The peptides Ac-Trp-Tyr-NH₂ and Ac-Trp-Tyr-Ser-NH₂, which form the N-terminal region of a folding nucleus in β-lactoglobulin, were studied in the gas phase using IR/UV double resonance spectroscopy and initial results were presented at a previous symposium. Molecular dynamics (AMBER 99/99SB, CHARMM 27) and ab initio calculations (RI-B97-D/TZVPP, pbe GGA/cc-PVDZ) resulted in an improved interpretation of the spectra and assignments for the observed conformers. Results are compared to similar molecules such as Ac-Trp-NH₂ and Ac-Phe-Phe-NH₂.

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