Poster 5

Conformational Studies by NMR of the Novel Antimicrobial Synthetic Peptide PGAa

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PGAa which was designed with N-terminal sequence template of the antimicrobial peptides from insects, frogs and mammalian families, has an antifungal activity and highly cationic structure. Recently, it has been reported that PGAa has effects Gram-positive(G(+)), Gram-negative(G(-)) bacteria, Candida and another yeast. However, PGAa has more efficiently bactericidal activity to G(+) than G(-). Based on the previous report, we focused on the pathogenic yeast. In result, Candida albicans 28838 showed the highest antifungal activity among many Candida albicans and Candida guilliermondi showed high antifungal activity at 12.5ug/ml. The solution structures of PGAa were determined in 40% trifluoroethanal(TFE)/H2O mixture, dodecylphosphocholine(DPC) micelles as well as aqueous solution by circular dichroism(CD) and nuclear magnetic resonance spectroscopy(NMR spectroscopy). PGAa exists as a random coil in water solution based on far ultravisible(UV)-CD spectroscopy and NMR data. The three-dimension structures of PGAa in TFE and DPC were calculated by simulated annealing protocol with NOE constraints and NH/HD exchange data. PGAa exhibited a long α-helical structure in both TFE and DPC micelle environments. This studies show that the stacking of hydrophobic side chains induces α-helix in the micelle environments. Therefore, we suggest that the α helix formation of PGAa could play a critical role for biological activity.