

# Molecular Dynamics Study of Snail Mucus Peptides Self-Assembly

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The increased emergence of antibiotic-resistant bacterial strains renders inefficient the existing traditional antibiotics. The situation is enforced by a substantial decline in the development of new antibacterial agents. Therefore, in recent years considerable efforts are focused on the development of alternative therapies for the treatment of infectious diseases. The characteristics, the broad spectrum and largely nonspecific activity of the antimicrobial peptides (AMPs), qualify them as possible candidates for therapeutic alternatives and their potential against multi-drug resistant pathogen infections has attracted a lot of interest.

AMPs come in nature in the form of multicomponent secretory fluids that exhibit certain biological activity. Additional complications arise when the studies are exploratory and probe desired interaction patterns at the stage of protein design, that is – when the 3D structure of the peptide is not known, but only its amino acid sequence (primary structure). The first step in this case is deducing the possible biological fold of the peptide.

In preparation for a large-scale investigation of the antimicrobial activity of certain snail-mucus derived peptides, we study solvation behavior of the individual components of the natural multicomponent fluid by means of molecular dynamics simulations. Formation of aggregations and their structure might be decisive in understanding the antimicrobial mode of action of the components and of the compound as a whole. We present the results about the component with the biggest electric charge (9 amino acid residues, with charge +2). We observe a self-assembly process in a simulation box with 27 molecules of the peptide.

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