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Short Talk 4 - To understand the antimicrobial activity of the salivary protein Histatin 5

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Histatin 5 is a saliva protein that acts as the first line of defence against oral candidiasis caused by *Candida Albicans*, and it also possesses bactericidal effects. The antimicrobial activity has been ascribed to the high content of basic amino acids. Histatin 5 also participate in the formation of a protective layer on smooth tooth surfaces, and thereby prevent microbial colonization and stabilize mineral-solute interactions. It is established that various transitional metals, such as zinc, nickel, copper, and iron are intrinsically present in the saliva and it is hypothesized that the metal binding abilities of Histatin 5 plays an important role for the candidacidal mechanism. Histatin 5 binds zinc and copper and possesses definitive metal binding motifs for copper and nickel as well as for zinc. In this presentation I will discuss how we use computer simulations on both the atomistic and coarse-grained level in combination with experimental techniques such as scattering and surface adsorption techniques to achieve a molecular understanding of the systems of interest. Furthermore, I will present our latest results regarding Histatin 5 in solution, its interaction with multivalent ions, and the interaction with bilayers corresponding to model cell membranes. The possibility of using Histatin 5-spermidine conjugate as an anti-fungal drug will also be highlighted.

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