Self-organisation in polypeptide substances: towards understanding biological activity of antimicrobial peptides

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Antimicrobial peptides (AMPs) are essential components of innate immunity in most multicellular organisms and represent an ancient nonspecific host defense mechanism against infectious pathogens, that complements the highly specific cell-mediated immune response. They are known to also exhibit anticancer, antiinflammatory and immunomodulatory role. In addition, despite the millions of years co-evolution, no signs can be seen of a wide-spread or even limited bacterial resistance against their action. All this makes natural AMPs a prime target for research and an ideal template for the design of sustainable antibiotic biologicals.

There is experimental evidence for antiviral, antibacterial, fungicidal, and even anti-tumor activity of multipeptide fractions from the mucus and the hemolymph of molluscs and arthropods. However, for the design and development of mucus-based biologicals, the identfication of the essentially active components in these compounds is needed. Here we present the first results of a pilot *in silico* study on newly identified peptides in two fractions from the mucus of the snail *Cornu aspersum*. The researched sample substances have no homologies with any known experimental structure in the Protein Data Bank. We employ molecular dynamics (MD) simulations to develop 3D structural models of these newly discovered peptides and commence a detailed investigation of their solvation behavior – individual and in constellations, to probe our based on earlier observation hypothesis for the self-organisation as a decisive initial stage in the AMPs' biological activity.

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