Virtual DCMIC Seminar Series 2021

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Structure determination of antimicrobial peptides in model membranes and live bacteria

Frances Separovic
School of Chemistry, Bio21 Institute,
University of Melbourne, Australia

Antimicrobial peptides (AMPs) have been extensively studied as promising alternatives to traditional antibiotics. Solid-state NMR has been used to characterise their effect on lipid bilayers, their primary target. Such studies are important to provide high-resolution details within a model system but correlation with *in vivo* situations remains speculative, especially in view of the complex modulation observed with slight changes in conditions such as pH, temperature, lipid composition or peptide concentration. Studying AMPs in live bacteria is, therefore, important but presents several challenges, such as sensitivity and bacterial lifetime. Studies of AMPs in live *E. coli* or *S. aureus* bacteria using solid-state NMR techniques will be presented. The impact of the AMP maculatin 1.1 (Mac1) on bacteria was monitored by ^{31}P while structural details on the peptide were obtained using dynamic nuclear polarization (DNP) enhanced ^{13}C and ^{15}N solid-state NMR experiments. Finally, a novel strategy to perform in-cell DNP NMR experiments was established by using spin-labelled peptides; and $\{^{15}N\}^{13}C$ REDOR measurements have been performed to measure the distance between several pairs of $^{13}C{=}O$ and ^{15}NH within the Mac1 amino acid sequence, which indicate a transmembrane helical structure in bacteria.

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