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Preferred Conformations of Cyclic Ac-Cys-Pro-Xaa-Cys-NHMe Peptides: a Model for Chain Reversal and Active Site of Disulfide Oxidoreductase

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The conformational study on cyclic Ac-Cys-Pro-Xaa-Cys-NHMe (Ac-CPXC-NHMe; X = Ala, Val, Leu, Aib, Gly, His, Phe, Tyr, Asn, and Ser) peptides has been carried out using the ECEPP/3 force field and the hydration shell model in the unhydrated and hydrated states. This work has been undertaken to investigate structural implications of the CPXC sequence as the chain reversal for the initiation of protein folding and as the motif for active site of disulfide oxidoreductases. The backbone conformation DAAA is in common the most feasible for cyclic CPXC peptides in the hydrated state, which has a type I β-turn at the Pro-Xaa sequence. The proline residue and the hydrogen bond between backbones of two cystines appear to play a role in stabilizing this preferred conformation of cyclic CPXC peptides. However, the distributions of backbone conformations and β-turns may indicate that the cyclic CPXC peptide seems to exist as an ensemble of β-turns and coiled conformations. The intrinsic stability of the cyclic CPXC motif itself for the active conformation appears to play a role in determining electrochemical properties of disulfide oxidoreductases.