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Poster 4

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

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Mastoparan B (MP-B), an antimicrobial cationic tetradecapeptide amide isolated from the venom of the hornet *Vespa basalis*, is an amphiphilic α-helical peptide. MP-B possess a variety of biological activities such as mast cells degradation histamine release, phospholipase A_2 and C, erythrocyte lysis and binding to carmodulin. In order to study the relationship between the structure and biological activity, we used the three analogues by replacing amino acids with alanine (4Lys→Ala: 4MP-B, 12-Lys→Ala: 12MP-B, 9Trp→Ala: 9MP-B). Tertiary structures of MP-B and its analogues in trifluoroethanol (TFE)-containing aqueous solution 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, T_1 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 -helical structure are essential for the biological activity of MP-B.