A molecular dynamics simulation was performed on MMP-2 using TAMU supercomputing service. Energy minimization of MMP-2 was followed by the heat treatment at 300 K for 100 ps.

**DISCOIDIN DOMAIN RECEPTOR (DDR-2)**

- Receptor activated with a three-helical collagen binding to the extracellular discoidin domain
- Plays a key role in communication of cells and controls cell behavior: cell growth, differentiation, and metabolism
- Essential for controlling formation of spindle midzone during anaphase of cell mitosis in eukaryotes

**RESEARCH PURPOSE**

The proteins studied are major components of key processes that occur in the body such as tumor invasion, angiogenesis, cell migration, regulation of cytoskeleton, and remodeling of the extracellular matrix. Once the proteins are built, simulations on these proteins can be performed to analyze static and dynamic properties, thus elucidating how their dynamic motion and mechanics are related to their cellular function.

**METHODS**

- RCSB is a protein data bank “repository for 3-dimensional structural data of large biological molecules”
  - 1976: 24 files
  - 2014: 405,732 files
- The PDB file is retrieved from RCSB database and provides “cor” and “psf” files
- RCSB Protein Data Bank - RCSB PDB - 1CK7 Structure Summary.
- CHARMM provides a method to model the “cor” and “psf” files so that varying conditions such as heat fluctuations, energy minimization, and protein vibrations can be modeled for analysis of static and dynamic properties
- RCSB PDB Research Collaboratory for Structural Bioinformatics
- VMD is used for molecular modeling and includes tools for working with volumetric and sequence data

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**CITATIONS**

- RCSB Protein Data Bank - RCSB PDB - 1CK7 Structure Summary.