Supplementary Information

Structure of supramolecular astaxanthin aggregates revealed by molecular dynamics and electronic circular dichroism spectroscopy

Grzegorz Zajac,[1] Ewa Machalska,[1] Agnieszka Kaczor,[1,2] Jiří Kessler,[3] Petr Bouř, [,3] Malgorzata Baranska[*,1,2]*

[1] Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, Krakow 30-387, Poland

[2] Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University, Bobrzynskiego 14, Krakow 30-348, Poland

[3] Institute of Organic Chemistry and Biochemistry, Academy of Sciences, Flemingovo náměstí 2, Prague, 16610, Czech Republic

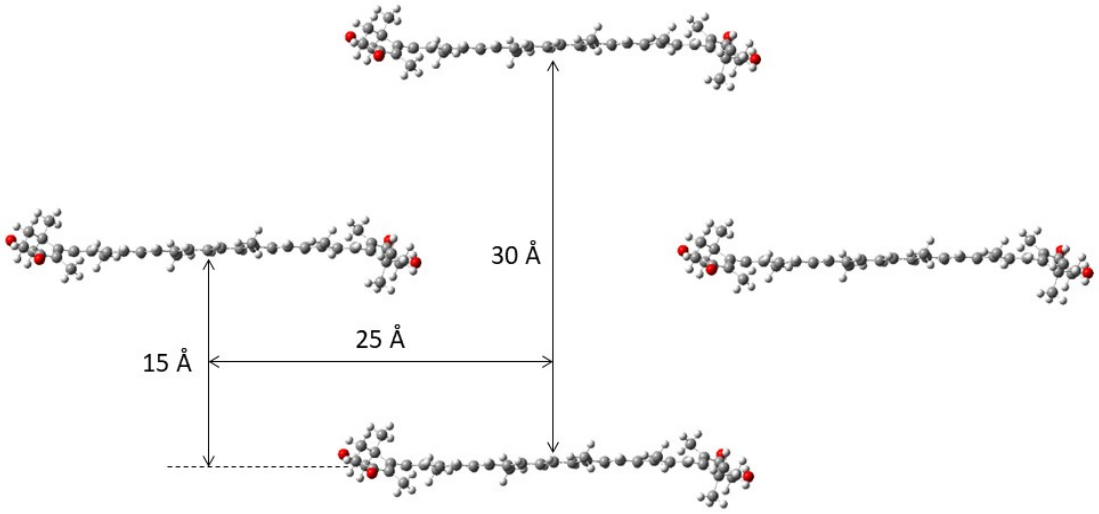

Fig. S1 Details of the J-aggregate model structure.

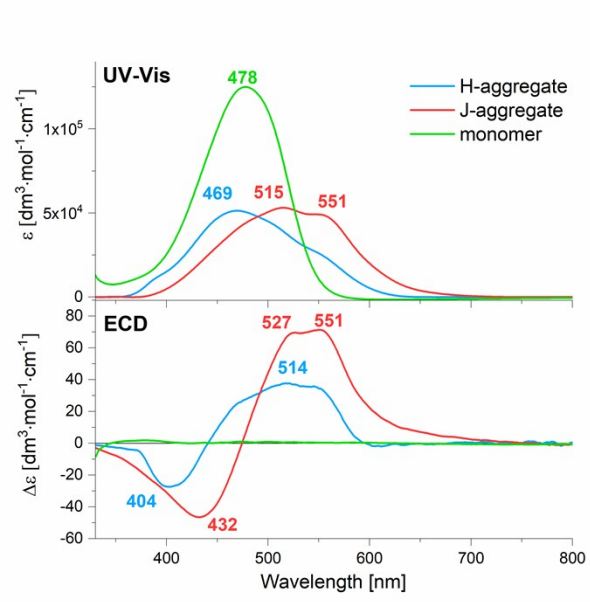

Fig. S2 Experimental UV-Vis and ECD spectra of the H-, J-aggregate and monomer of AXT.

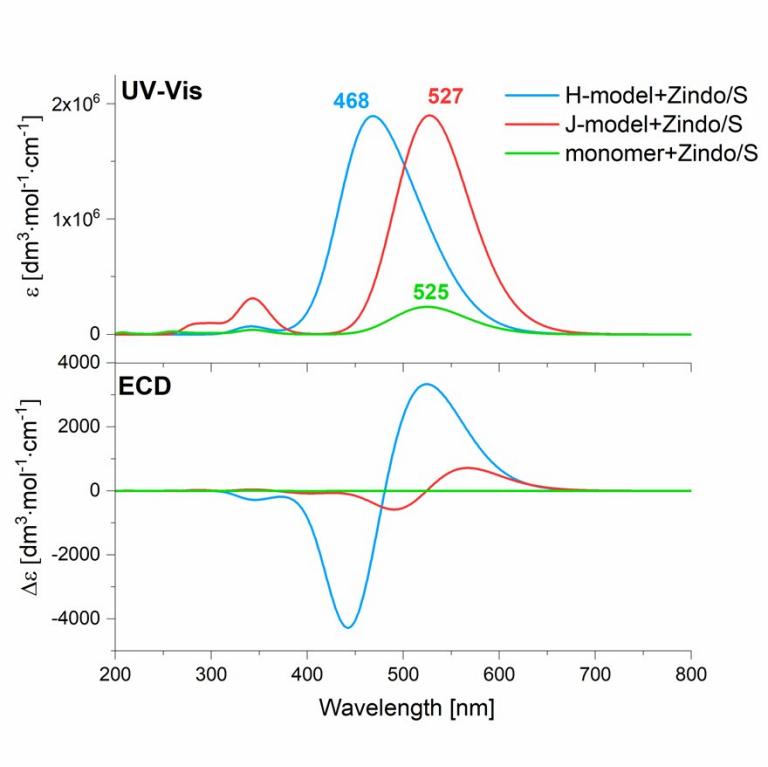

Fig. S3 Calculated UV-Vis and ECD spectra of the H- and J-aggregates arbitrary models and monomer at the ZIndo/S theory level.

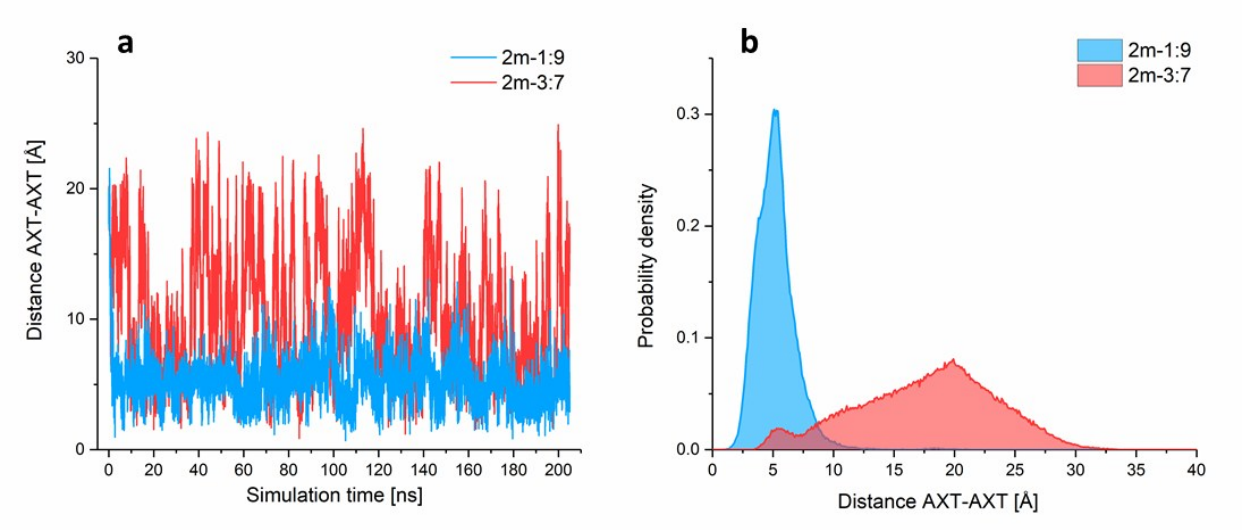

Fig. S4 AXT-AXT distance curves versus MD simulation times, and AXT-AXT distance histograms for 1:9 and 3:7-dimer models.

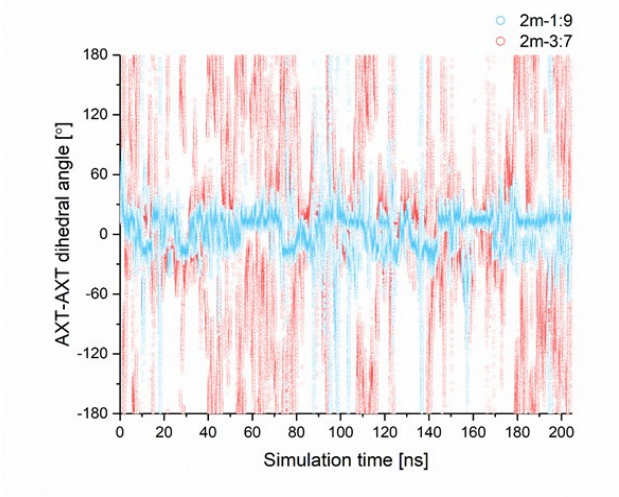

Fig. S5 AXT-AXT dihedral angle curves versus MD simulation times for 1:9 and 3:7-dimer models.

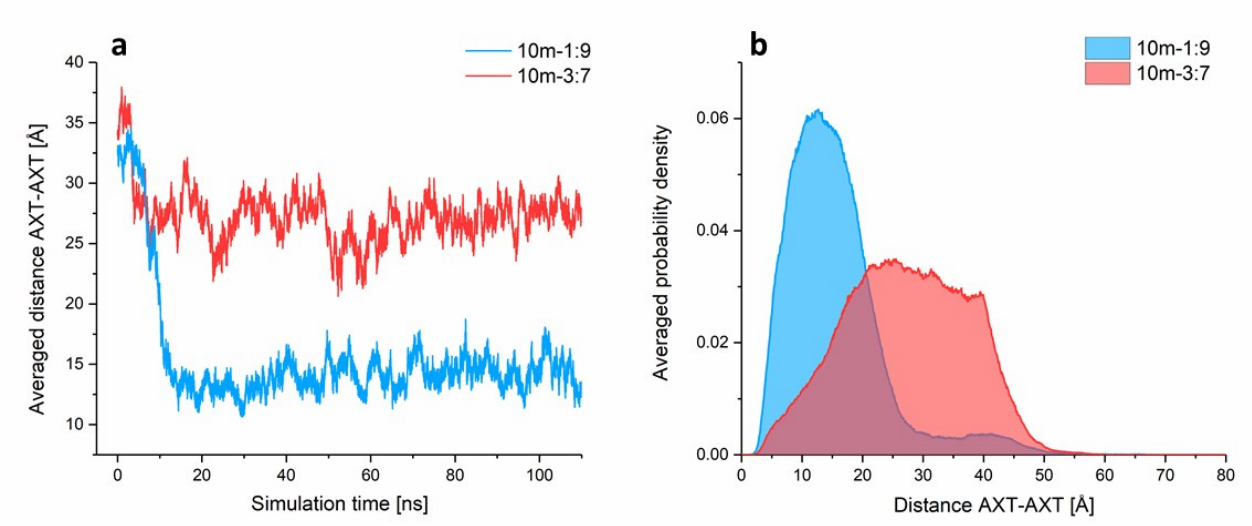

Fig. S6 Averaged AXT-AXT distance curves versus MD simulation times, and AXT-AXT distance histograms for 1:9 and 3:7-decamer models.

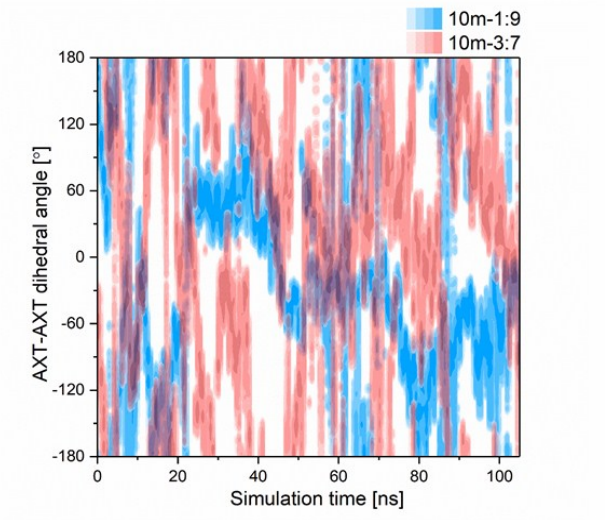

Fig. S7 AXT-AXT dihedral angle density curves versus MD simulation times for 1:9 and 3:7-decamer models.

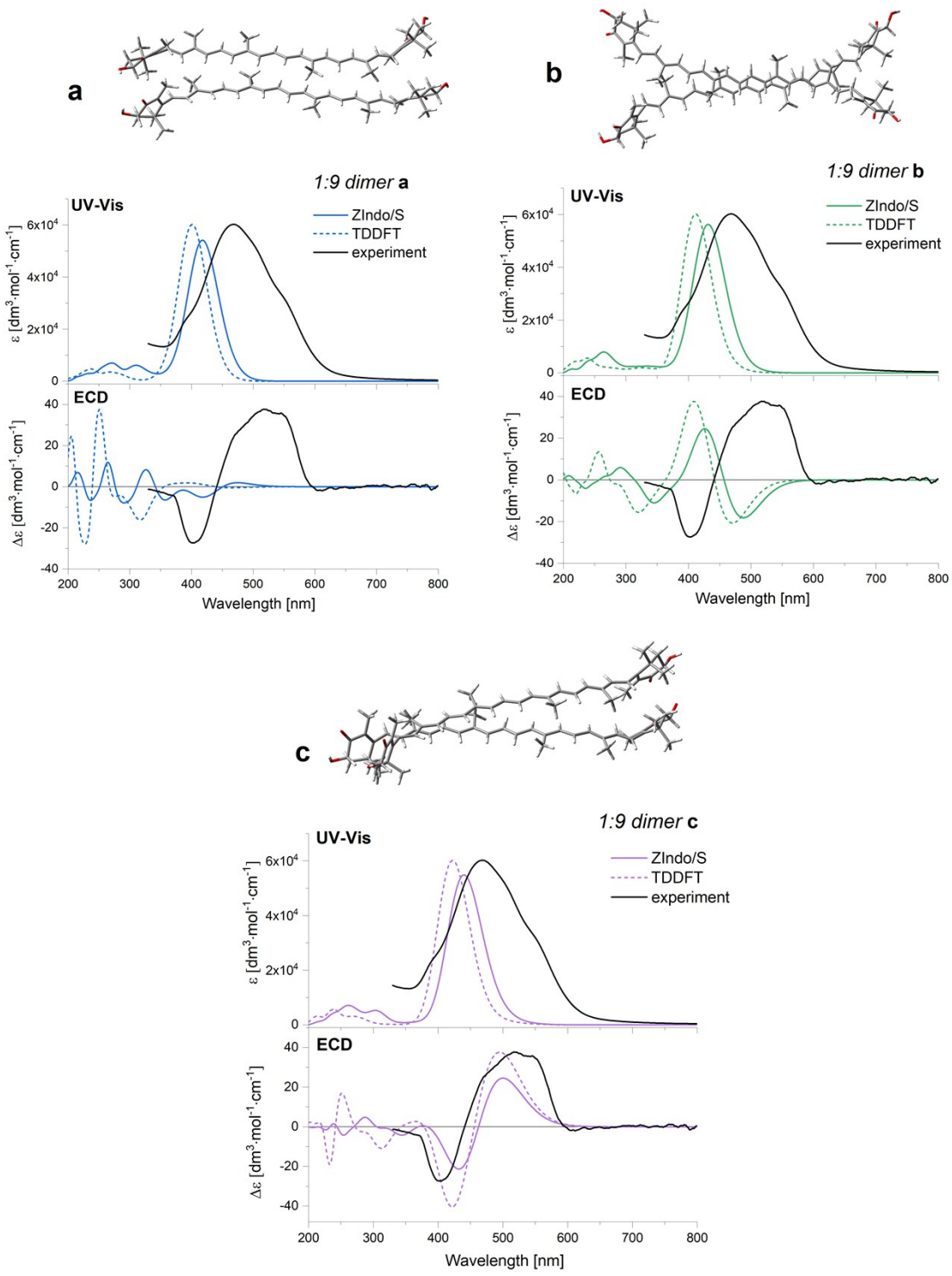

Fig. S8 UV-Vis and ECD spectra of typical structures taken from the 1:9 (a-c) dimer MD simulation models.

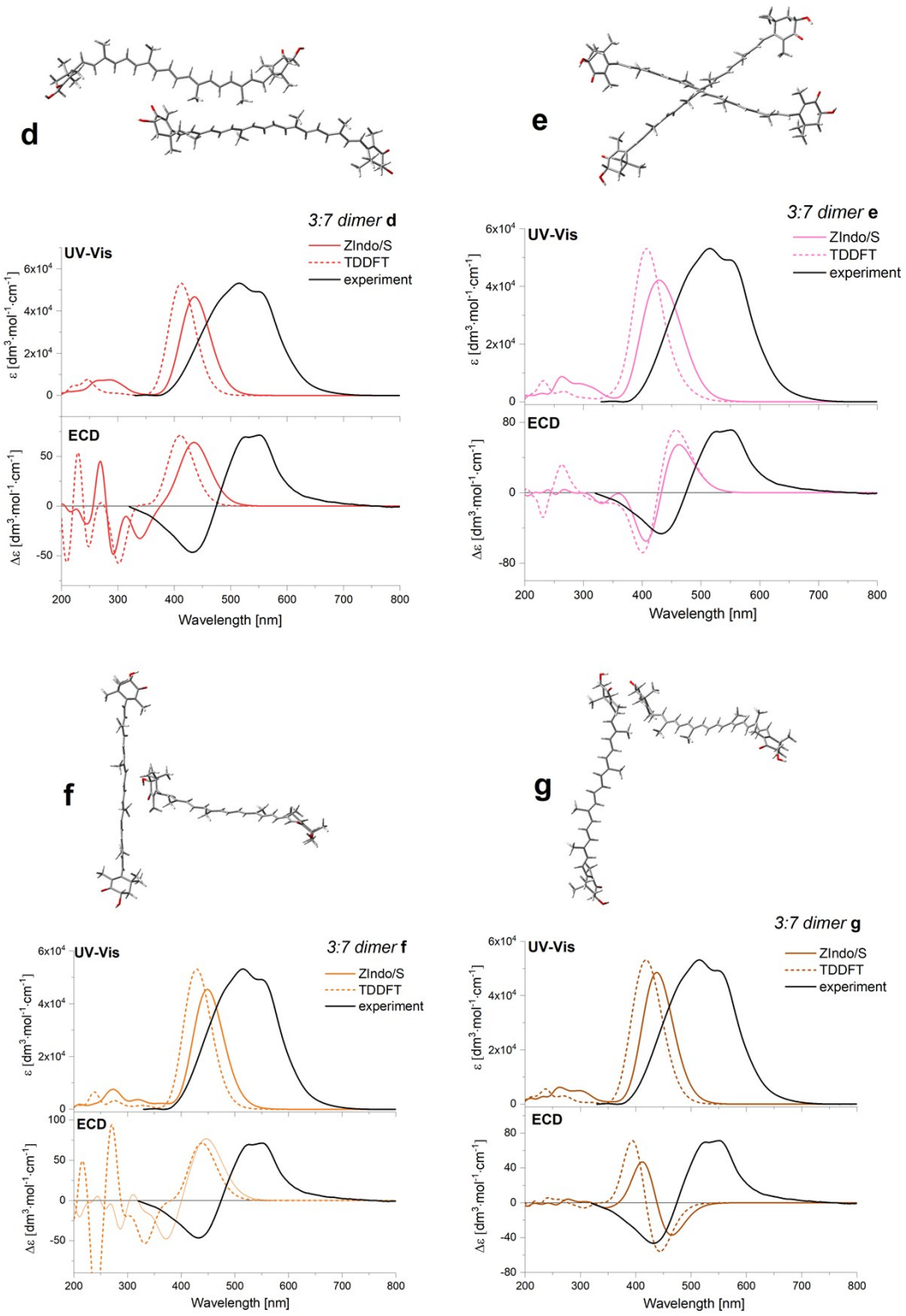

Fig. S9 UV-Vis and ECD spectra of typical structures taken from the 3:7 (d-g) dimer MD simulation models.

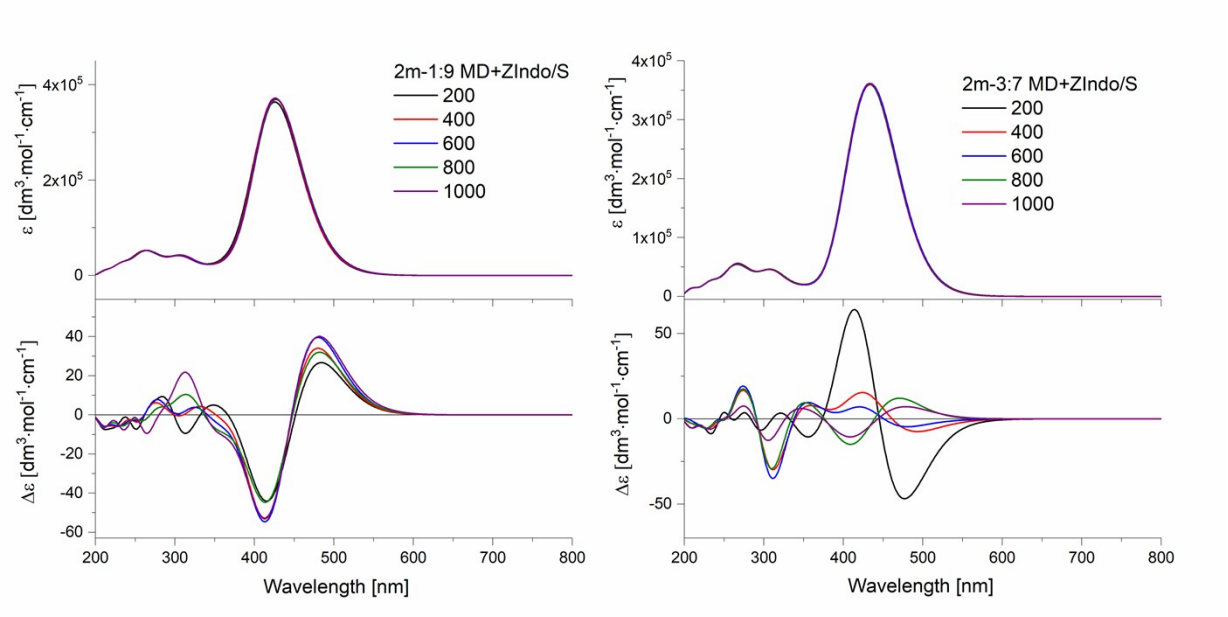

Fig. S10 UV-Vis and ECD spectra of simulated AXT dimers (1:9 left panel, 3:7 right panel) at ZIndo/S theory level, averaged over 200, 400, 600, 800 and 1000 MD clusters.

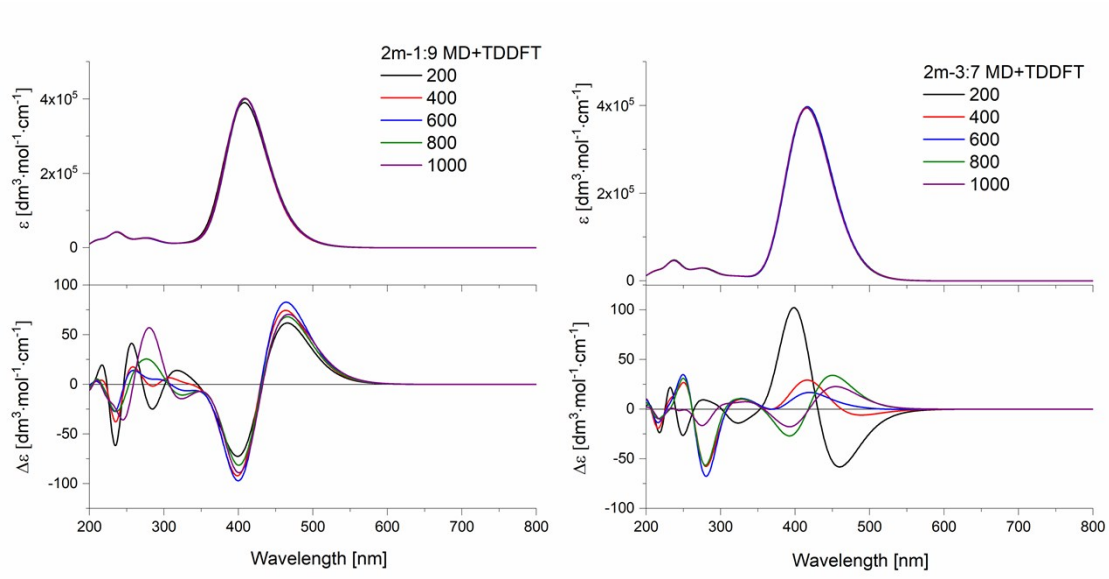

Fig. S11 UV-Vis and ECD spectra of simulated AXT dimers (1:9 left panel, 3:7 right panel) at TD-DFT theory level, averaged over 200, 400, 600, 800 and 1000 MD clusters.

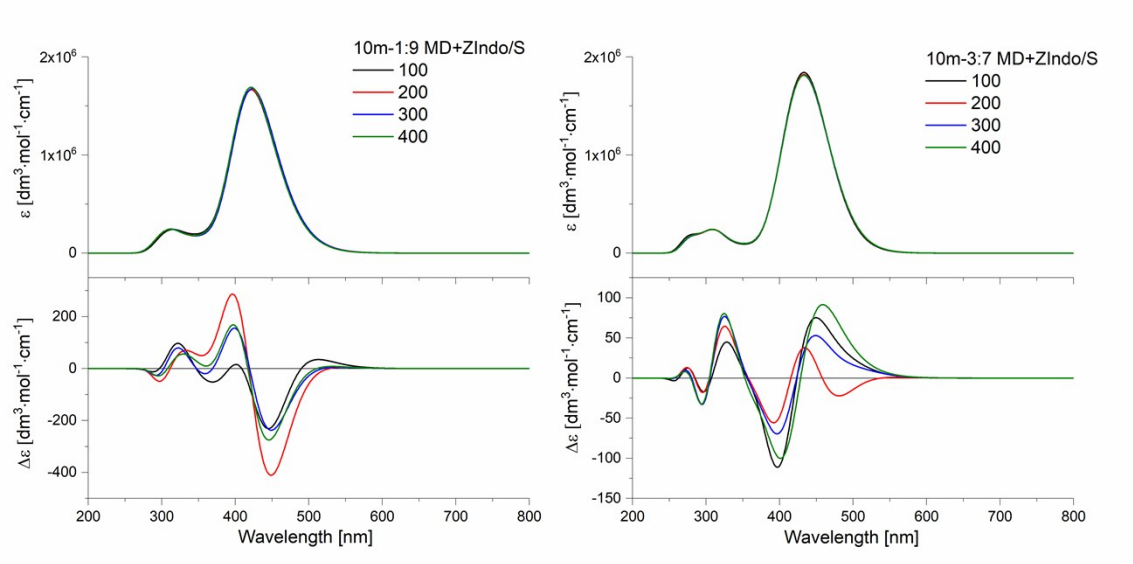

Fig. S12 UV-Vis and ECD spectra of simulated AXT decamers (1:9 left panel, 3:7 right panel) at ZIndo/S theory level, averaged over 100, 200, 300 and 400 MD clusters.

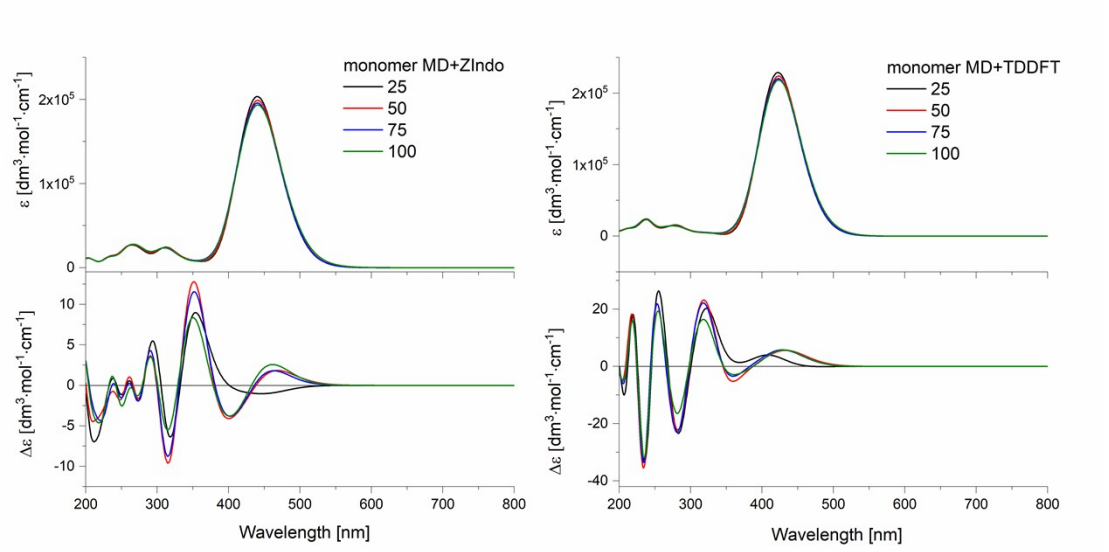

Fig. S13 UV-Vis and ECD spectra of simulated AXT monomers at ZIndo/S and TD-DFT theory level, averaged over 25, 50, 75, 100 MD clusters.

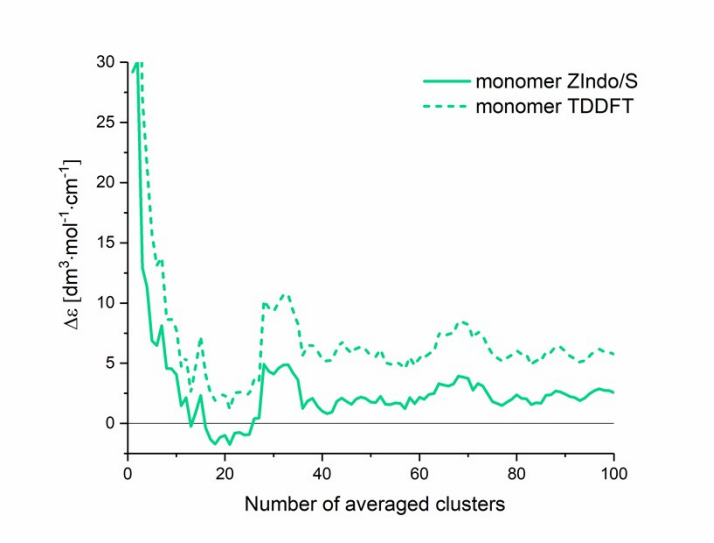

Fig. S14 ECD intensities (Δε) of simulated AXT monomers at 462 nm (ZIndo/S) and 431 nm (TD-DFT), as a function of the number of averaged clusters.

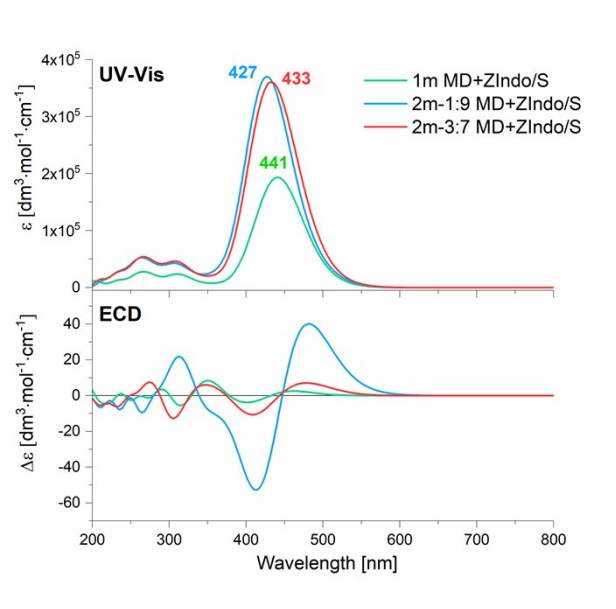

Fig. S15 Calculated UV-Vis and ECD spectra of the 1:9 and 3:7-dimer models and monomer at the ZIndo/S theory level, averaged over 1000 (dimers) or 100 (monomer) single spectra of extracted MD clusters.

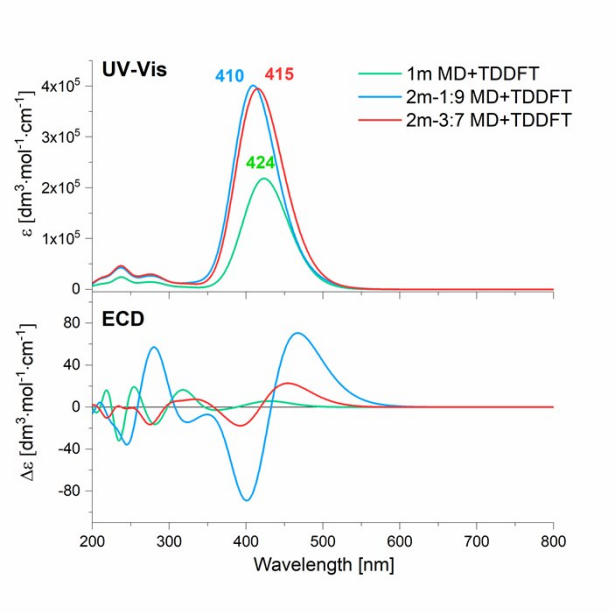

Fig. S16 Calculated UV-Vis and ECD spectra of the 1:9 and 3:7-dimer models and monomer at the TDDFT/CAM-B3LYP/ Def2SVP theory level, averaged over 1000 (dimers) or 100 (monomer) single spectra of extracted MD clusters.

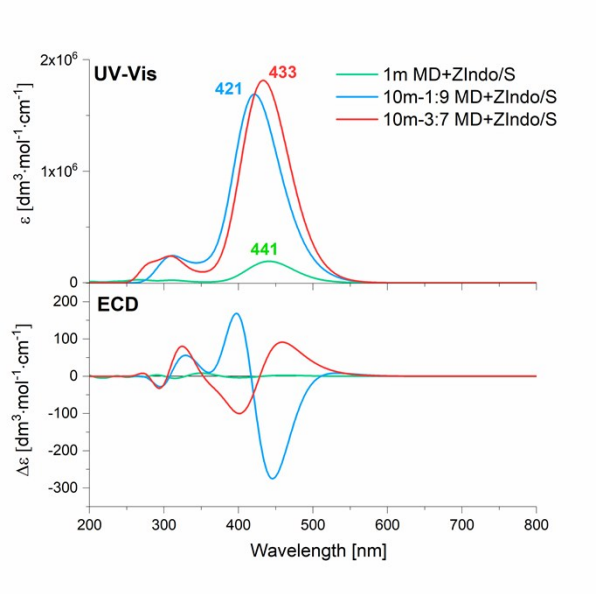

Fig. S17 Calculated UV-Vis and ECD spectra of the 1:9 and 3:7-decamer models and monomer at the ZIndo/S theory level, averaged over 400 (decamers) or 100 (monomer) single spectra of extracted MD clusters.

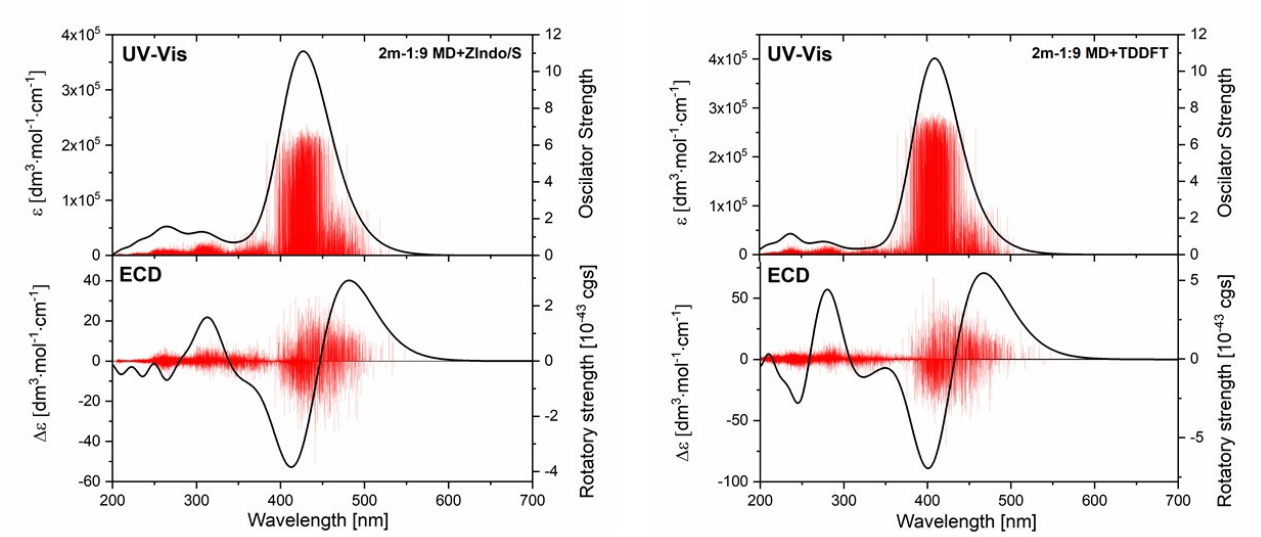

Fig. S18 Averaged UV-Vis and ECD spectra, together with oscillator and rotatory strengths intensity, from all extracted MD clusters of *1:9-dmier* model, calculated at the ZIndo/S and TD-DFT theory level.

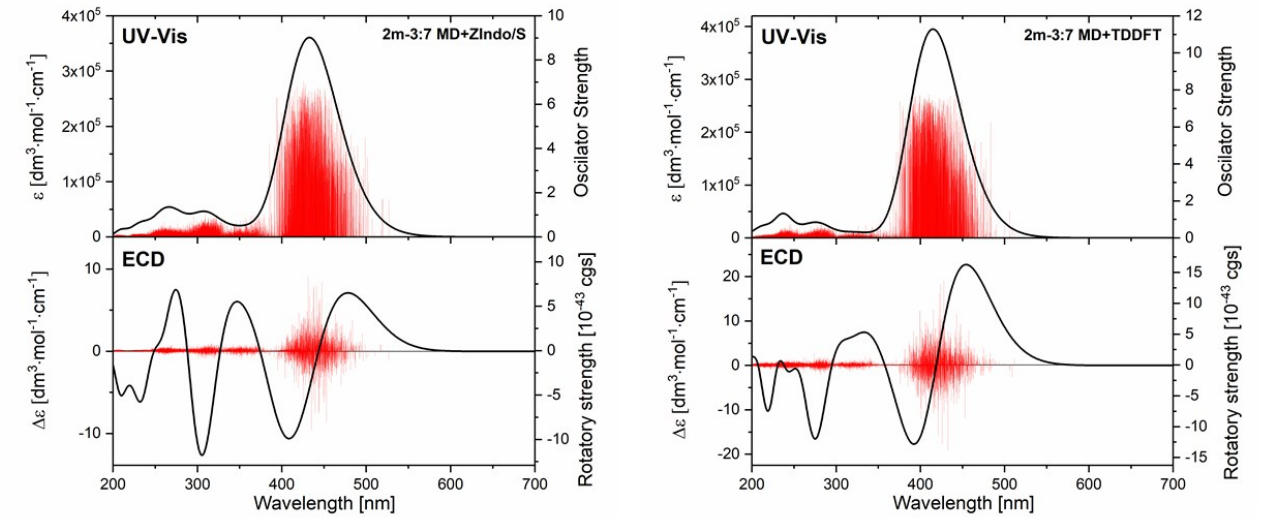

Fig. S19 Averaged UV-Vis and ECD spectra, together with oscillator and rotatory strengths intensity, from all extracted MD clusters of *3:7-dmier* model, calculated at the ZIndo/S and TD-DFT theory level.

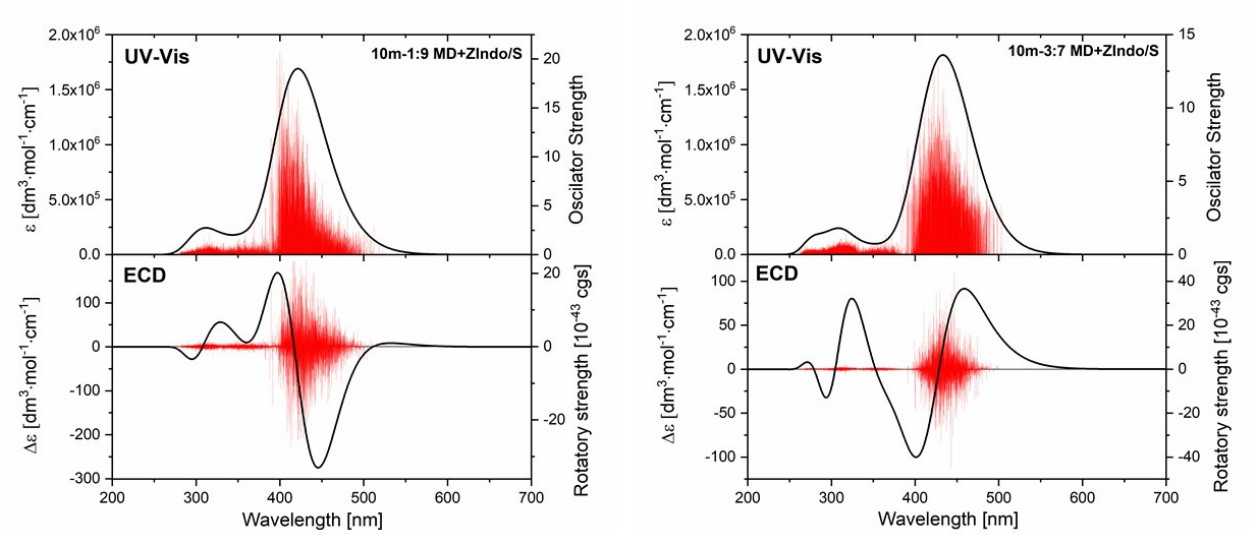

Fig. S20 Averaged UV-Vis and ECD spectra, together with oscillator and rotatory strengths intensity, from all extracted MD clusters of *1:9-decamer* and *3:7-decamer* models, calculated at the ZIndo/S theory level.

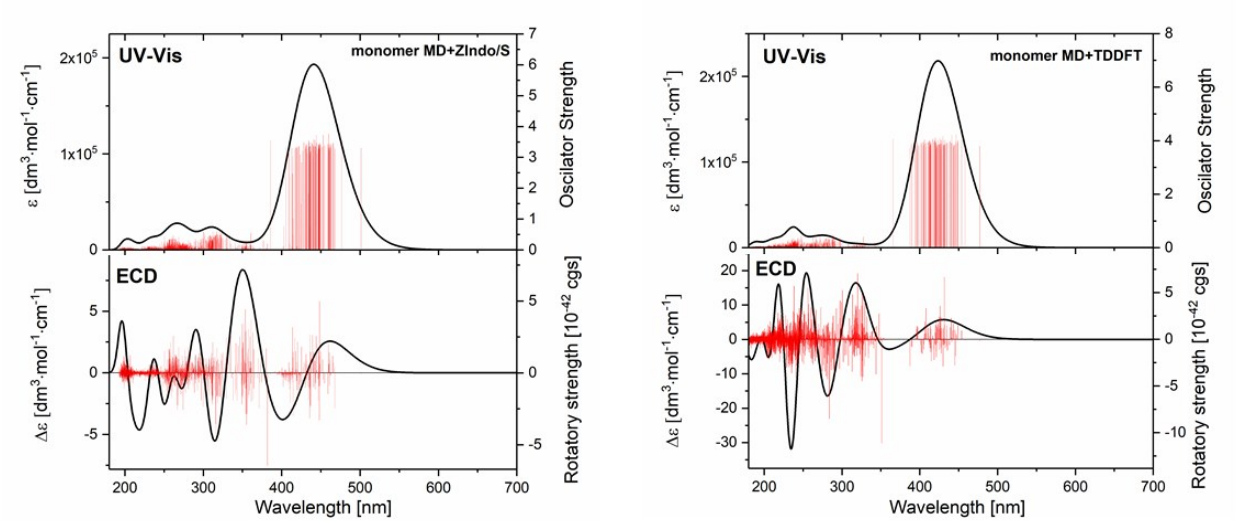

Fig. S21 Averaged UV-Vis and ECD spectra, together with oscillator and rotatory strengths intensity, from all extracted MD clusters of *monomer* models, calculated at the ZIndo/S and TD-DFT theory level.

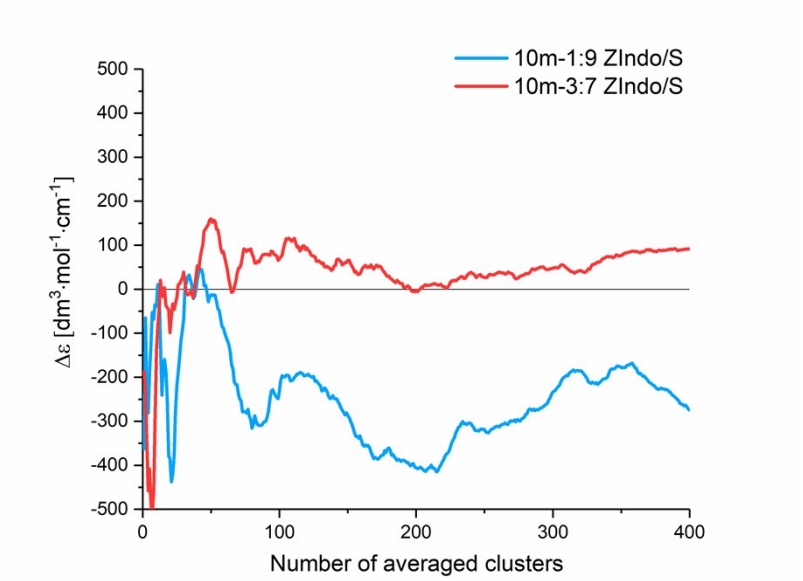

Fig. S22 ECD intensities (Δε) of simulated AXT decamers at 446 nm (1:9) and 459 nm (3:7), dependent on the number of averaged clusters.