Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Single-Conformation Spectroscopy of Cold, Protonated ^{D}PG-containing peptides: Switching β-turn Types and Formation of a sequential Type II/II' Double β-turn

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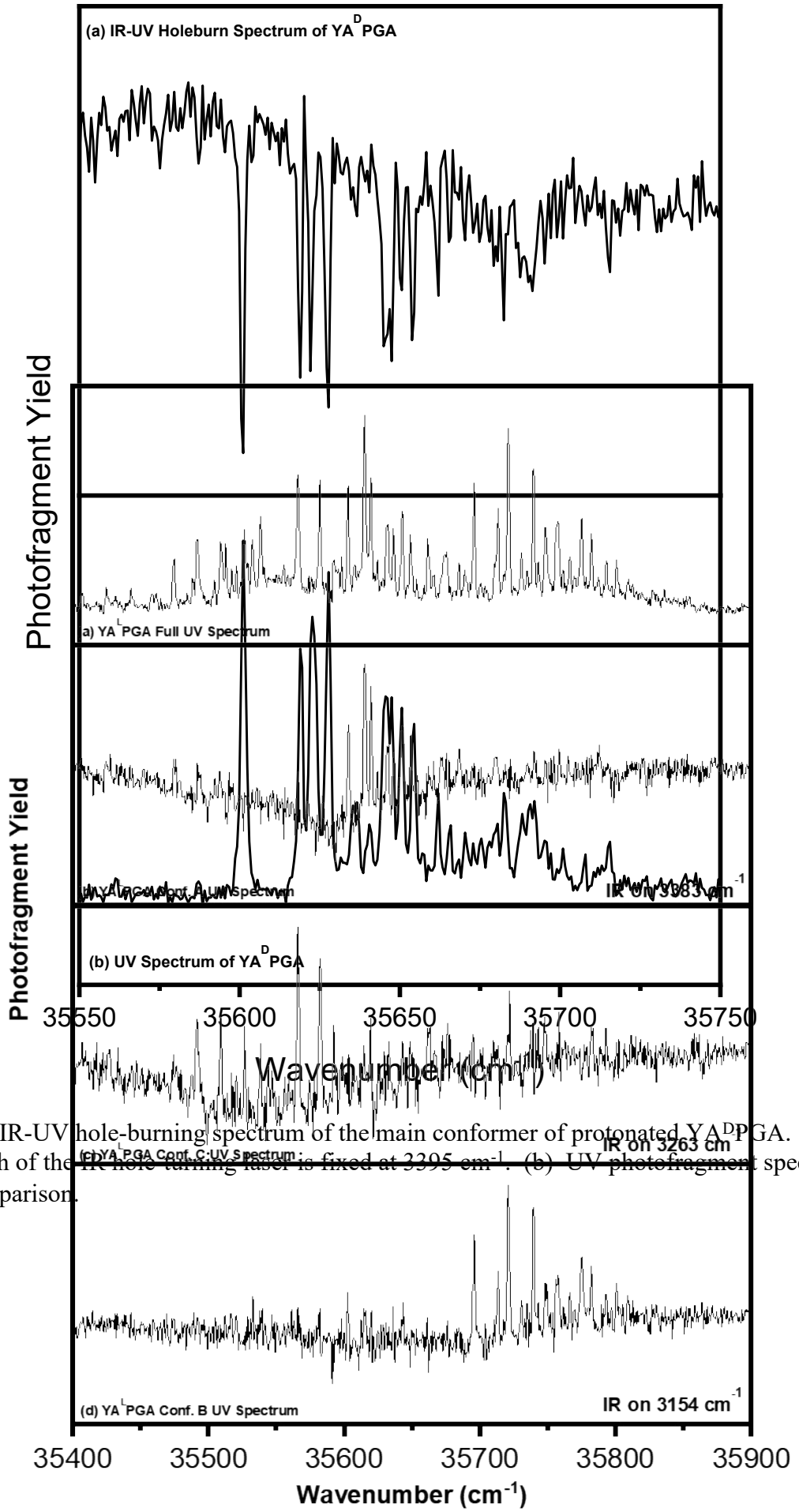

Figure S1. (a) IR-UV hole-burning spectrum of the main conformer of protonated YA^{D}PGA. The wavelength of the IR hole-burning laser is fixed at 3395 cm^{-1}. (b) UV photofragment spectrum shown for comparison.

Figure S2. (a) UV photofragment spectrum of protonated $YA^{L}PGA$. IR-UV hole-burning spectra of conformers (b) A, (c) B, and (d) C, with IR hole-burn laser fixed at the indicated wavenumber position. These spectra prove that there are three unique conformers of $[YA^{L}PGA+H]^{+}$.

Type II, $A^{D}P$	0.00	0.00
Type II' ^{D}PX	14.3	0.54

Table S1. Zero-point corrected relative energies (ΔE_0) for the secondary structural motifs of each molecule.

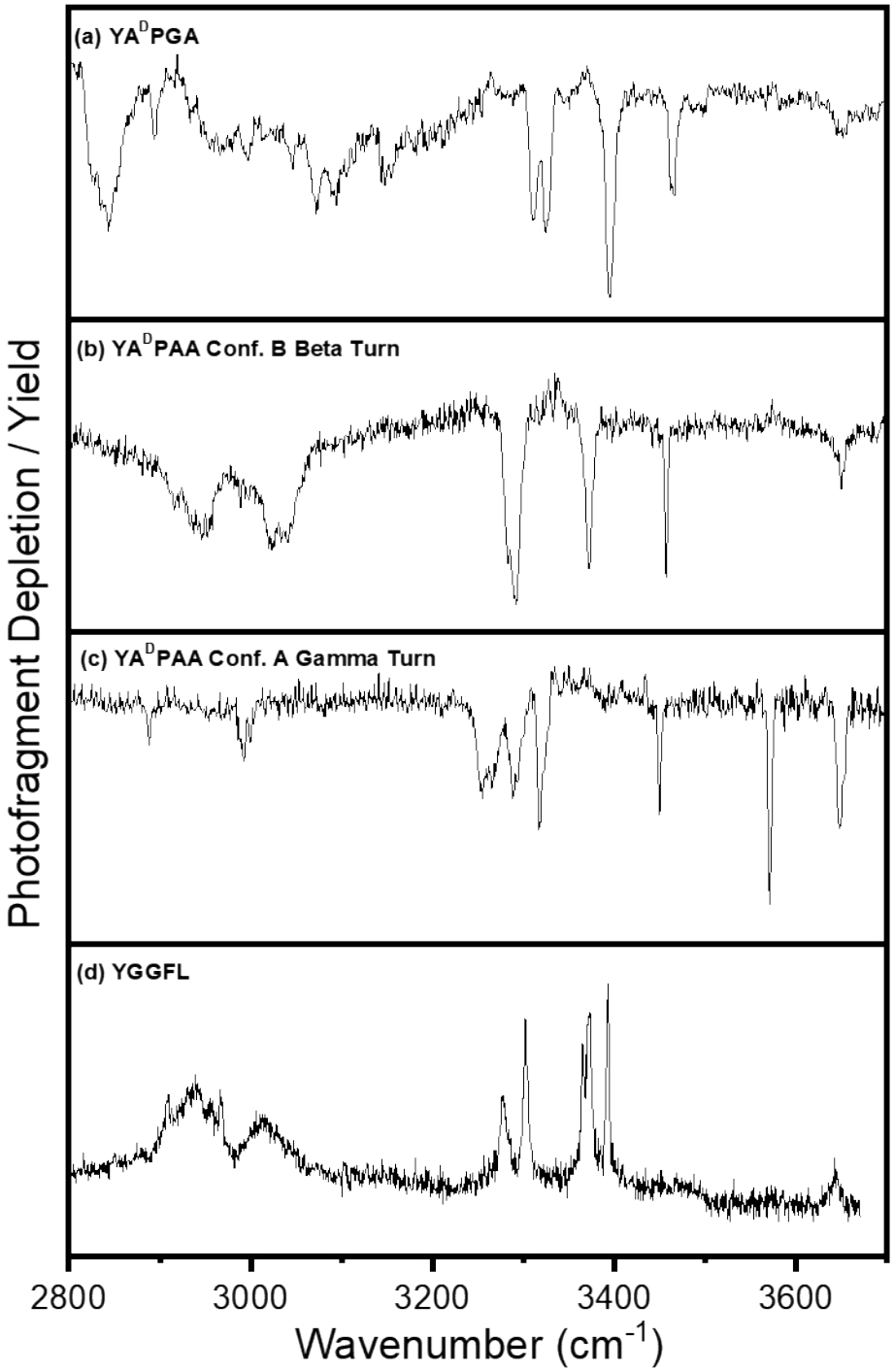

Figure S3. Comparison of the infrared spectra of various turn types.

Conformation specific infrared spectra of (a) the Type II β-turn found in YA^{D}PGA, (b) the Type II' β-turn found in Conformer B of YA^{D}PAA (c) the double γ-turn found in Conformer A of YA^{D}PAA and (d) the Type II' β-turn found in YGGFL. In all cases, the peptides are protonated at the N-terminus.

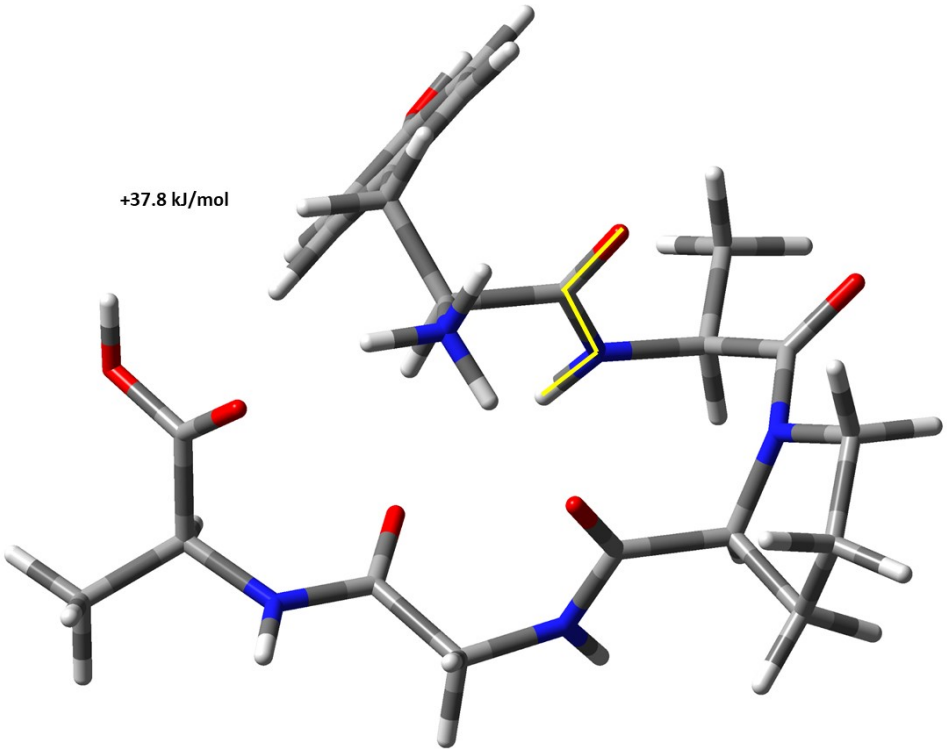

Figure S4. YA^{L}PGA conformer B with trans amide bond

Optimized calculated structure of conformer B of [YA^{L}PGA + H]$^{+}$ with a trans amide bond (yellow lines) between Y_1 and A_2 instead of the cis amide bond in the assigned structure.

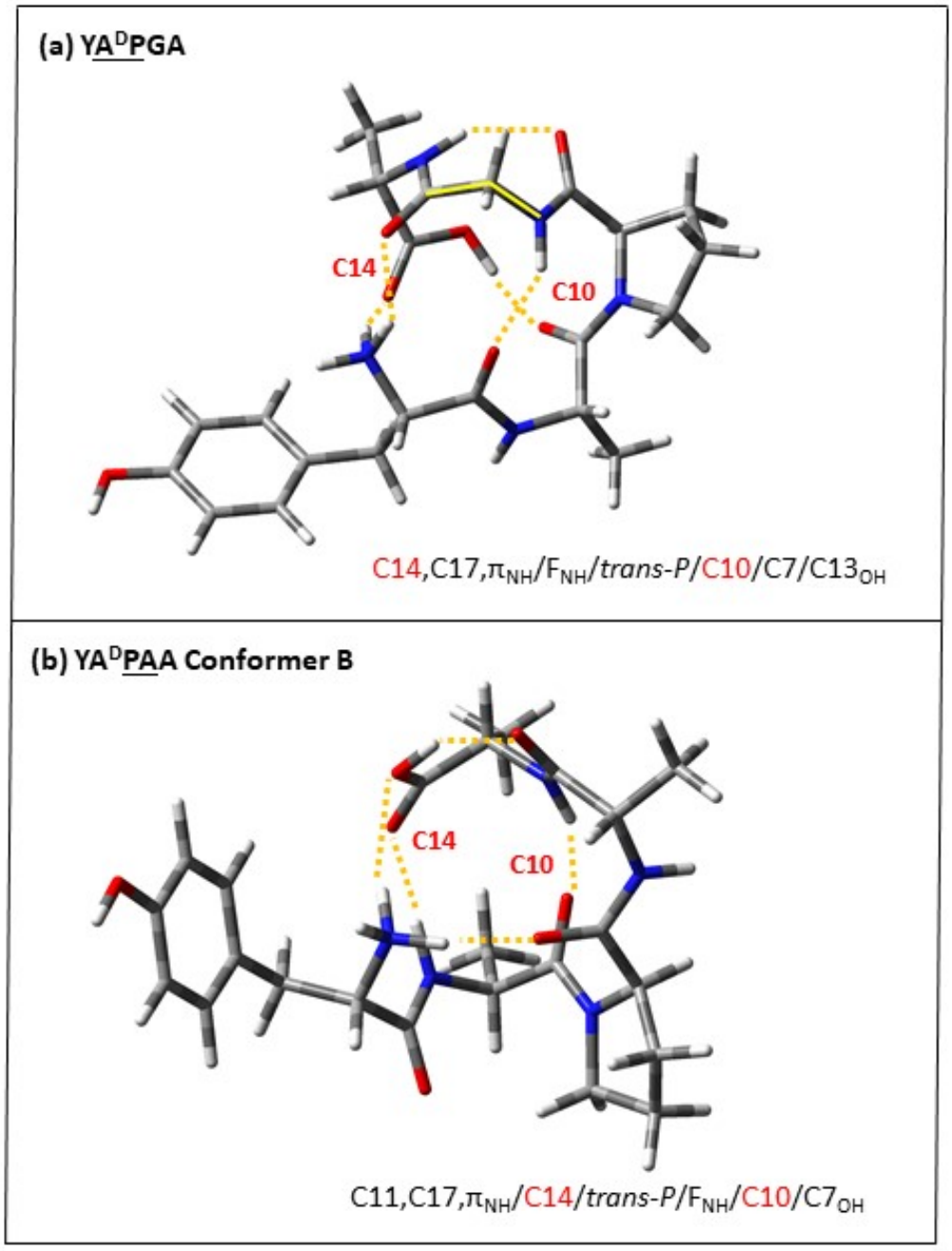

Figure S5. Comparison of the β-turns formed by (a) YA^{D}PGA and (b) Conformer B of YA^{D}PAA. The underlined region denotes the location of the turn. Short-hand notation describing the hydrogen bonding pattern of both molecules is shown with the β-turn forming hydrogen bonds labelled in red.