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MOLECULAR BIOMECHANICS AND THERMODYNAMICS OF CELL ADHESION

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ABSTRACT

Cell adhesion regulates cell fate by controlling migration, signaling, proliferation and differentiation. Over the last two decades, numerous receptors, ligands and signaling molecules controlling adhesion have been discovered. However, nearly all computational models addressing adhesion have focused exclusively at the continuum level and have ignored the molecular mechanics and thermodynamics of these complex cell-matrix interactions. This lack of molecular detail has resulted in limited application of computational models in developing a fundamental understanding of adhesion and related processes.

Using a suite of computational studies, combining principles of biomechanics, thermodynamics and statistical physics, we study the molecular mechanics of receptor ligand interactions, force generation and integrin clustering in two and three dimensional cell adhesion. Our novel approach is scalable, and while it incorporates molecular detail, solvent effects and conformational restrictions, it can be easily scaled to cells cultured in two and three dimensional environments. By incorporating the entropic, conformational, solvation, long and short-range interactive components of integrins as well as the extra-cellular matrix molecules, we are able to predict adhesive free energy as a function of a number of key variables such as surface coverage, interaction distance, molecule stiffness and size and solvent conditions. Our method allows us to simultaneously study integrins and ligands, as well as functionalized nanoparticles of different sizes and chemical identities [1]. The results of our simulations not only provide a fundamental understanding of biomechanics of adhesion at the molecular level but also suggest possible strategy for designing novel biomaterials [2-3].

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