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Conformation-Specific Infrared and Ultraviolet Spectroscopy of Cold [YAPAA+H]$^+$ and [YGPAA+H]$^+$ Ions[1] ANDREW DEBLASE, CHRISTOPHER HARRILAL, JOHN LAWLER, NICOLE BURKE[2], SCOTT MCLUCKEY, ZWIER TIMOTHY, Purdue Univ — Incorporation of the unnatural D-proline stereoisomer into a peptide sequence is a typical strategy to synthesize model β-hairpin loops. Using conformation-specific IR and UV spectroscopy of cold ($\approx$ 10 K) gas-phase ions, we unravel the inherent conformational preferences of the ^{D}P and ^{L}P diastereomers in the protonated peptide [YAPAA+H]$^+$ because only intramolecular interactions are possible in this isolated regime. Consistent with the solution phase studies, one of the conformers of [YA^{D}PAA+H]$^+$ is folded into a β-hairpin turn. However, a second predominant γ-turn conformer family is identified. The [YA^{L}PAA+H]$^+$ stereoisomer discourages β-hairpin formation. We show that the *trans* (^{D}P)$\rightarrow$*cis* (^{L}P) isomerization is sterically driven and can be reversed by substituting [YG^{L}PAA+H]$^+$ for [YA^{L}PAA+H]$^+$. Therefore, we provide a basis for understanding residue-specific alterations in the potential energy surface and reveal new insights into the origin of β-hairpin formation from the bottom-up.

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