Targeting Cardiovascular Disease Receptors with Antimicrobial Peptides (AMPs) : Molecular Docking and Dynamics Insights	
Authors	**Doni Dermawan, Nasser Alotaiq**
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Abstract: Infection-related cardiovascular diseases (CVDs) represent a significant health challenge,necessitating novel therapeutic strategies targeting key receptors involved in inflammation andinfection. Antimicrobial peptides (AMPs) offer a promising approach, potentially disruptingpathogenic processes. This study aimed to investigate the efficacy of AMPs as therapeutic agents by examining their interactions with critical CVD-related receptors. A comprehensive computational approach was utilized to assess the interactions between AMPs and receptors associated with CVDs.Molecular docking studies were conducted to evaluate AMP binding to target receptors: ACE2,CRP, MMP9, NLRP3, and TLR4. The top-performing AMPs were further analyzed through 100 ns molecular dynamics (MD) simulations, and their binding affinities were quantified using MM/PBSA calculations. The analysis revealed that Tachystatin, Pleurocidin, and Subtilisin A exhibit strong binding affinities to key CVD-related receptors, including ACE2, CRP, and MMP9. These AMPs demonstrated the potential for disrupting receptor-peptide interactions critical to infection and inflammation. MD simulations confirmed the stability of AMP-receptor complexes, with MM/PBSA calculations showing significant binding energies. Future directions include conducting in vitro and in vivo studies to validate the therapeutic efficacy and safety of these AMPs in clinical settings.