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[研究简报]

影响多肽与花粉钙调素亲和性的因素
——多肽的圆二色性及核磁共振研究

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The Factors Influencing the Peptide Affinity for Pollen Calmodulin
—— Peptide Conformation Study by CD and 2D-NMR

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Abstract　Synthetic buckwheat pollen peptide BPP-1 (A-P-V-L-Q-I-K-K-T-G-S-N) and its analogues BPP-2[(*D*)A-P-V-L-Q-I-K-K-T-G-S-N-NH_2], BPP-3 (A-P-A-L-Q-L-K-K-N-G-S-Q-G-NH_2) showed different binding behavior to rape-pollen calmodulin (pCaM). Fluorescence titration experiments demonstrated that BPP-1 had no affinity for pCaM while its C-terminal amide, BPP-2, had fair affinity for pCaM (dissociation constant of pCaM-peptide complex, $K_d = 2.9 \times 10^{-1}$ μmol/L) due to the decrease in C-terminal polarity. But compared with BPP-3 ($K_d = 8.1 \times 10^{-2}$ μmol/L), which was also a peptide amide, BPP-2 had a much lower binding ability. In order to investigate other factors influencing peptide affinity for pCaM besides polarity (or hydrophobicity), CD and 2D-NMR spectroscopes were used to study the conformations of BPP-1 and BPP-3. It revealed that molecular flexibility could affect peptide's ability to bind pCaM. BPP-1 displayed rigid extended peptide bonds in the middle region where the basic amino acid pair Lys^7-Lys^8 is located, flanked by flexible peptide segments on both terminals; while the middle five-residue region of BPP-3 exhibited as very flexible segment. Such a structural character might facilitate BPP-3 to adopt a conformation contributive to the interaction of two Lys residues with the acidic residues of pCaM in its peptide-binding site and resulted in higher affinity. As this study revealed, both of the two peptides showed the lack of ordered structure in the aqueous solution. It seemed that there was no relationship between peptide affinity for CaM and the propensity of peptide chain to form α-helix. This contradicted what most previous researches approved that α-helix was an important character of peptide with high affinity for CaM.

Keywords　Peptide; Affinity; Flexibility; 2D-NMR; CD

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