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)$_2$H$^+$ Experimental spectrum (black line) Simulated spectra of $\pi$-(c-LD)$_2$H$^+$ (red line) b) c-(LL)$_2$H$^+$ Experimental spectrum (black line) Simulated spectra of $\pi$-(c-LL)$_2$H$^+$ (red line) and $\tau$-(c-LL)$_2$H$^+$ (blue line)
**Figure S2**: Most stable structures of the protonated dimers a) (c-LD)$_2$H$^+$ and b) (c-LL)$_2$H$^+$ calculated at the ri-b97-d-D3BJ/def2-TZVPPD level of theory in a solvent continuum. Simulated IR absorption spectra for c) the most stable (c-LD)$_2$H$^+$ structure and d) the most stable (c-LL)$_2$H$^+$ 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.