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

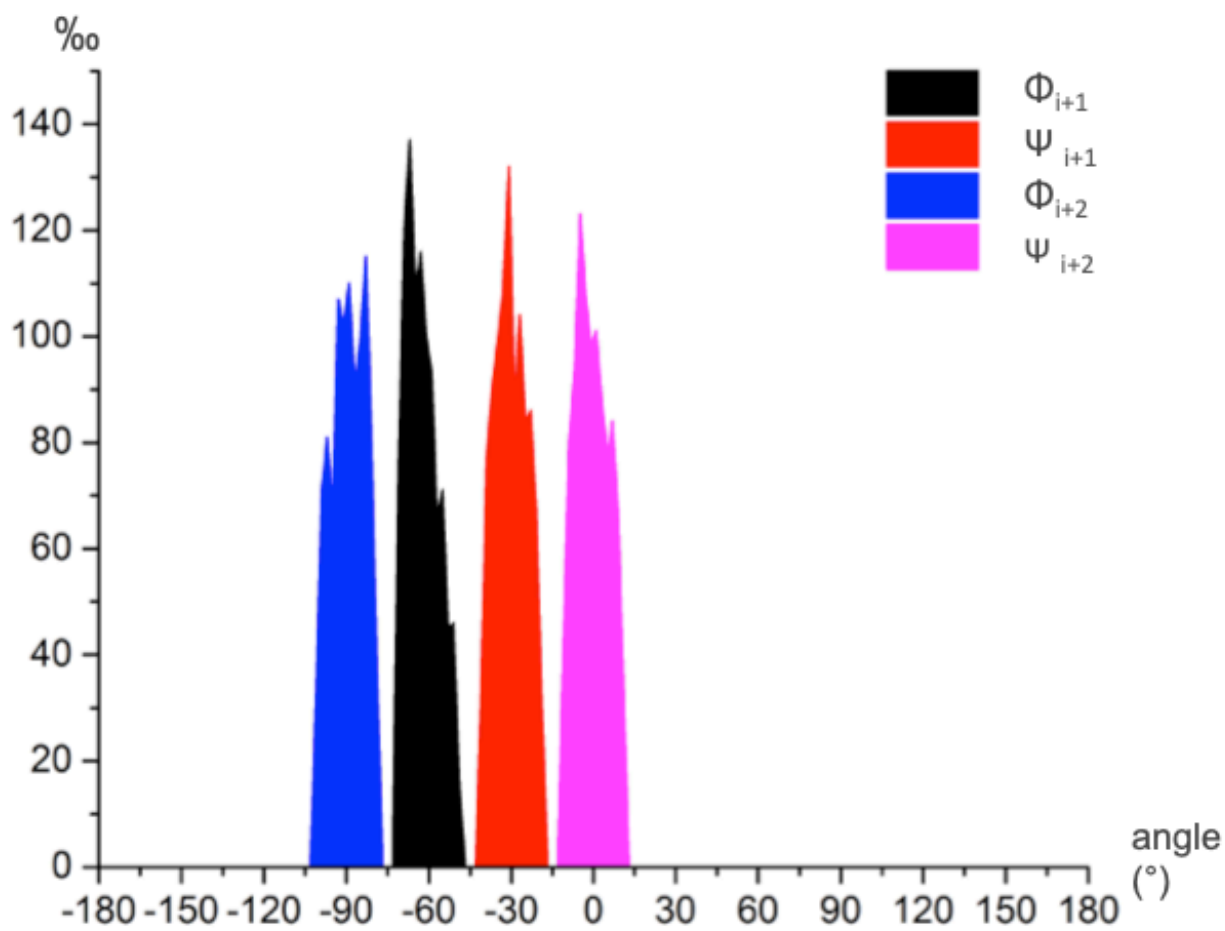**Figure S3**. Dihedral angles (in °) distributions (in ‰) for Ace-A-A-NHMe in type II β-turn conformation.

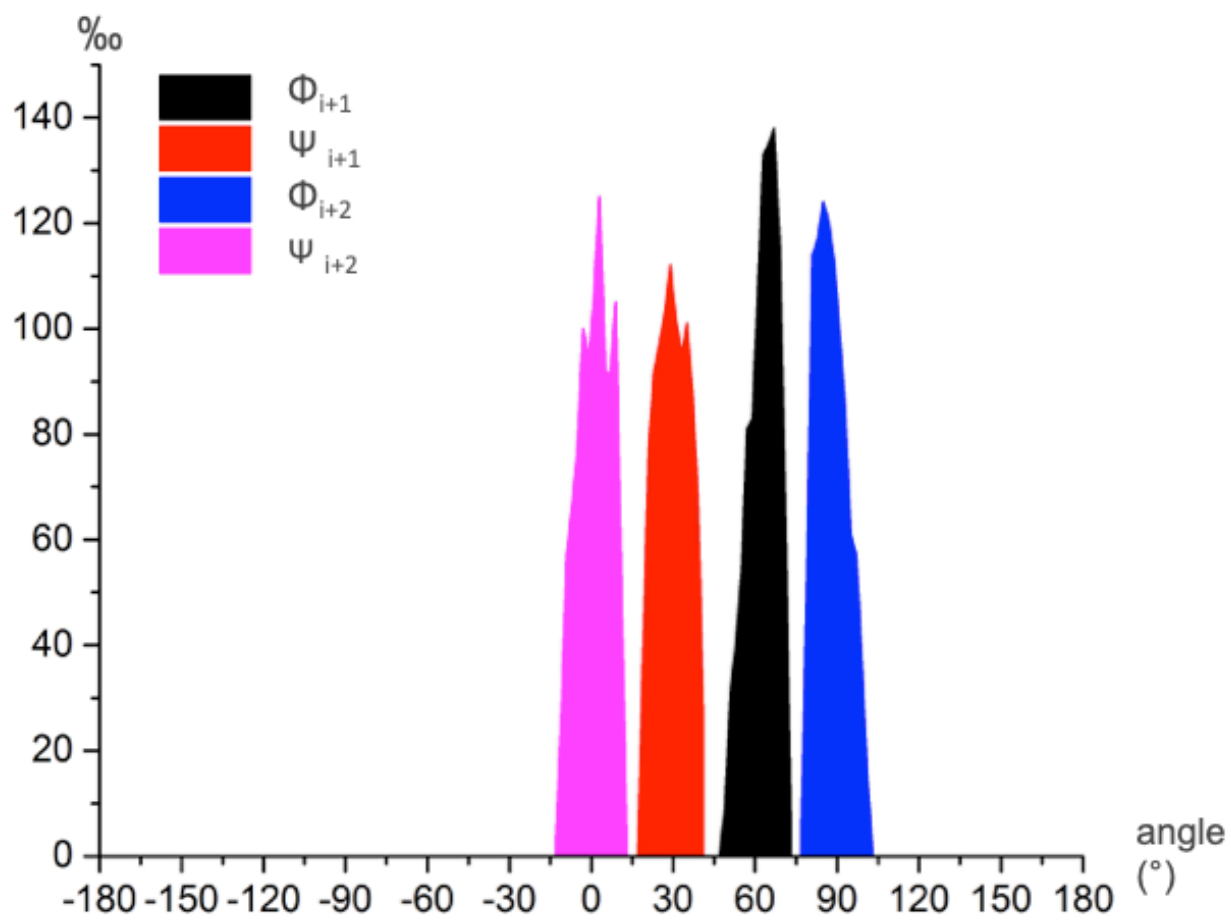**Figure S4**. Dihedral angles (in °) distributions (in ‰) for Ace-A-A-NHMe in type II' β-turn conformation.

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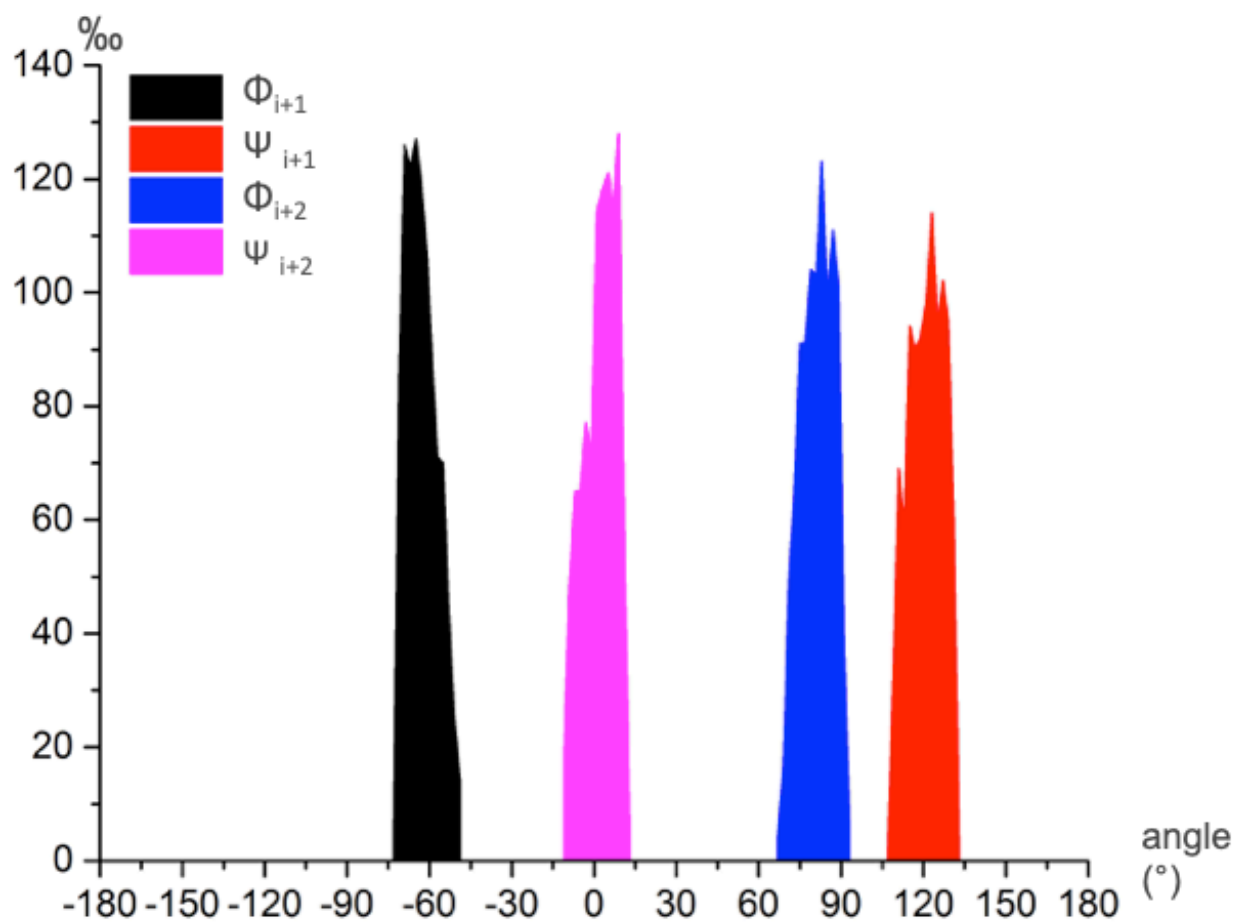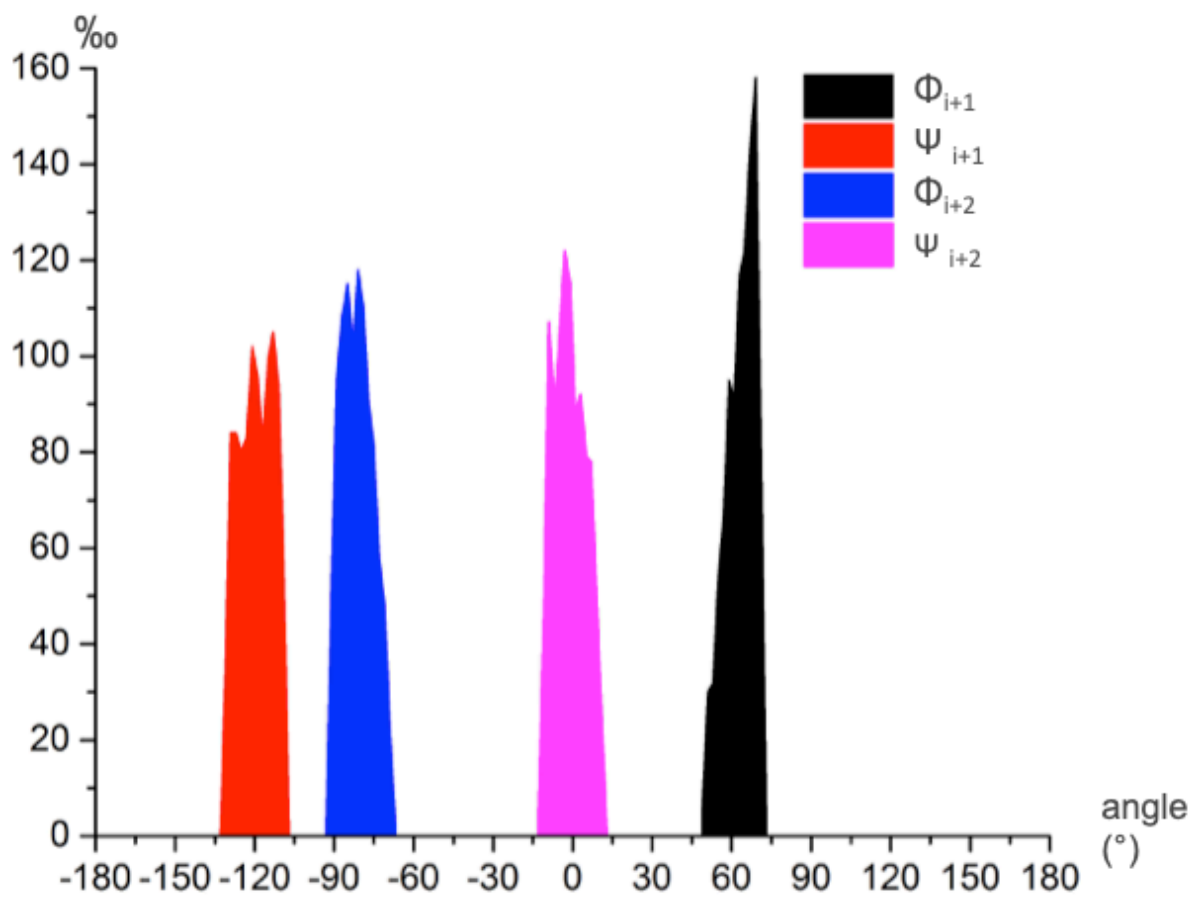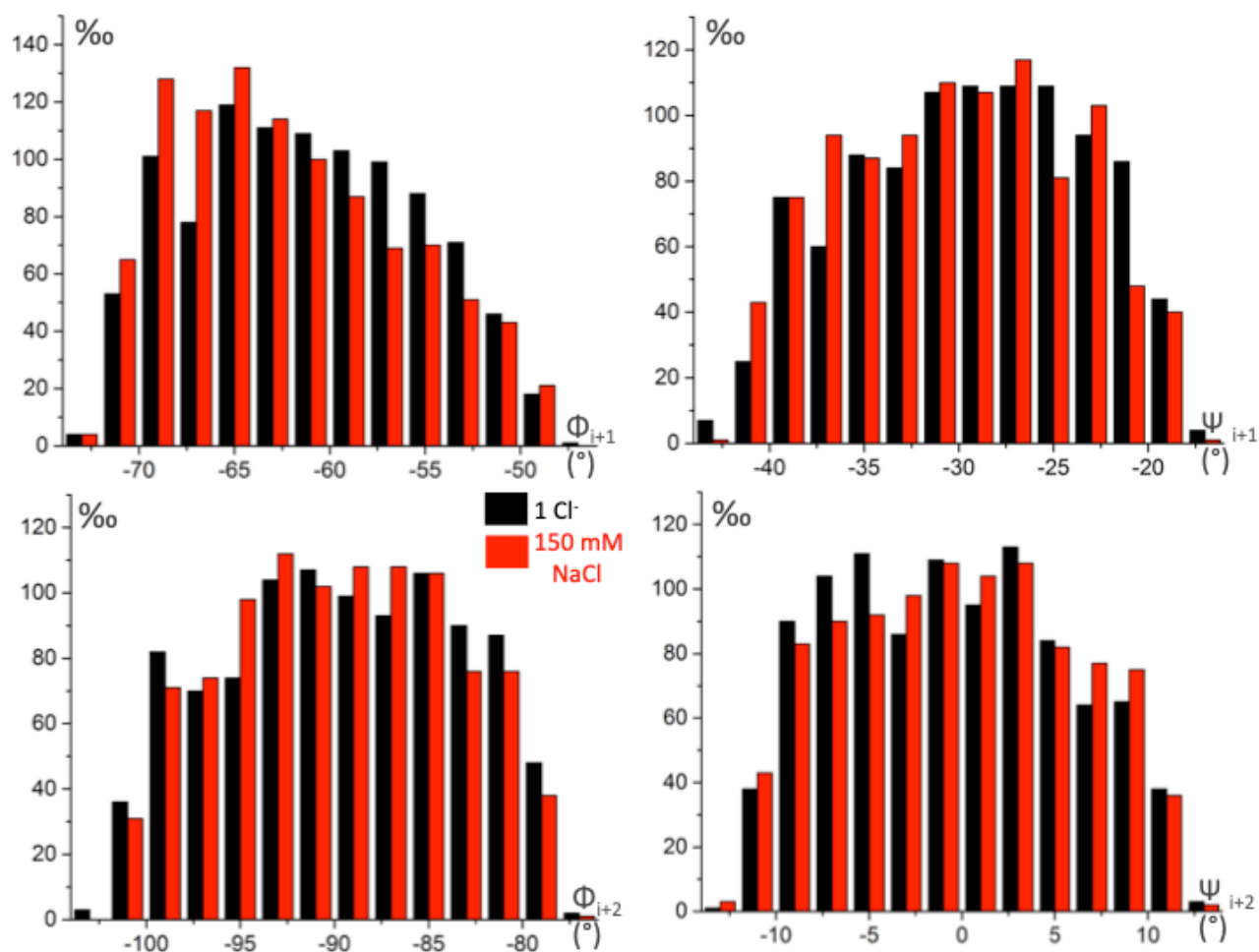
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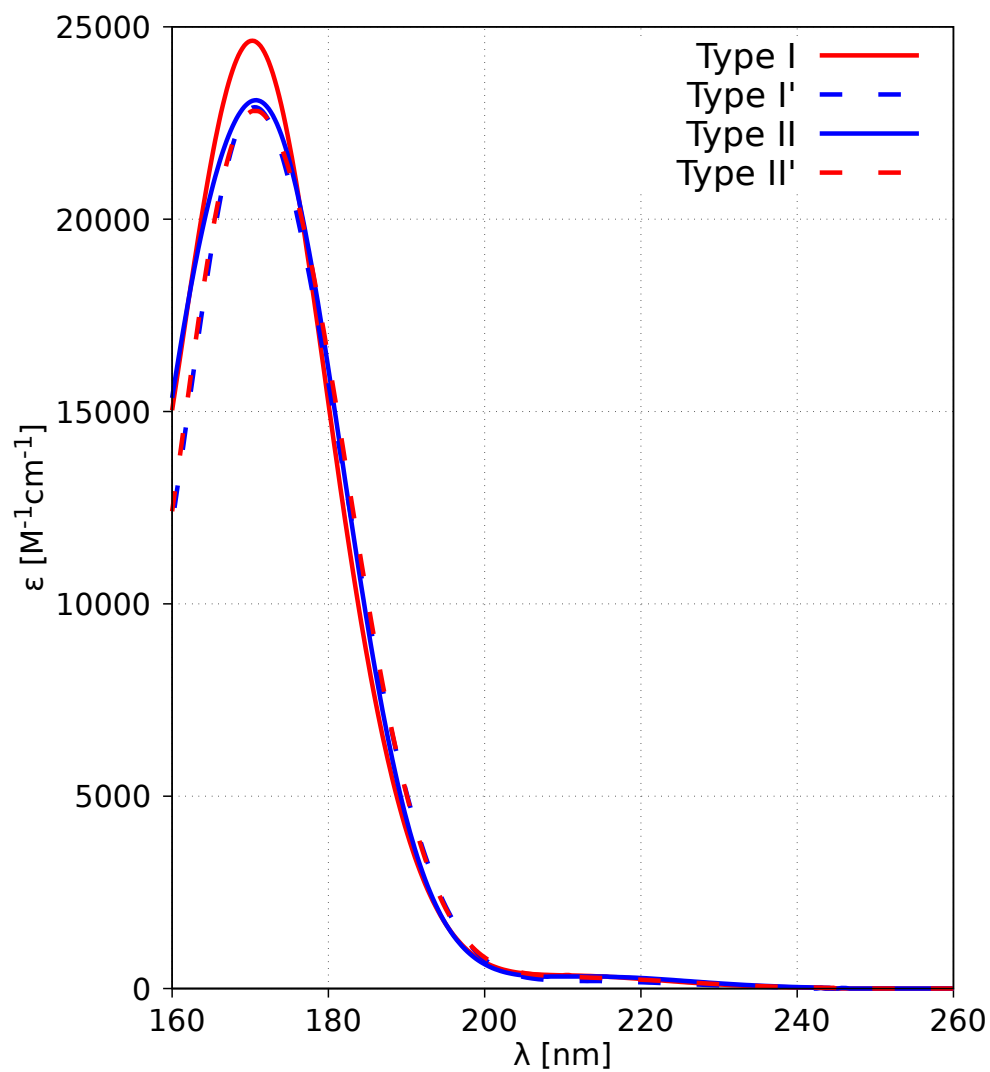
Figure S7. Distributions (in %) for the intensity ratio between the negative and positive ECD bands, κ (see eq. 5 in the paper) for the four considered β-turn types.
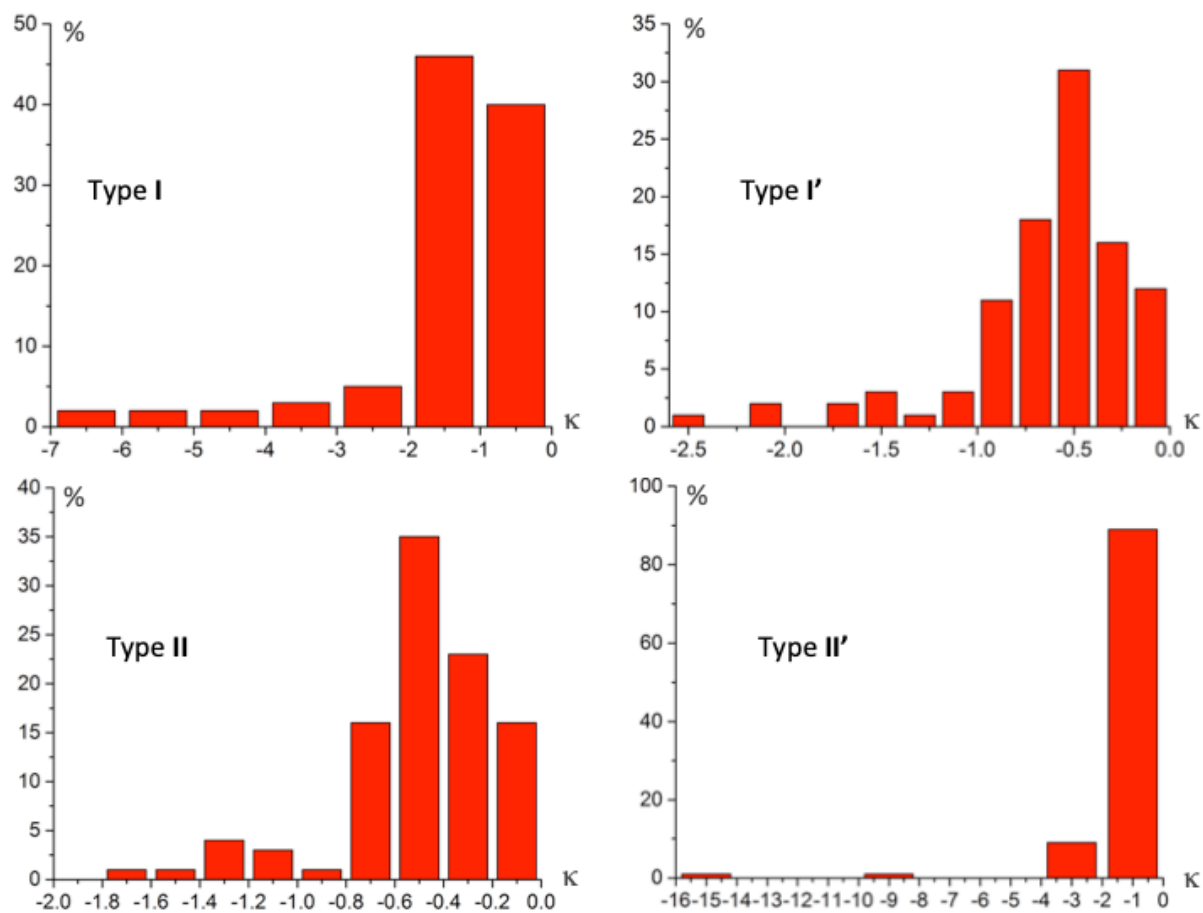
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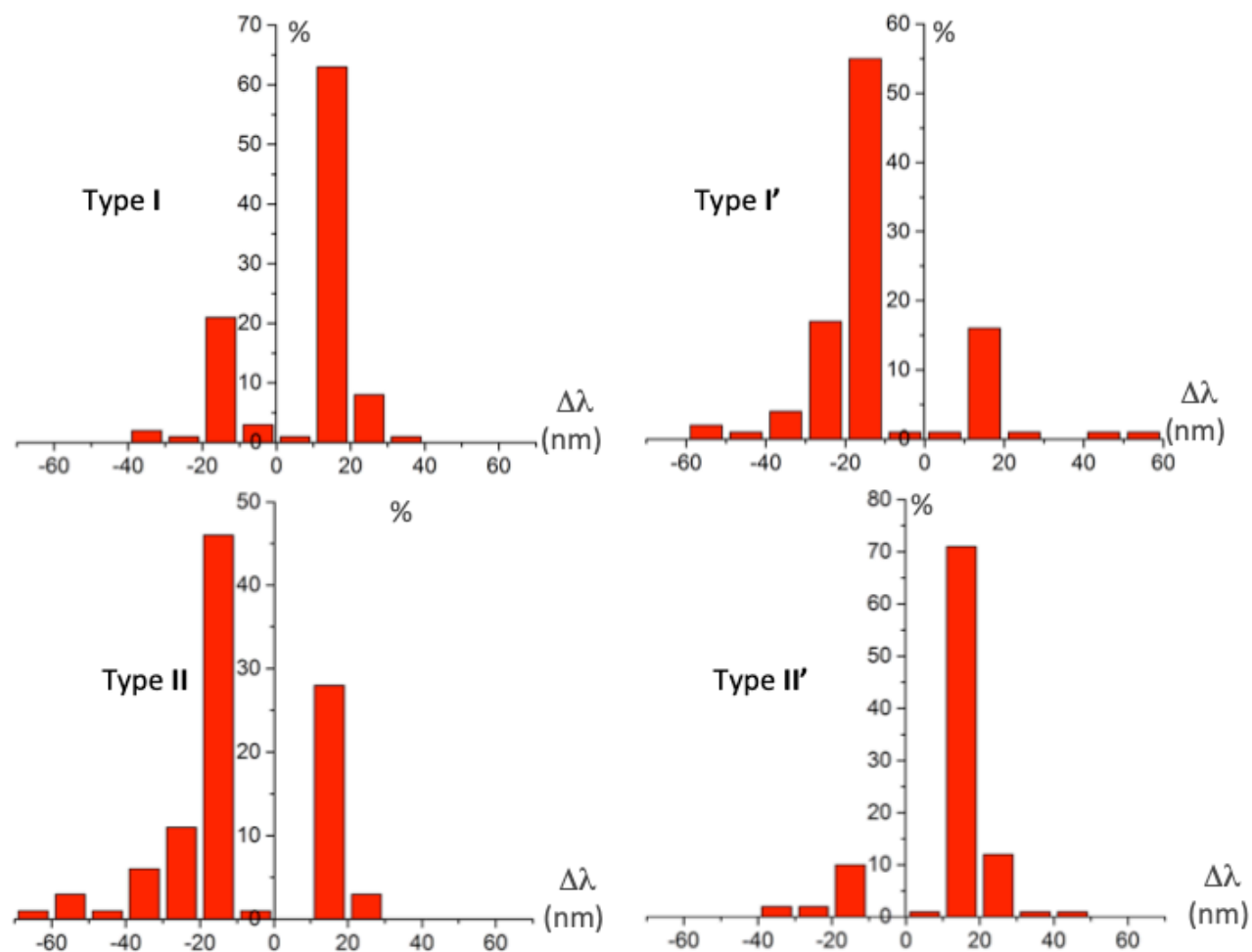
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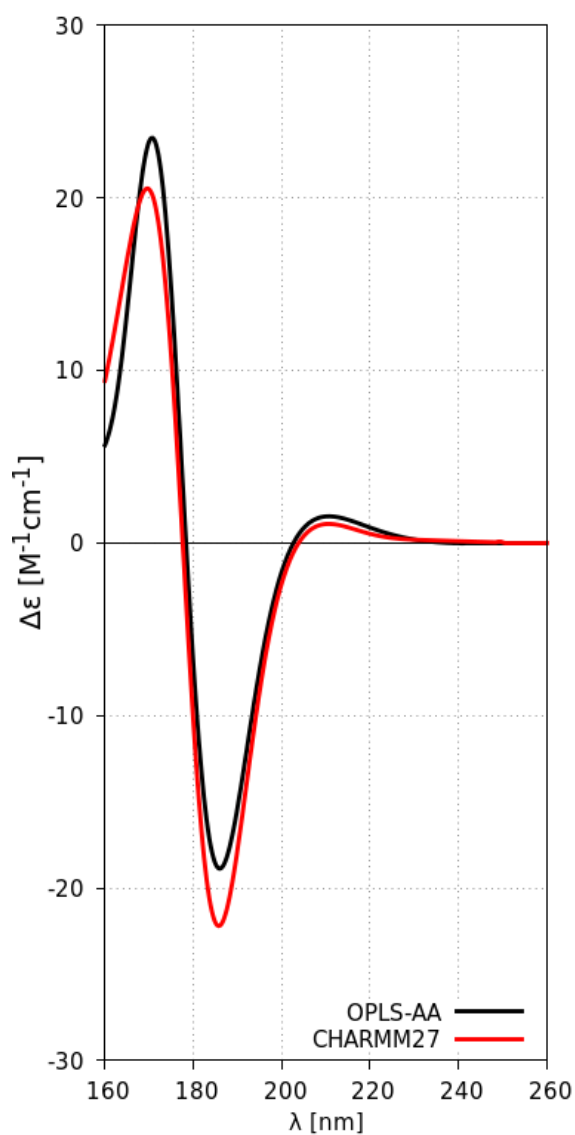
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