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# Self-Association of Antimicrobial Peptides in Mono- and Multicomponent Solutions: a Computational Study

*Thursday, 1 September 2022 15:00 (15 minutes)*

Antimicrobial peptides (AMPs) are a diverse class of short proteins, that are a key element of the nonspecific innate immunity in most organisms, displaying a wide range of antimicrobial, antifungal, antiviral and even anticancer effects. Lately, AMPs have attracted great research interest in the context of strategies to combat multi-drug resistant bacterial infections. AMPs come in nature in the form of multicomponent secretory fluids that exhibit certain biological activity. Although these small proteins are usually cationic and amphiphilic, their antimicrobial action is not completely understood, neither is their behaviour in bodily liquids prior to attacking the target membrane. We studied various linear AMPs behavior in mono- and multicomponent solutions, prior to their engagement with the pathogenic membrane, by means of long-scale molecular dynamics simulations. We observed that the peptide monomers self-associate into clusters, which consist of a non-polar hydrophobic core and exposed to the solvent charged and polar residues. We consider the so-formed structures as the perfect transport system – locking the hydrophobic uncharged residues in the core of the cluster prevents the interaction with the uncharged eukaryotic membranes, and positioning the charged residues on the cluster surface enables for electrostatic interaction with the bacterial surface. The very formation of the clusters but also the peptide folding, promoted by the amphiphilic structure in the aggregates, allow for an increase of the local concentration of AMPs to be delivered to the target membrane in a functionally active conformation.

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