

Abstract Submitted
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Phosphate mediated self-organizing scaffolds in bio-organic antimicrobial peptide (KSL) – a coarse-grained MC simulation¹ BARRY FARMER, GLENN JOHNSON, DONALD EBY, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — A coarse-grained model was used to predict the self-organization of a cationic oligopeptide, KSL (sequence, KKVVFKVKFK) in phosphate buffer. Monte Carlo simulations consisted of a range of peptides concentrations ($C_{KSL} = 0.01- 0.07$) and a fixed phosphate concentration ($C_w = 0.1$). Specificity of the interaction between each residue and the phosphate solvent are considered via an interaction matrix for the well-depth of the LJ potential. The stochastic motion of the oligopeptides is described using Metropolis algorithm and the end-state equilibrium is the self-assembly of peptides into the scaffold aggregates via non-covalent bonding. We examine the energy and mobility profiles of each peptide residue, their characteristic surrounding within the range of interaction, radial distribution function, radius of gyration and global dynamics of the peptides. We find that the density of the aggregate decays exponentially from its central core if strong phosphate interaction is considered. The radius of gyration for the peptide scaffold structure decreases systematically on increasing the phosphate interaction.

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