

**Characterization of β -turns by electronic circular dichroism spectroscopy:
A coupled molecular dynamics and time-dependent density functional theory
computational study**

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Supplementary information file

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Figure S1. Dihedral angles (in $^{\circ}$) distributions (in %) for Ace-A-A-NHMe in type I β -turn conformation.

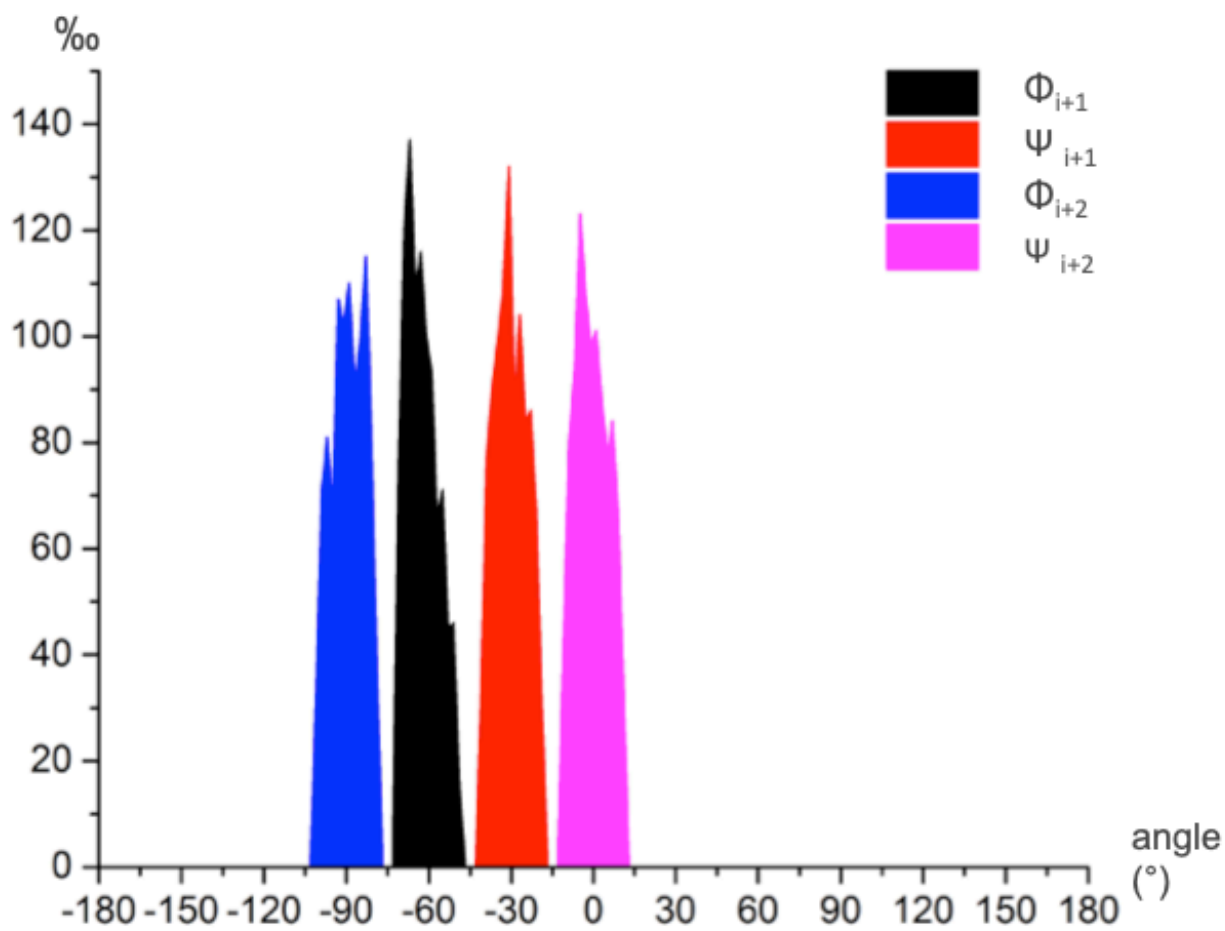


Figure S2. Dihedral angles (in °) distributions (in %) for Ace-A-A-NHMe in type I' β -turn conformation.

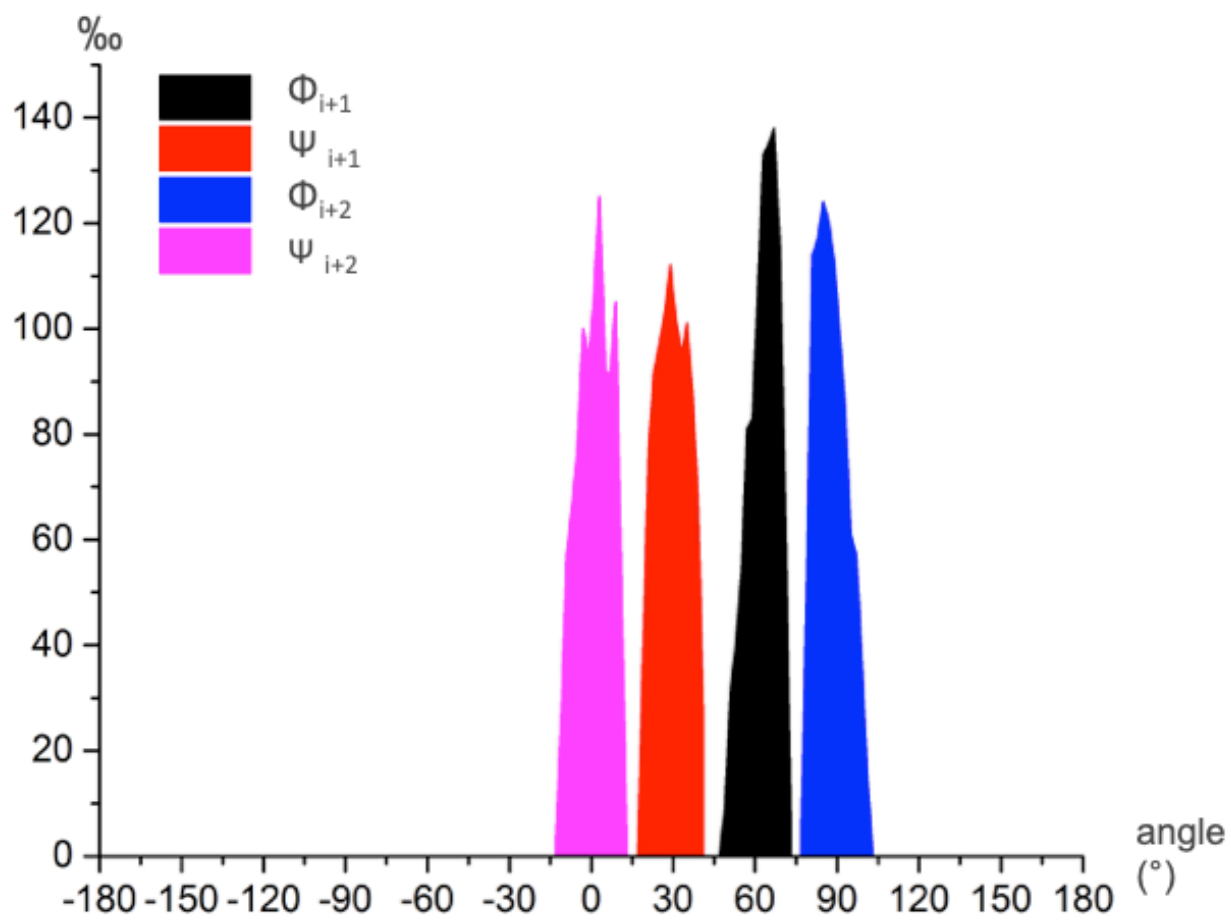


Figure S3. Dihedral angles (in $^{\circ}$) distributions (in %) for Ace-A-A-NHMe in type II β -turn conformation.

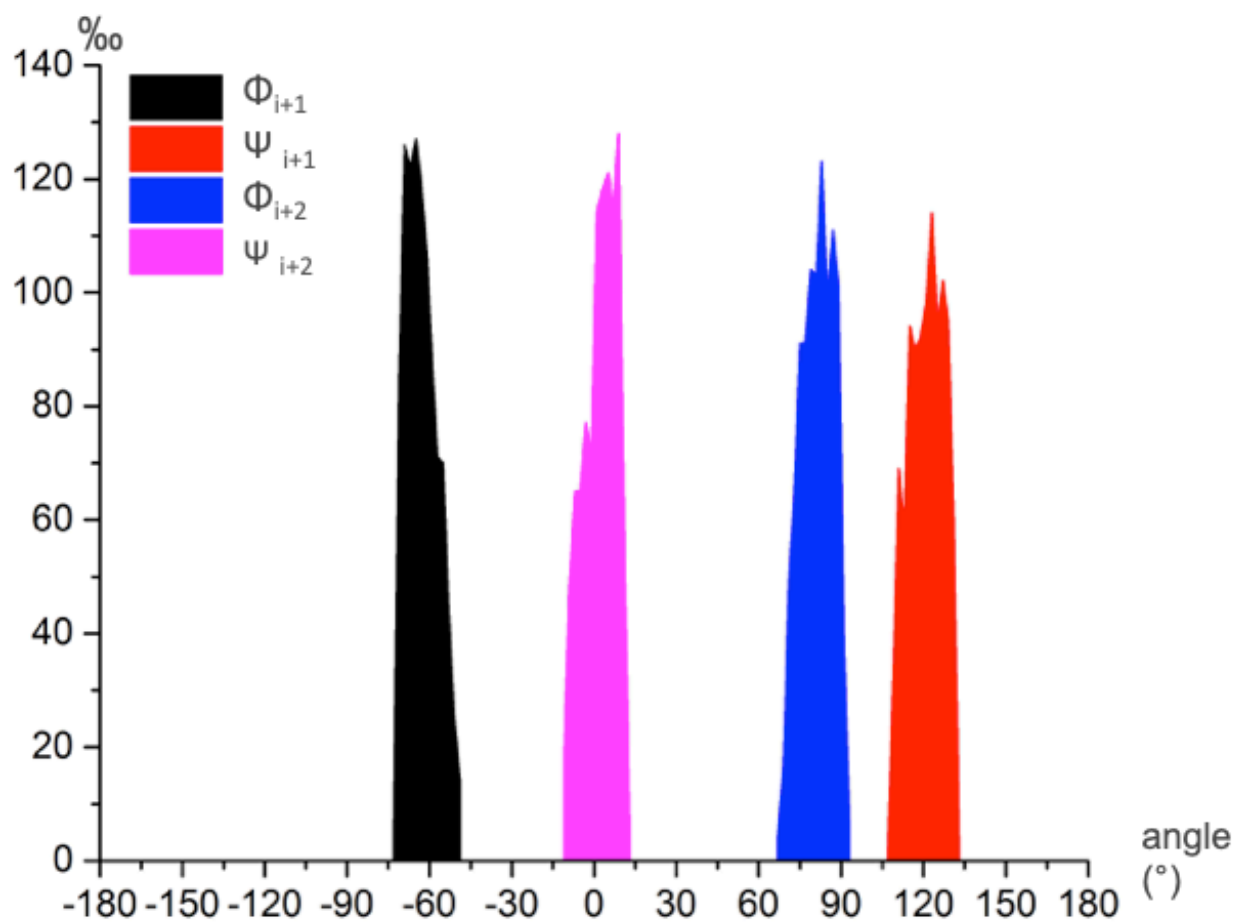


Figure S4. Dihedral angles (in $^{\circ}$) distributions (in %) for Ace-A-A-NHMe in type II' β -turn conformation.

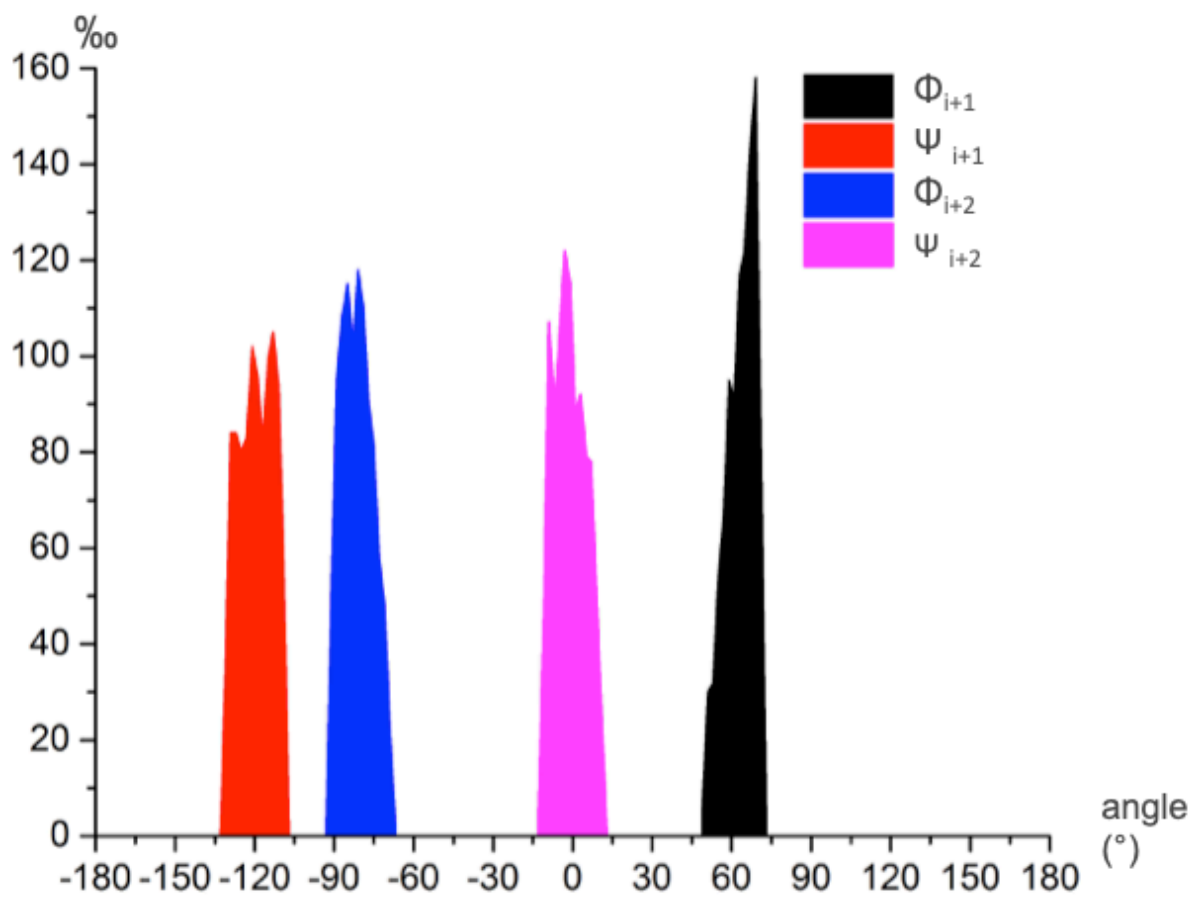


Figure S5. Dihedral angles (in $^{\circ}$) distributions (in %) for Ace-K-A-NHMe in type I β -turn conformation with only one Cl^- as counteranion (in black) and in a 150 mM NaCl solution (in red).

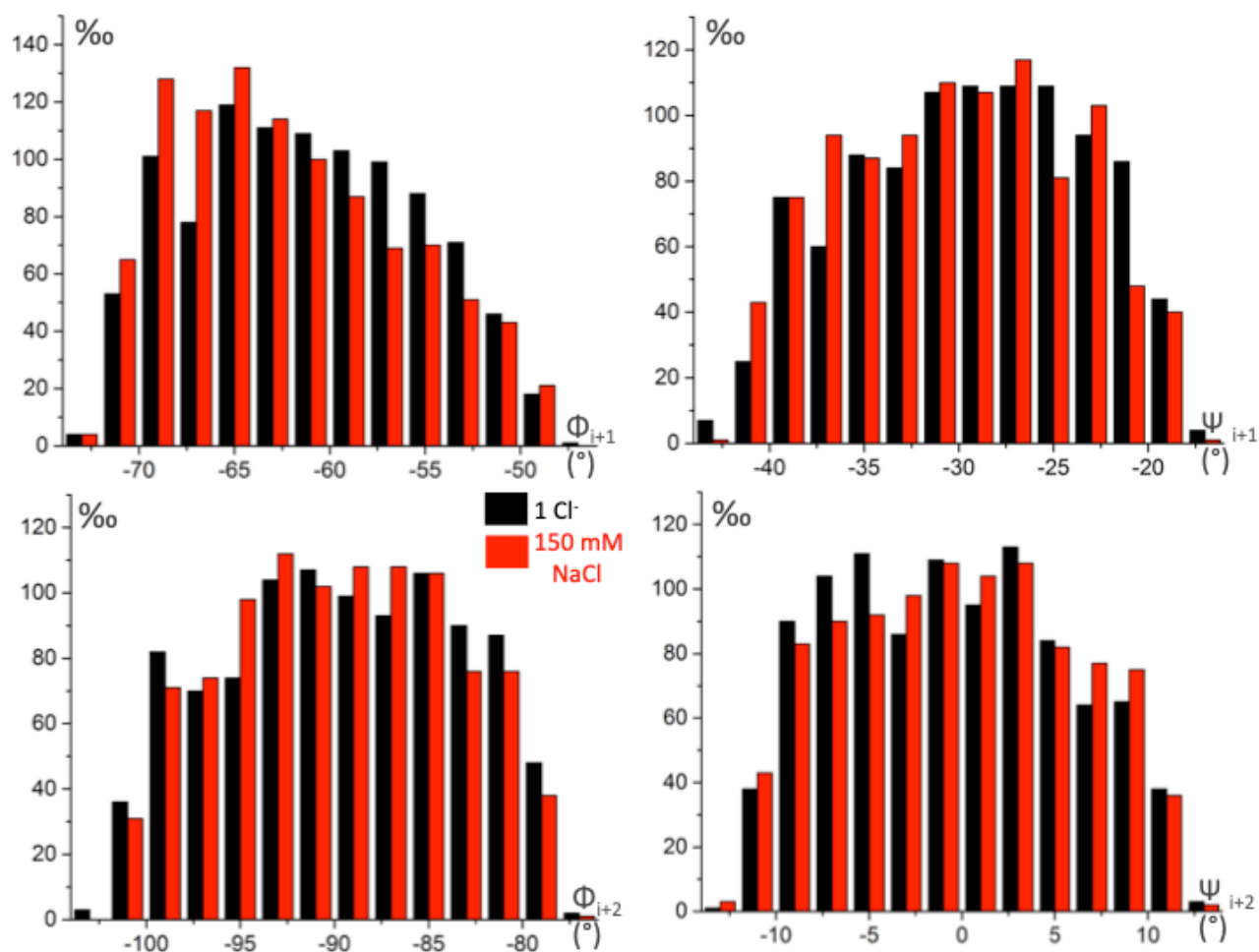


Figure S6. Averaged absorption spectra for Ace-A-A-NHMe for the four β -turns types considered here.

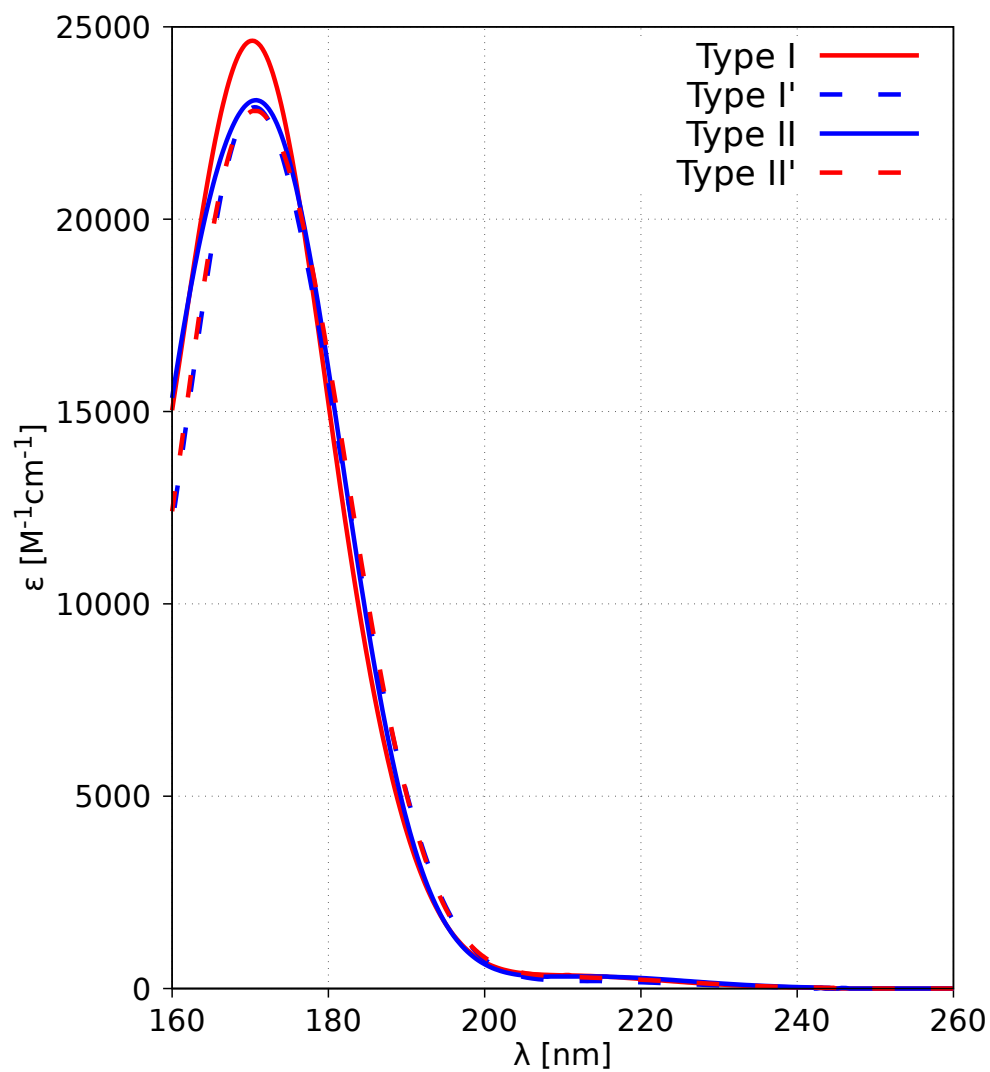


Figure S7. Distributions (in %) for the intensity ratio between the negative and positive ECD bands, κ (see eq. 5 in the paper) for the four considered β -turn types.

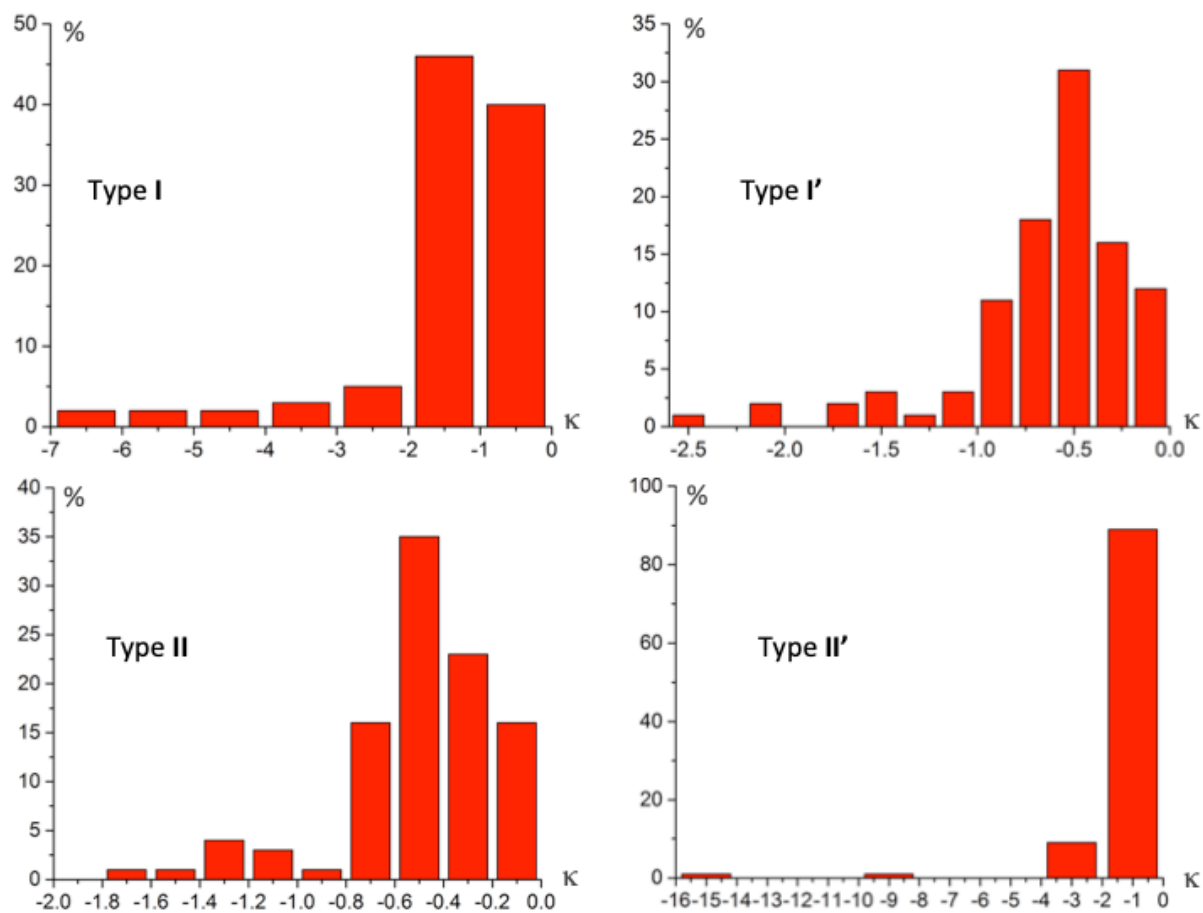


Figure S8. Distributions (in %) for the wavelength difference between the negative and positive ECD bands, $\Delta\lambda$ (in nm, see eq. 4 in the paper) for the four considered β -turn types.

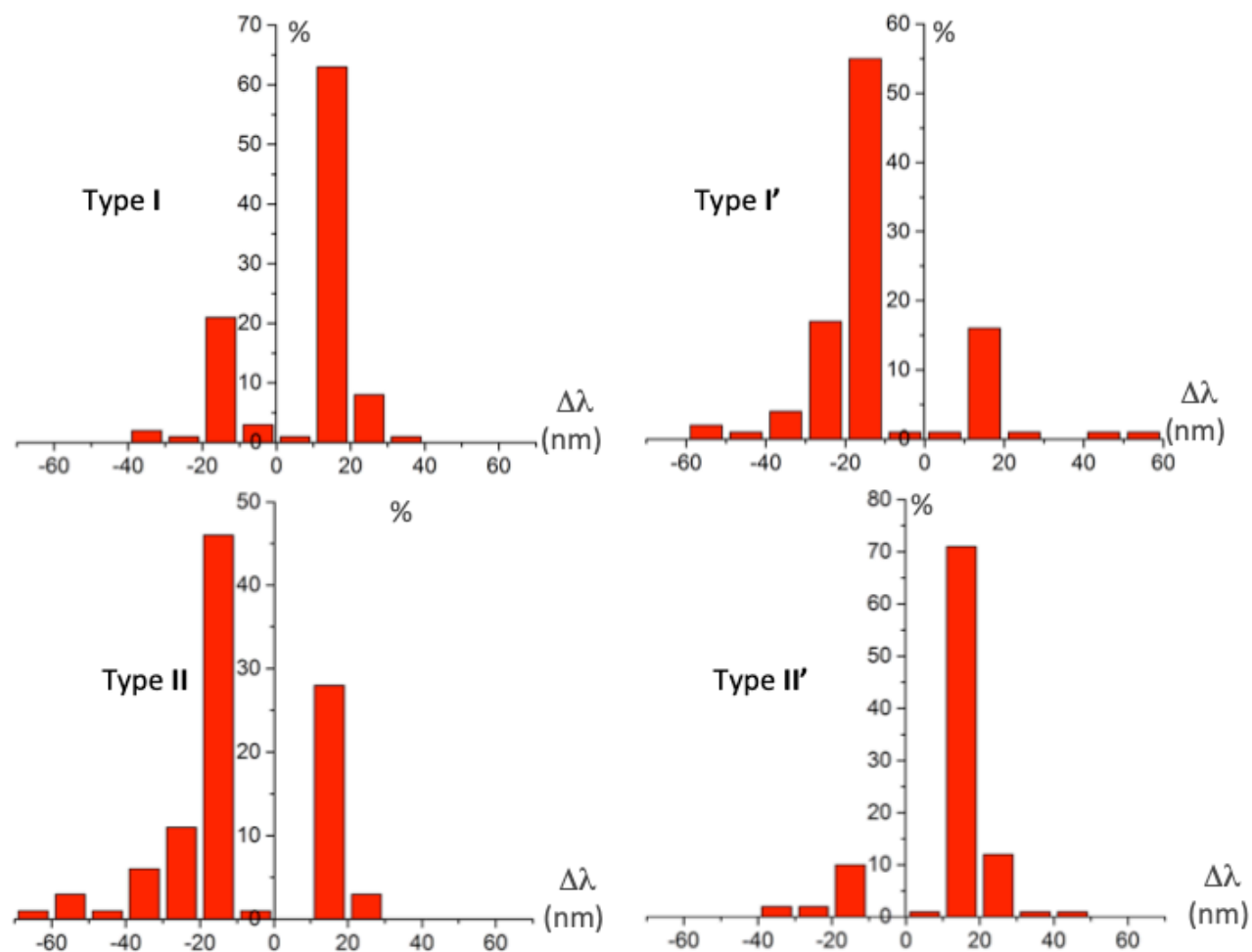


Figure S9. Comparison of averaged ECD spectra for the minimal model Ace-A-A-NHMe for the β -I turn conformation obtained from a restrained MD simulation (with allowed deviations of $\pm 10^\circ$ around the canonical Φ_{i+1} , Ψ_{i+1} , Φ_{i+2} and Ψ_{i+2} dihedral angles) using either the OPLS-AA or the CHARMM27 force fields.

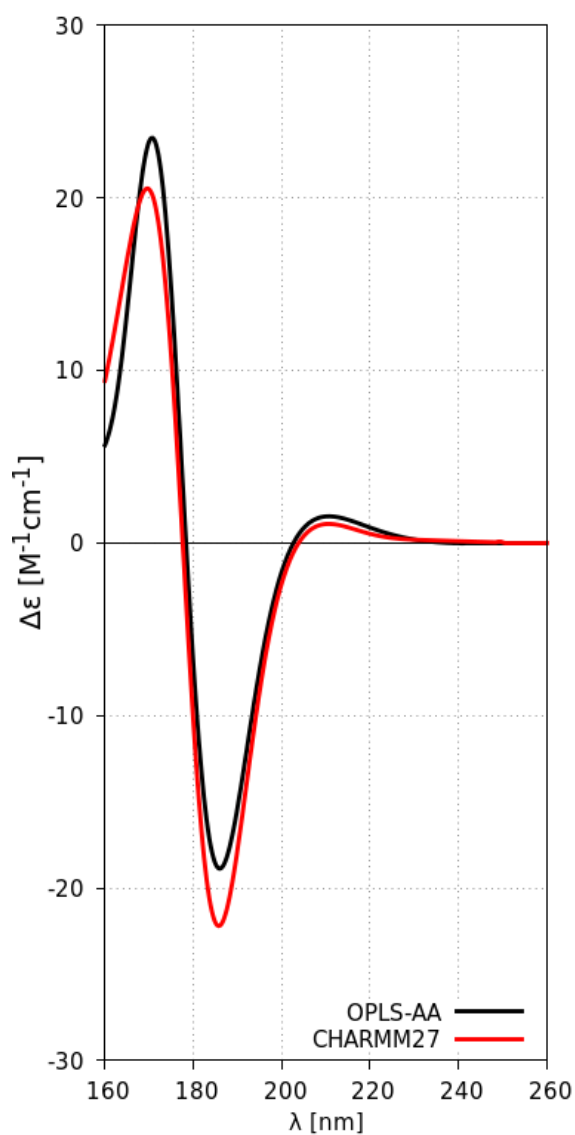


Figure S10. Averaged ECD spectra for β -turn type I computed with (using the RESPONSE module) and without (using the PROPERTIES module) the PE-EEF extension.

