MD simulation of antimicrobial peptides with NMR constraints

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Our BioNMR group is currently studying antimicrobial peptides with membrane disrupting properties. These peptides are thought to form pores or alter the membrane structure in such a way that depolarization of the membrane potential leads to cell death. Such peptides might serve as novel antibiotics, able to kill drug-resistant bacteria. The secondary structure of these peptides is studied by CD (circular dichroism) spectroscopy, while orientational parameters like the insertion and rotation angles can be determined by NMR and oriented circular dichroism (OCD). The experimentally obtained parameters are time-averaged over milliseconds to seconds and do not give any direct information about dynamics. MD simulations of these systems allow us to observe membrane insertion and possible pore forming of antimocrobial peptides with high temporal and spatial resolution. A comparison to the experimental data allows validation and improvement of the computational model.