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Understanding the interactions between the intrinsically disordered peptide Histatin 5 and lipid bilayers, the effect of amino acid sequence and electrostatic interactions

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Histatin 5 (Hst5) is a histidine-rich, 24 amino acid protein, classified as an intrinsically disordered protein (IDP). It is a cationic salivary protein found to play a crucial role in fungicidal activity, and its activity to inhibit the growth and viability of *Candida albicans* has been evaluated using a variety of techniques. The underlying mechanism is however not very well known. The aim of this project is to understand the underlying mechanism of the role of the histidines and the interaction with the lipid bilayer system.

The results obtained from neutron reflectometry and QCM-D have shown that the interaction between the peptide and the lipid bilayer is completely governed by electrostatic effects. This was done by changing the charge content in the bilayer and the ionic strength of the buffer. At low ionic strength, the peptide penetrates the bilayer and cumulate close to the solid silica substrate underneath the lipid bilayer. The effect of the number of histidines, and hence the charge of the peptide, have been studied with QCM-D. Results show that the interaction with the bilayer is strongly affected by the number and position of the histidines in the peptide. The peptide adsorption is reduced when the number of histidines is conserved, but the peptide sequence is scrambled, as well as when some selected histidines are replaced by glutamines, which is the pH-insensitive counterpart to histidine. Results on how the different variants of Hst5 adsorb to surfaces and the free energy profiles for the interaction is obtained from coarse-grained Monte Carlo simulations.

UV/Vis-spectrophotometry measurements have shown that the interaction between Hst5 and a lipid bilayer initiates a peroxidation reaction, this is also affected by the number of histidines in the sequence.

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