Investigation of Adhesion Peptide Interactions with Hydroxyapatite through Computational Molecular Dynamics

Hamkins, Jaya (School: Crescenta Valley High School)

Nanomedicine revolutionizes treatment of cardiovascular disease through the design of peptide-labelled nanoparticles that bind to hydroxyapatite (HA), the form of calcium in atherosclerotic plaques. This project evaluates binding efficacies of broad-range adhesion peptides (SVSVGMKPSPRP, STLPIPHEFSRE, and VTKHLNQISQSY) to hydroxyapatite through the use of molecular dynamics (MD) software. Peptide and hydroxyapatite slab structures were generated using configuration software PEPFOLD3 and molecule editing software Avogadro, respectively. Three 5 ns simulation trials were run for each peptide using MD software GROMACS to model atomic force-field interactions between the peptide and the hydroxyapatite in water solvent. Binding efficacy was evaluated through visual observation and calculation of the surface separation distance (SSD) between the peptides and the HA slab. Binding is indicated by a separation of less than 1 nm between the amino acid binding site and HA slab. SVSVGMKPSPRP exhibited binding at its lysine (K) and arginine (R) residues. STLPIPHEFSRE exhibited binding at its first serine (S), and VTKHLNQISQSY exhibited binding at lysine (K) and histidine (H). Consistent adhesion interactions were evident in all three trials of SVSVGMKPSPRP, two trials of VTKHLNQISQSY, and one trial of STLPIPHEFSRE. The simulations confirmed that all three peptides possess binding capabilities and identified the binding sites. SVSVGMKPSPRP exhibited the smallest surface separation distance from hydroxyapatite over multiple trials, thereby demonstrating the greatest binding efficacy, and suggesting the greatest potential for clinical use. These results are contingent upon the initial peptide structures and would benefit from extended simulation periods and in vitro confirmation.

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