## [P39] Interaction studies of bacterial proteins with antimicrobial peptides by NMR

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The steadily increasing problem of bacterial resistance to common antibiotics intensifies the search for alternative ways to control resistant pathogens, causing thousands of deaths each year.

A promising way to overcome this rising imminence is the use of antimicrobial peptides (AMPs) as leads. AMPs are especially useful because of their property to selectively inhibit metabolic pathways crucial for reproduction and metabolic survival of pathogens. [1]

The aim of this study is the inhibition of essential synthetic cycles of gram positive bacteria, which should be achieved by interfering the interaction of the acyl carrier protein with an artificial peptide. To study the binding process of the peptide to the protein, primarily saturation-transfer difference (STD) NMR spectroscopy, a very versatile technique for the observation of protein-ligand binding, is applied. [2]

In order to study the complexes, first the unbound peptide structures had to be examined. This was done using NMR-parameters as input for chemical shift based structure elucidation systems TALOS [3], CS-Rosetta [4] or CS23D [5], a typical result is shown in Figure 1.

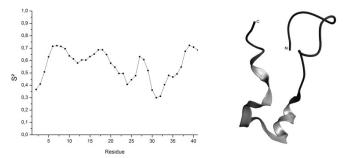


Figure 1: Left diagram: S<sup>2</sup> order parameter from TALOS indicating flexibility of the peptide backbone. The picture on the right shows a structure estimation of the peptide from CS23D web server.

Bibliography:

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