-1100
-1120
-1140
-4420
-4440
-4460
10
12
14
16
18
20

Figure S2

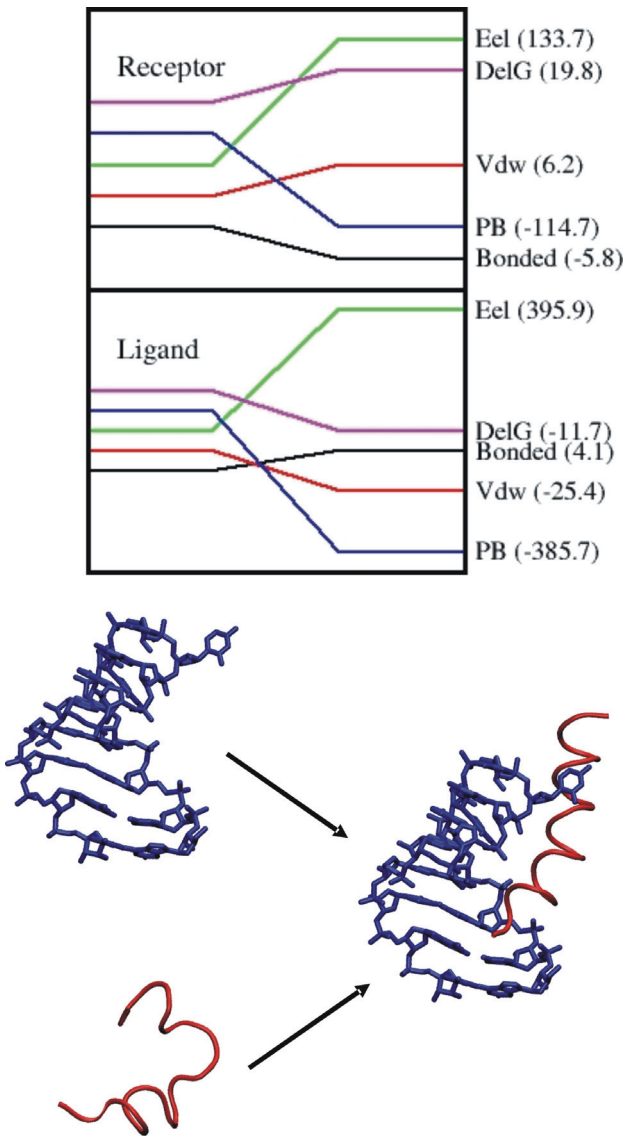
Receptor
Eel (133.7)
DelG (19.8)
Vdw (6.2)
PB (-114.7)
Bonded (-5.8)
Ligand
Eel (395.9)
DelG (-11.7)
Bonded (4.1)
Vdw (-25.4)
PB (-385.7)

Figure S3

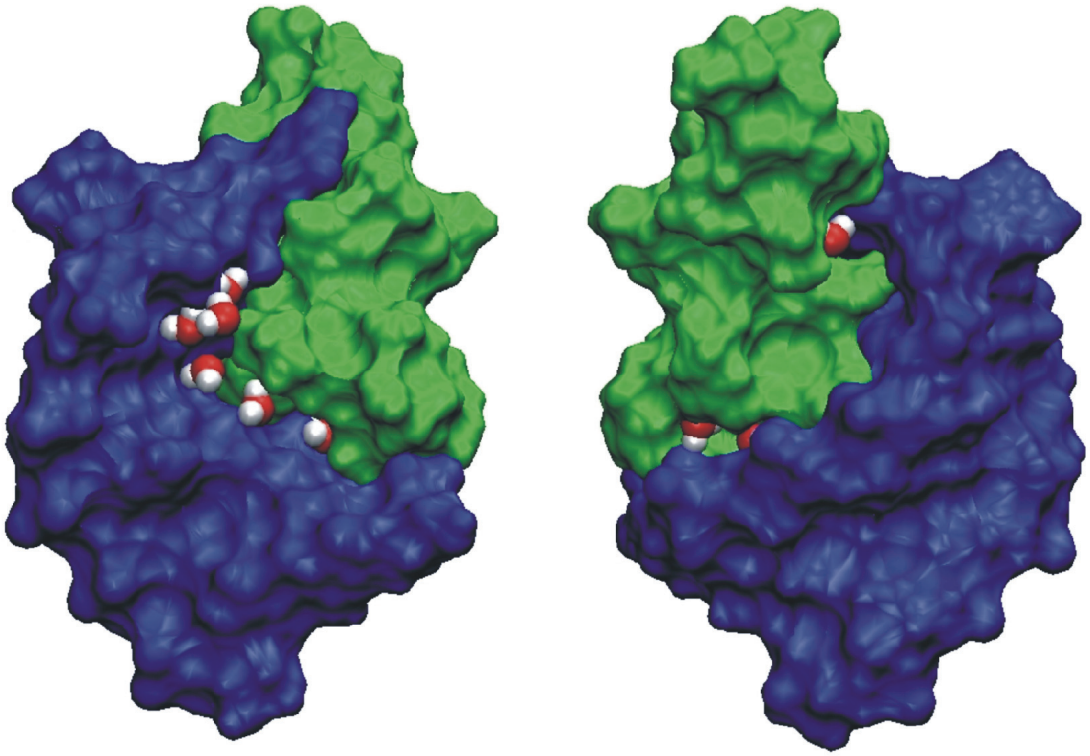

Figure S4