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Design of β-turn II peptides using α,β-dehydro-amino acids: synthesis and solution conformation of ΔPhe containing peptides Boc-Gly-ΔPhe-Val-OCH_3 (I) and Boc-Phe-ΔPhe-Phe-OCH_3 (II)

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To provide a detailed comparison of conformations of ΔPhe containing peptides in chloroform ($CDCl_3$) and dimethylsulfoxide ($(CD_3)_2SO$) the peptides Boc-Gly- ΔPhe-Val-OCH_3 (I) and Boc-Phe- ΔPhe-Phe-OCH_3 (II) were synthesized in solution phase by the azlactone method. The conformation investigation was carried out using NMR spectroscopy and the deductions were based on intramolecularly hydrogen-bonded NH groups and Nuclear Overhauser Effect (NOE) studies. Temperature and solvent dependence studies were performed in $(CD_3)_2SO$ and $CDCl_3$-$(CD_3)_2SO$ mixtures. The results of these investigations indicated that the peptides (I) and (II) adopt similar conformations. Furthermore, the conformations were found to be very similar in both solvents. The results also confirmed that the ΔPhe at (i+2) position induces constrains which favor the formation of a β-turn II conformation. The NMR results in solution showed a good agreement with the conformations of ΔPhe containing peptides as observed in the crystalline state. These results highlight the significance of Δ-residue based steric factors in deciding the conformational properties of Δ-residue containing peptides.