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In Silico Study of the Early Stages of Aggregation of beta-Sheet Forming Antimicrobial Peptide GL13K

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Antimicrobial peptides (AMPs) are of growing interest as potential candidates that may offer more resilience against antimicrobial resistance than traditional antibiotic agents. In this article, we perform the first *in silico* study of the synthetic β sheet-forming AMP GL13K. Through atomistic simulations of single and multi-peptide systems under different conditions, we are able to shine a light on the short timescales of early aggregation. We find that isolated peptide conformations are primarily dictated by sequence rather than charge, whereas changing charge has a significant impact on the conformational free energy landscape of multi-peptide systems. We demonstrate that the loss of charge-charge repulsion is a sufficient minimal model for experimentally observed aggregation. Overall, our work explores the molecular biophysical underpinnings of the first stages of aggregation of a unique AMP, laying necessary groundwork for its further development as an antibiotic candidate.

Keyword-1

Computational Biophysics

Keyword-2

Protein aggregation

Keyword-3

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