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Structure of an Antimicrobial Peptide Buforin II

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The structure of an antimicrobial peptide buforin II has been studied by ^{1}H NMR and CD spectroscopy. Buforin II is flexible and random structure in H_2O but the parts of buforin II become helical structure in trifluoroethanol (TFE)/H_2O (1:1, v/v) solution. From the restrained molecular dynamics calculation using NMR data, we obtained the possible conformation of buforin II in TFE/H_2O solution. The calculated structure contains an α-helix in Val-12 to Arg-20 segment and irregular helix in Pro-11 to Gly-7 segment. These helical region shows amphiphilicity. The possible conformation of this antimicrobial peptide in amphiphiilic environment is discussed.