A-3

Studies of Tertiary Structures of Mastoparan B and Alanine Analogues by NMR Spectroscopy

Kyeunghee Yu, Shin-Won Kang[1], Nam-Gyu Park[2], Yangmee Kim
Department of Chemistry, Konkuk University
[1]Department of Chemistry, Pusan University
[2]Department of Biotechnology and Bioengineering, Pukyong National University

Mastoparan B (MP-B), an antimicrobial cationic tetradecapeptide amide isolated from the venom of the hornet *Vespa basalis*, is an amphiphilic α-helical peptide. In order to study the relationship between the structure and biological activity, we used the three analogues by replacing amino acids with alanine (4LysAla: 4MP-B, 12-LysAla: 12MP-B, 9TrpAla: 9MP-B). Tertiary structures of MP-B and its analogues in TFE/water, micelle, and bicelle environment have been determined by NMR spectroscopy and molecular modeling and indicate that 4MP-B and 12MP-B adopts higher content of amphiphilic α-helix structures than MP-B while 9MP-B has a random structure. NOESY, T1 relaxation data, and fluorescence data indicate that tryptophan residue has close contacts with hydrophobic side chains of phospholipid in the membrane. 9MP-B has less hemolytic activity relative to MP-B. It can be suggested that hydrophobic interactions between MP-B and phospholipid and the appropriate hydrophobicity of peptide to induce α-helical structure are essential for the biological activity of MP-B.