Cell adhesion to motile nano ligands: Effects of ligand size and concentration in solution

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***Short Abstract* — Cells interact with both tethered and motile ligands in their extra-cellular environment to initiate and regulate signaling, adhesion and migration. A quantitative and fundamental understanding of these receptor-ligand interactions is necessary for drug discovery, tissue engineering and biomaterial fabrication. We present a mean field approach to quantify the fundamental thermodynamics of the interaction between the cell surface receptors and motile ligands in solvent.**

***Keywords* — Cell matrix interactions; Nano-ligands; Gibbs Free Energy; Cell adhesion.**

SUMMARY OF RESULTS AND CONCLUSION

Our studies show that the free energy of interaction between the receptors and the motile nano-sized ligands depends strongly on the ligand size at nanometer scale and the behavior at low and high concentration shows disparity that cannot be explained by simple scaling laws. We find that at allowed concentrations for motile ligands of all sizes (from 0.8nm to 2.0nm), it is always larger sizes that is more preferred. Gibbs free energy monotonously increases as concentration goes up. There's an apparent change from small sizes (e.g. 0.8nm, 1.0nm) to large sizes (e.g. 1.5nm, 2.0nm) at high concentrations. The smaller size systems undergo a transition from bound receptor dominant region to free dominant with the increase of the surface coverage of receptor and concentration of ligand. On the other hand, systems containing larger ligands are always bound receptor dominant. From the Helmholtz free energy aspect, although systems of any size demonstrates similar decreasing trend at low concentration, the larger sizes show more stability, while smaller size systems all have a basin, i.e. minimum at high concentration. In addition our calculations also show the effect of the explicit binding energy of receptor and ligand. For any ligand size, the G. free energy shows a very well linear behavior, while the H. free energy has more structure. Our calculations provide insights into understanding cell-matrix interactions at a fundamental level as well as to identify potential avenues for fabrication of nano-ligands for therapeutic and bio-technological purposes.

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