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

How Change in Chirality Prevents β-Amyloid Type Interaction in a Protonated Cyclic Dipeptide Dimer

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Supplementary Information

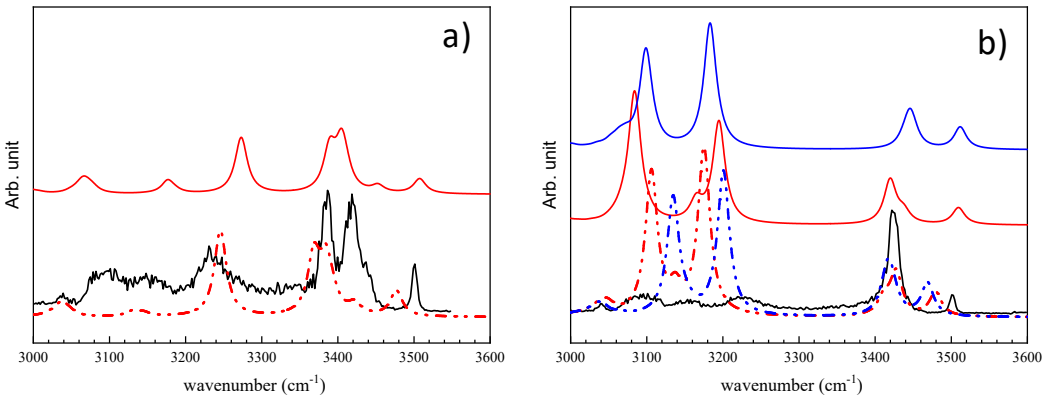

Figure S1: comparison between the IR absorption spectra simulated at the ri-b97-d-D3BJ/def2-TZVPPD (full lines) and the B3LYPD3BJ/6-311++G(d,p) levels of theory (dotted lines) in the hydride stretch region. a) c-$(LD)_2H^+$ Experimental spectrum (black line) Simulated spectra of π-$(c\text{-}LD)_2H^+$ (red line) b) c-$(LL)_2H^+$ Experimental spectrum (black line) Simulated spectra of π-$(c\text{-}LL)_2H^+$ (red line) and τ-$(c\text{-}LL)_2H^+$ (blue line)

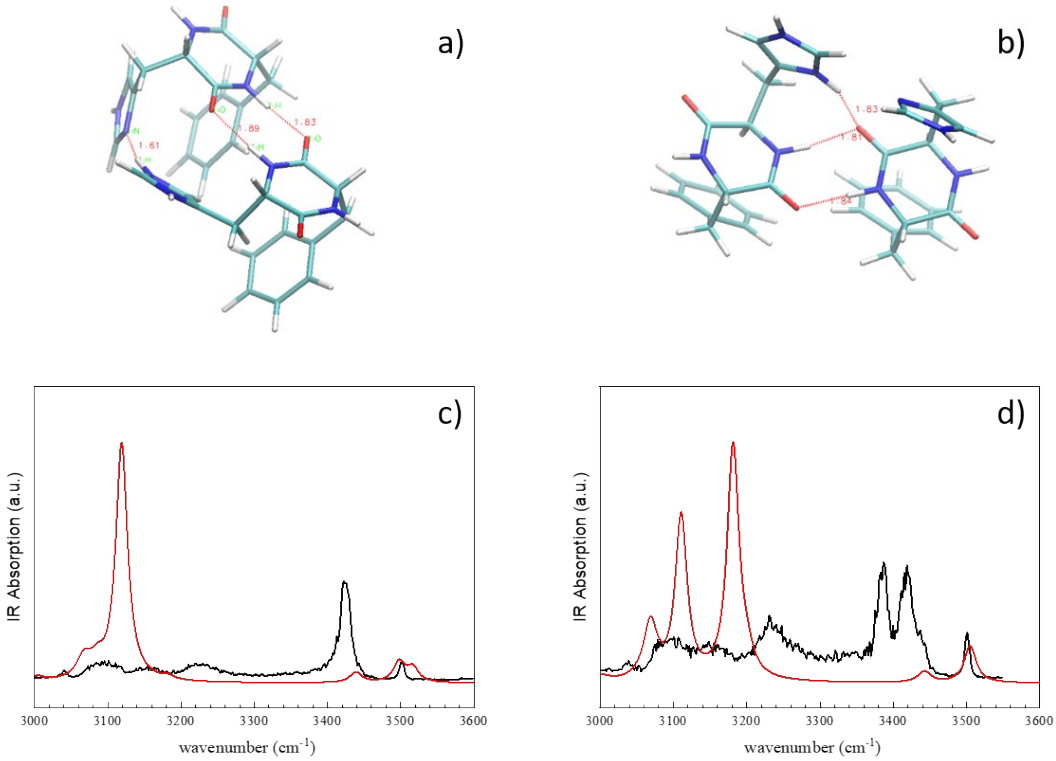

Figure S2: Most stable structures of the protonated dimers a) $(c\text{-}LD)_2H^+$ and b) $(c\text{-}LL)_2H^+$ calculated at the ri-b97-d-D3BJ/def2-TZVPPD level of theory in a solvent continuum. Simulated IR absorption spectra for c) the most sable $(c\text{-}LD)_2H^+$ structure and d) the most stable $(c\text{-}LL)_2H^+$ structure. The frequencies are scaled by 0.978.

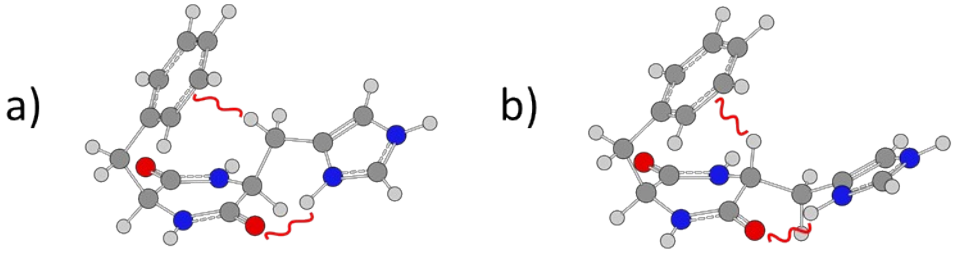

Figure S3: Most stable structures of the protonated monomer a) (c-LL)H^+ and b) (c-LD)H^+ calculated at the B3LYP-D3/6311++G(d,p) level of theory.