INTERPRETATION OF THE IR/UV SPECTRA OF Ac-Trp-Tyr-NH_2 and Ac-Trp-Tyr-Ser-NH_2 USING MOLECULAR DYNAMICS AND AB INITIO METHODS.[a]

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The peptides Ac-Trp-Tyr-NH_2 and Ac-Trp-Tyr-Ser-NH_2, 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.[b] 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-NH_2 and Ac-Phe-Phe-NH_2.

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[b]J.A. Thomas, D.W. Pratt, E. Gloaguen, B. Tardivel, F. Piuzzi, and M. Mons 63^{rd} International Symposium on Molecular Spectroscopy, FB11, 2008.